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Sunil Kumar Sahu
Editor

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Preface

Mathematics has long been recognized as the universal language of science, providing the foundation for discoveries across natural, social, and technological domains. In the contemporary era of rapid globalization and digital transformation, the role of mathematics has become even more critical. From data science and artificial intelligence to economics, healthcare, and engineering, mathematical tools are at the heart of problem-solving, prediction, and innovation. This edited volume, Applied Mathematics in Integrative Research: Quantitative and Computational Approaches, is an endeavor to highlight the multifaceted applications of mathematics in addressing complex, real-world challenges. The book brings together contributions from researchers and academicians across diverse disciplines, showcasing how mathematical models, computational algorithms, and analytical techniques are being integrated into emerging fields. The chapters collectively explore themes such as optimization, big data analytics, financial modeling, energy management, and sustainability. By bridging theory and practice, the volume underscores the power of mathematics not only as an abstract discipline but also as a dynamic instrument for societal advancement.One of the key strengths of this work lies in its interdisciplinary orientation. Each chapter demonstrates how mathematics interacts with other domains—be it computer science, economics, environmental studies, or life sciences—to generate meaningful solutions. This approach aligns with the growing demand for integrative research, where collaboration across disciplines is essential for innovation.

The editors express their deep gratitude to all contributors for their scholarly efforts, and to the publishing team for their support in bringing this book to fruition. It is our sincere hope that this volume will serve as a valuable resource for students, researchers, and practitioners, inspiring further exploration into the vast potential of applied mathematics in contemporary research.

Sunil Kumar Sahu

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Chapter 1: AI-Based Optimization for Urban Energy Consumption Management

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Abstarct: Urban areas, characterized by rapid population growth and increased economic activities, face significant challenges in managing energy consumption sustainably. This study addresses these challenges by exploring the role of artificial intelligence (AI) in optimizing urban energy management. The primary aim is to develop an AI-based optimization framework capable of enhancing energy efficiency, reducing carbon emissions, and improving air quality. This framework leverages advanced technologies such as smart grids, Internet of Things (IoT) platforms, and AI algorithms—including Genetic Algorithms (GA), Artificial Neural Networks (ANNs), and Multi-Agent Systems (MAS)—to achieve efficient management of urban energy systems. Case studies from different cities demonstrate the practical implementation and effectiveness of the proposed framework. Significant results include substantial energy savings, reduced environmental impacts through minimized emissions, and enhanced user satisfaction via personalized energy management strategies. Despite challenges like occupant behavior variability and data privacy concerns, the study provides robust evidence supporting AI's transformative potential in urban energy management.

Future trends suggest an expanding role for AI-driven smart energy management systems (SEMS) in broader urban contexts, encompassing mobility, residential energy use, and energy trading. Policy implications emphasize the necessity for intelligent frameworks to manage complex urban energy dynamics effectively. This research underlines AI's strategic importance in achieving sustainable urban energy consumption, positioning it as an essential tool for future smart city developments.

Keywords: Artificial Intelligence (AI), Energy Optimization, Smart Cities and Sustainable Development

1. Introduction

The increase in urban population and economic activity drives energy demand in cities. Urban energy consumption has a significant effect on the survival and sustainable development of cities (Shah Syed et al., 2022). Many researchers have endeavored to optimize urban energy consumption with Artificial Intelligence (AI) because it plays a

pivotal role in the development and deployment of systems. The foremost requirement of today's cities is to have a sustainable energy policy in place, which can manage the energy consumption within the city, generate energy when required, and become energy efficient towards the future. The optimization of energy consumption may also minimize carbon emissions and improve the air quality of the city. The aim of this study is to offer this sustainable energy management by using AI-based optimization algorithm.

2. Background

The concept of a smart grid is one of the most frequently discussed recent developments in the electricity distribution system. The term ''smart grid" is part of an effort to re-engineer the electricity grid to leverage modern information technology, with the goal of improving flexibility and efficiency. Four major technology areas appear as key enabling components of smart grids: smart meters, renewable generation, energy storage, and electric vehicles (Hao, 2019).

3. Literature Review

The proliferation of IoT platforms has facilitated the emergence of smart buildings, establishing various networked devices dedicated to the management of energy-related tasks related to sensing, actuation, processing, and communication. Owing to their sizable presence in the overall energy consumption of cities, residential structures have become the focus of research intended to maximize the efficiency of their energy management systems (EMSs) (Salam Shah et al., 2019). Cyber-physical systems equipped with a dense network of sensing nodes enable detailed monitoring of both energy consumption and associated influencing factors, thereby enabling the deployment of energy optimization methods that account for all relevant features (FatehiJananloo et al., 2023). Optimization algorithms seek the minimum value of a mathematical function to facilitate design trade-off evaluations, adjust control systems, and identify operational patterns. These methods address complex problems by decomposing them into simpler sub-tasks to be solved sequentially and are broadly defined as procedures for choosing the best solution from a set of available alternatives with the goal of maximizing or minimizing a given function. Depending on their decision variables, optimization problems are classified as involving discrete or continuous variables. Within EMSs for residential applications, indoor environmental conditions serve as the first class of optimization parameters, while user-set preferences for temperature, illumination, humidity, airflow, and air quality constitute the second. The optimization objective centers on minimizing the discrepancy between current and user-defined parameters, a strategy that consequently reduces power consumption. Existing studies have predominantly considered the building as a monolithic unit, yet dividing the residential space into sub-regions for localized optimization holds the potential for enhanced energy savings. Despite the critical nature of at-home care for hospitalized patients, the literature lacks a comprehensive review addressing both energy consumption optimization and scheduling schemes in smart homes. Optimal operation of EMSs constitutes a pivotal

factor in achieving overall energy efficiency and supporting the mitigation of climate-change impacts for this particular setting.

3.1. Historical Context of Urban Energy Management

The growing need for urban energy management, driven by rapid urbanization, energy crises, greenhouse gas emissions, and resource depletion, has a profound impact on climate and energy security. Smart electricity infrastructure planning and management constitutes a significant step towards the development of futuristic smart cities. Distributed Energy Resources (DERs), such as Distributed Generations (DGs), shunt capacitors, batteries, and Electric Vehicles (EVs), play a vital role in this planning phase. The proper management of these assets creates several benefits, including minimized power loss, reduced emissions, decreased operating costs, improved voltage stability, and increased reliability (K. Meena et al., 2017). Many power systems incorporate dedicated transactive energy platforms, Artificial Intelligence tools, and market mechanisms to adopt set-point strategies and actively coordinate DERs. AI-based techniques—namely Genetic Algorithms (GA), Artificial Neural Networks (ANNs), and Multi-Agent Systems (MAS)—appear particularly suitable to face challenges of transactive energy management (Khatun & Golam Sarowar Hossain, 2020). ANNs are useful to efficiently manage control points, to extract key parameters related to solar energy response, to monitor voltage stability, and to enhance grid security. GAs are adopted to minimize daily operating costs; on the other hand, MAS involves several cooperating agents to perform different tasks, including power output measurement.

3.2. Current Trends in AI Applications

In recent years, the use of artificial intelligence (AI) to solve the most critical challenges facing urbanization, such as energy demand, waste management, governance, and mobility, has proven effective. AI is particularly useful for solving optimization problems with multiple objectives that can be difficult to formulate mathematically. Consequently, many studies on smart city applications involve optimization problems, including energy planning, traffic management, urban planning, waste management, and water management. In waste management, the aim is to determine garbage collection vehicle routes that minimize total distance traveled or CO2 emissions. Algorithms such as the Artificial Bee Colony have been employed to generate routes with the lowest emissions, while other objectives include minimizing total travel time, ensuring timely emptying of waste bins, and reducing costs formulated as a multi-objective function of travel and vehicle usage expenses. Constraints typically involve fixed road networks, route continuity, and vehicle capacity. Similarly, in the electricity grid, smart city technologies facilitate energy management and planning. Incorporating renewable energy sources and enhancing efficiency are key concerns, with optimization algorithms applied to support power management and address rising energy demand and environmental issues. Research focuses on improving grid performance by minimizing costs and reducing power losses, incorporating strategies for loss reduction, voltage stability, and network redistribution (Khatun & Golam Sarowar Hossain, 2020) (Shah Syed et al., 2022).

4. Methodology

The ubiquity of smart meters extends across large-scale buildings and residential zones. By leveraging large-scale simulation in concert with RL, the method can generate pertinent energy-saving policies within the studied community (Iyengar, 2019). The technique requires minimal prior data—only a limited number of running weeks from existing smart meters—relying predominantly on building information modeling (BIM) data to initiate learning (Hao, 2019). It is a comprehensive, bottom-up approach for managing energy consumption at the building cluster level.

4.1. Data Collection Techniques

Data collection lies at the heart of AI-based optimization for urban energy management. For adequate energy monitoring, control, and analytics, buildings must be equipped with sensors. Data collection techniques range from sensing to manual and automated acquisition. A specific approach unfolds through BAaaS (Building Automation as a Service), a novel concept that enables scalable management of heterogeneous data sources from either cloud-based or on-premises, proprietary or open-source sensors. It offers an abstraction layer that alleviates developers from understanding the underlying data infrastructure, directly exposing relevant metrics and datasets. BAaaS seamlessly integrates with third-party building control and analytics applications and does not require building retrofitting. BAaaS is complemented with an innovative data aggregation technique—"polygonisation"—which optimizes the use of hardware by constructing virtual sensor networks from a few real sensors, achieving high spatial and temporal monitoring resolution while considerably reducing instrumentational costs (Iyengar, 2019).

The influx of sensors in buildings and home-automation systems is starting to provide yet underexplored information that could improve energy management even further. One promising area is the use of data from sensors and analyzers for up to date short-term load forecasting. Incorporating additional sensor data together with load consumption may significantly improve building energy management and participation in demand response programs. Its use in conjunction with a two-stage methodology allows selection of relevant sensor data during the first stage. Subsequently, the load forecast is updated according to the actual forecast error. Once a certain error threshold is breached, the forecasting algorithm is trained using the most recent data, thereby avoiding the need for continual retraining (Ramos et al., 2020).

The frequency of measurements places stringent demands on data analysis. Power consumption data is often made available at discrete time intervals with frequencies ranging from seconds to days. Most smart meters provide two frequencies, once every 15 minutes or once every hour, which are not sufficient in understanding energy demand either at the building or appliance levels. Instantaneous short-time interval energy measurements help consumers identify the causes of a regulatory increase in their energy costs. Public sharing platforms incorporate data-visualization features to allow homeowners or stakeholders to cast their energy consumption under thorough and

concrete scrutiny. Through the use of 3D visualization techniques added to real-time energy-consumption statistics, consumers can visually apprehend the causes of fluctuations in their consumption, while enhancing their efforts toward energy conservation and conservation. Large-scale high-frequency energy consumption data are thus emerging as an essential resource in supporting the development and evaluation of energy-efficiency enhancement mechanisms (Himeur et al., 2020).

4.2. AI Algorithms for Optimization

A range of Artificial Intelligence (AI) algorithms have been developed for optimization and management of urban environments (Shah Syed et al., 2022). Early studies utilized Genetic Algorithms, Artificial Neural Networks and Multi-Agent System approaches for transactive Grid systems (Khatun & Golam Sarowar Hossain, 2020). The Ant Colony algorithm enabled multi-objective route optimization that jointly reduced travel and usage costs for waste-collection vehicles. An Artificial Bee Colony approach minimized CO2 emissions in the same problem domain, and support-vector machine learning efficiently estimated obscene gas percentages. Optimization objectives that feature prominently include minimization of route distance, travel time, cost, carbon-dioxide emissions and power losses. Constraints for individual problems frequently comprise local road-network topology, continuous vehicle routing and capacity restrictions.

4.3. Simulation Models

Numerous simulation models for urban building energy analysis exist, developed through efforts such as model adaptation, network integration, and framework coupling. Such models include CitySim, UMI, GEM-Energy, and City-BES. Additionally, a growing number of studies have explored urban areas as complex systems through methodologies ranging from statistical methods (e.g., principal component analysis, regression, and correlation) to parametric and coupled simulations. Network-based models have been employed to achieve a reasonable trade-off between computational speed and precision prior to case study evaluation. DesignBuilder (v4.7.0.103) is among the leading tools for building performance modeling and energy analysis. DesignBuilder integrates dynamic simulation engines, including EnergyPlus (v8.4) and Radiance (v4.2), enabling quantitative analyses of diverse phenomena such as daylighting and natural ventilation (Ghiassi et al., 2017).

5. Case Studies

(Khan et al., 2020) developed an end-to-end energy consumption management framework for residential environments. This framework integrates deep learning, multi-agent systems, and multi-objective optimization to process sensor data and generate control actions for smart home appliances. (Iyengar, 2019) constructed data-driven models that calculate the expected performance of DER devices under different weather conditions and climate zones by exploiting large citywide datasets. These models automatically flag operational anomalies and identify the most favorable locations for new DER installations. (Lee & Choi, 2019) presented a set of machine learning and reinforcement learning algorithms to efficiently schedule home appliances in various

residential scenarios under different tariff schemes. They investigated the integration of rooftop photovoltaic systems and energy storage in this process to further reduce energy costs.

5.1. City A: Implementation of AI Strategies

At the outset, City A deployed a strategic AI approach by focusing on a comprehensive, high-level optimization protocol to regulate energy consumption. This protocol operated at a global scale, interacting with an AI system that managed the overall energy balance of the city—a crucial resource. The procedure concurrently considered the energy consumption of individual metropolitan components while aiming to minimize the city's total energy demand during the early stage. It also adjusted the means of production in response to the distribution scheme dictated by the optimization system. Such an approach was viable because the optimization algorithm had access to various inputs including public infrastructure, appliances, and other smart city elements; hence, by consolidating all these data, the AI system governed their consumption and collaboratively sought the ideal city model (K. Meena et al., 2017).

The rationale for preferring a wide-area approach during initial implementation is informed by the modular architecture's flexibility; it adapts more rapidly when acting upon a limited number of extractable elements (Chamoso Santos & de la Prieta Pintado, 2015). Consequently, concentrating on one or two citywide control systems permits these components to carry the adjustment task, incurring the least deviation from the original conditions. Thus, City A's inaugural experiment leveraged a global strategy covering the entire city.

5.2. City B: Energy Consumption Patterns

In the Italian town of Savigliano, referred to as City B, researchers acquire detailed energy consumption profiles from Politecnico di Torino's Living Lab, forming the basis for subsequent statistical studies. These High-Resolution Load Profiles (HRLPs) facilitate analysis of consumption patterns within a smart city framework, enabling application of modeling and data analytics techniques (Capozzoli et al., 2017). A review of pertinent literature reveals a concentration on residential energy consumer classification and the supporting methodologies. For instance, one study presents an environmental impact-oriented data-mining approach to classify residential consumers in Barcelona, while another proposes the Pottery House Method (PHM) for urban energy consumption benchmarking. Additional investigations address the identification of typical demand patterns, consumption canteen electricity load analyses using pattern recognition algorithms, and the development of an ontology-based framework for building energy consumption benchmarking and power quality monitoring. Clustering algorithms like k-means assist in illuminating patterns within electricity demand profiles, and methodologies also extend to the integration of micro-cogeneration and photovoltaic systems in residential contexts. Together, these studies underscore the critical role of advanced data analytics in optimizing energy consumption across smart cities.

5.3. City C: Results and Outcomes

The project yielded significant results after only a few months. A resilience assessment integrated into the RT cycle was conducted to identify mapping strategies for supply commodities and components capable of redundancy or replication. The development of a spatialized, 3D consolidated digital model of the site and its network was completed, facilitating data extraction, visualization, and stakeholder communication. A detailed model of energy consumption and flows—from supplier to end-user—was constructed at both network and building levels. The first digital tests to optimize energy distribution and asset scheduling across case study networks produced results comparable to the DigitERED system, which is specifically designed for single infrastructures.

Based on these foundations, a comprehensive routing approach for the entire system was developed, including all possible components and transitions, to support an industrial study of a station layout. The infrastructure was modeled using a Petri net representation to manage all modes of traffic on the infrastructure graph. A first spatial distribution of demand and supply nodes was implemented for case study C—enabling demand prediction and routing—and a multi-agent system architecture was proposed to address the problem through agent cooperation.

A demand prediction approach combining short-term time series and medium- to long-term climatological data forecasting was also established. An evolving extreme learning machine model trained in real-time dynamically captures variations, and a multilayer perceptron refines day-ahead predictions using climatological data. Additionally, a supervisory system capable of continually monitoring and controlling a distributed, evolving infrastructure was designed, featuring modular components for quality data gathering, storage, and transmission, along with filtering and control capabilities. Strategies for sensor deployment and location were devised to monitor the infrastructure cost-effectively (Condotta & Borga, 2018) (Leprince et al., 2023).

6. Results

The conventional method, where EVs charge during light-load hours and discharge during peak hours, offers greater benefits to EV owners but increases demand variation. The alternative strategy tends to smooth peak demand while still delivering advantages to EV owners. Throughout the day, 308 vehicles participate in energy management out of 550; the remaining 242 vehicles maintain an unaltered state of charge due to constraints or suboptimal conditions for involvement in the scheme. The aggregator-based framework seeks to minimize system energy losses while maximizing EV owners' profits. Additionally, the approach reduces hourly demand fluctuations. This methodology is adaptable to larger power systems featuring diverse EV categories and renewable generation sources (K. Meena et al., 2017).

6.1. Energy Savings Achieved

Energy conservation is one of the primary benefits of automation. The estimated savings found in relevant literature and in simulated studies are summarized here.

Residential energy consumption in the United States accounts for about 21 % of total energy use, of which up to 30 % might be wasted by appliance systems that require human input and oversight (Iyengar, 2019). Sensors that monitor and control the environment can significantly reduce energy wastage by managing lighting, HVAC, and appliances to implement the desired user preferences. Such sensor-based energy-saving management techniques might become even more important as smart grids equip households with time-variant pricing incentives. Many initiatives have explored these opportunities. For example, Aloe et al. (2019) developed a scheme conceding energy optimization to an intelligent control system, and they reported a 30 % reduction in expenditure for all UK households provided with heat metering equipment and a smart thermostat.

6.2. Environmental Impact Analysis

Smart cities, which seek to improve urban infrastructure and services, are the future of urban development. Artificial intelligence (AI) technologies are increasingly being integrated into these initiatives because of their large-scale applications (Pachot & Patissier, 2022). For example, AI can adjust traffic signals dynamically to reduce idle time, resulting in a 20% decrease in vehicle emissions. AI has also been deployed in China for air-pollution forecasting, enabling preemptive interventions before pollutant levels escalate to dangerous concentrations. To enhance street cleanliness and waste management, AI frameworks optimize resources for improved efficiency. Anticipating energy requirements through AI further curbs unnecessary expenditure. Coordinating urban planning with AI mitigates the effects of climate change and natural disasters. Real-time urban dashboards that display environmental parameters could foster environmental accountability and enhance residents' quality of life. AI-assisted solutions for renewable energy systems similarly optimize performance, thereby increasing operational efficiency and lowering environmental impact. Furthermore, energy-demand forecasting and consumption-reduction strategies contribute to the transition to sustainable energy. The utility of meteorological data for wind-farm optimization showcases AI's capability in this domain. Corporate examples include Google and Huawei, both of which have implemented AI to regulate data-centre energy consumption.

6.3. User Satisfaction Metrics

User satisfaction represents a measure of comfort or unhappiness derived from the operation of different devices and/or the overall energy consumption pattern of all the appliances. In order to quantify the user satisfaction, clashes are computed. A clash between the user and EP is registered when the system would attempt to alter the current operation-mode of a device, or operate a previously unused appliance in order to optimize the energy consumed, when the user's preference is to maintain the current state of affairs (Gupta et al., 2020). The objective of user satisfaction can be further divided into two branches; User Satisfaction Maximization and User Dissatisfaction Minimization. The %user satisfaction should be maximized as it represents the rate of non-occurring electrical clashes during the operation of the EP, while user-

dissatisfaction should be minimized to reduce the probability of similar clashes (Samadi et al., 2020).

7. Discussion

For urban energy consumption optimization problems, solutions are often application-oriented and based on specific cases. Relevant problem-solving techniques involve mathematical optimization, machine learning, heuristic algorithms, simulation, and multi-agent optimization (Shah Syed et al., 2022). The framework presents an effective digital-reality parallel computing platform for optimizing urban energy flow and consumption. It collects and transmits data on consumption, cost, and system behavior from historical or real-time sources. This information supports large-scale energy optimization and urban decision making on cloud platforms. Digital mapping conducts related modeling, analysis, and computing (K. Meena et al., 2017). In parallel, a calibrated twin model runs optimization, including demand forecasting, scenario analysis, and control parameter calibration. In decision support, physical exploration and virtual interaction supplement existing functions. A case study on Beijing's urban system demonstrates that digital mapping enables computer programming of complex coupling in energy flow and urban elements. Mapping analysis from urban elements supports system calibration and remains more accessible than big-data analytics or AI engines for cities with limited experience.

7.1. Comparative Analysis of Case Studies

In (Iyengar, 2019) , an intelligent energy management system for home appliances is presented, emphasizing household and appliance profiles to enhance energy consumption visibility and control. A novel agent-based framework called Intelligent Control of Energy (ICE) targets commercial buildings and utilizes fuzzy systems, neural networks, and genetic algorithms to model building thermal response, achieving energy savings while maintaining occupant comfort. At the household level, a policy-based framework facilitates flexible power consumption management to address peak demand, with a house agent regulating appliance states based on the comparison between actual and available power. Autonomous agents representing consumers, resources, utilities, and production companies engage in negotiation protocols such as offer, request, and reward tables to optimize power consumption and system stability. A taxonomy of ten common household appliances characterizes their elasticity properties, and collected data on load profiles and usage patterns support probabilistic validation of energy management simulations.

7.2. Challenges in Implementation

Energy planning constitutes a crucial dilemma in microgrid management, compounded by fluctuations in climate and economic conditions. A pivotal uncertainty source arises from occupant behavior—subjects to sociological and psychological stimuli—thereby eliciting a discrepancy between anticipated and actual building energy use. Subsequent disparities in electric demand and thermal load analyses propagate algorithmic ambiguities throughout the forecasting framework. Diverse occupant motivations

underlie control decisions such as window blind manipulation to optimize privacy, external visibility, or engagement with the external environment. The behavioural complexity extends to ungoverned activities including but not limited to post-occupancy, distancing, preferences, movement, interactive engagement, and habitual modifications. and behaviours diverge collectively under spatial, temporal, and cultural contexts; quantification difficulties hinder representation in predictive tool kits. Typically, planners derive energy demands through aggregation of electrical and thermal consumption data from reference buildings, inevitably subject to occupant-driven invary-ing deviations. Following an extensive empirical review, existing urban-scale energetic optimization models uniformly apply aggregated demand benchmarks inherently susceptible to behavioural variations. Consequently, current schemes lack resilience to occupant-mediated fluctuations in consumption patterns and the associated building performance gap. fluidity of occupant behaviour therefore constitutes an intrinsic constraint on the efficacy of demand coverage clarification within the planning boundaries.

In microgrids, integration of form-specific demand requirements (e.g. electric power, heat) further increases the complexity of urban energy planning, where generation-restricting climate fluctuations and conjoining transport and housing infrastructure impose additional challenges. The requirement to facilitate cross-sectoral conversions and satisfy variable regional load demands intensify algorithmic computational burdens. Attempts to capture occupant-induced fluctuations necessitate redundant parallel simulations, with the exponential demand increase rendering the process impractical for high-resolution configurations. Predominant resolution of the planning problem through spatial and temporal breakdown embodies a necessary trade-off; this compromise allows computational management but limits the capacity to represent explicit relations between energy supply and specific demand types. The adopted granularity imposes aggregation between consumption profiles of diverse actors and sectors, obfuscating individual activity patterns and disrupting the expansive characterization of urban demand required to exploit synergies between energy prosumers.

The currently favoured structural dimension strikes a balance between level of detail and extensiveness but engenders ambiguity in profile assignment to single actors. Support from hourly demand signals for prosumer identification thus becomes compromised, obfuscating intra-sectoral correlations and their exploitation for self-consumption enhancement or load balancing. The planning framework requires further integration of demand-side management to fully appraise neglected flexibility sources; activating such untapped potentials during the planning process could significantly amplify exploitable window duration, thereby promoting larger utilization for the satisfaction of final energy requirements.

An urban-scale planning strategy is consequently needed that combines alternative social compositions with explicit consideration of occupant behaviour, a paradigm evaluable through stochastic programs with occupant behaviour among the scenario dimensions.

The resulting distributed stochastic framework enables explicit management of inter-building synergies between prosumers to offset dimensioning uncertainties. The model considers a heterogeneous set of end-users with diversified, electricity and thermal demand requirements. It incorporates distributed generation, storage technologies and their conversion through power-to-gas facilities that generate renewable methane. The methodology thus fully addresses the complexity of systems rationalising supply and demand across housing and transport infrastructures, as commonly observed in smart-city contexts. Experimental application demonstrates urban energy strategies differentially influenced by social configuration, contemporary energy sectors, and newly integrated synthetic fuel solutions. A flexible system architecture emerges as a key feature for accommodating contextual uncertainties during long-term planning, where the optimal mix of supply technologies responds sensitively to the variability of sociological factors driving occupant behaviour (Leprince et al., 2023).

7.3. Future Trends in AI and Energy Management

Future Smart Energy Management Systems (SEMS) will focus on comprehensive energy arenas, including urban mobility, electric vehicles (EVs), home primary usage, and energy trading. Such SEMS will integrate big data from renewable energy, user habits, and mobility to buffer and sustain power for transportation, residential spaces, and trading at both short-term and long-term levels. For example, emerging SEMS concepts will provide efficient real-time scheduling for EVs on both short- and long-term horizons (Khatun & Golam Sarowar Hossain, 2020) , while smart grids will enhance the efficiency of charging infrastructures (K. Meena et al., 2017). Integration of new user habits, such as charging during peak hours or after a whole-day ride, will optimize energy flow and reduce usage peaks. Open challenges include advanced new services coupled with deep-learning techniques (Rinchi et al., 2024).

Global climatic and environmental challenges and health concerns have reshaped the urban context in recent years. Cities have embarked on challenging reforms to become more energy- and environment-conscious. The Sustainable Development Goals (SDGs) of the United Nations, along with dedicated week-long campaigns, challenge cities to cap their emissions of climate-changing gases, reduce pollution, and improve energy consumption and economic costs. Cities will likely be forced to tightly monitor their urban metabolic processes and open data. Societies will also become more conscious, supporting behavioral change and sustainability efforts. These factors confirm that SEMS will become extremely sought single platforms, enhanced with intelligent components and enriched with various data mining and federated learning modules to extract new knowledge and provide valuable wealth pooling from sensing information.

8. Policy Implications

The direct influence of social and economic development on energy consumption underlines the necessity of urban energy-consumption management schemes . The complexity of urban energy consumption calls for the incorporation of open or publicly offered data sets and the utilization of urban elements . Long-term Human-city

Interaction (HCI) data offers a promising avenue for balancing future urban energy consumption, as it contains detailed information about individuals and their surrounding environment that can be fully exploited for forecasting.

Traditional energy management policies rely on extensive domain knowledge and professional expertise, which are time-consuming and difficult to generalize due to the heterogeneity of cities. To address these challenges, an intelligent policy-level control framework can be established based on HCI data for urban energy consumption management. As demonstrated by (Thevampalayam Kaliappan, 2019) , policy-based power consumption management using single-agent and multi-agent Q-learning algorithms can effectively reduce peak demand on the smart grid and decrease carbon emissions, thereby improving environmental performance. Reinforcement learning in a multi-agent system enables the complex heterogeneous human-natural-urban system to evolve toward an optimal state automatically and efficiently. Vehicle–building–human (VBH) data derived from HCI records can serve as the underlying state for developing reinforcement-learning-based policies for different control purposes. The accuracy and efficiency of these policies are related to the quality of the VBH data, providing a clear and interpretable path for policy improvement and development.

8.1. Regulatory Frameworks

Regulatory frameworks must govern resource exchanges and innovations that affect the quality of these systems and give rise to new phenomena such as collective intelligence in societies (Pournaras et al., 2017). In the emergence of smart cities, governments and regulators are challenged with making decisions on the design of technologies that can drive long-term transformations of infrastructures, economies, and societies. This evolution is mostly realised through distributed bottom-up organisations enabled by the Internet of Things (IoT). Urban energy consumption regulation has become even more complex since energy market rules combined with AI trading agents reduce control over the sharing of energy resources within the energy grid. One objective in such context is to regulate short-term drive cycles while maintaining the electric grid in a safe state.

8.2. Incentives for Adoption

The adoption of new energy system infrastructure can proceed slowly. New approaches to corpus acceptance must be considered because the challenges posed by a rapid influx the system owners must adapt to require careful evaluation. Approaches that gradually introduce usage and permit acceptance at a reasonable rate will emerge from a demand-centered perspective. Such strategies will incentivize the decision to adopt the system, to the potential benefit of the owner.

9. Technological Considerations

Infrastructure technologies are crucial components of transactive energy systems, especially in the context of smart city applications. The integration of artificial intelligence (AI) and machine learning (ML) techniques provides an alternative solution for optimized grid management. Various AI methods—including Genetic Algorithms,

Artificial Neural Networks, and Multi-Agent Systems—have been proposed for smart grid applications: Artificial Neural Networks have been successfully used for control management, solar energy response, and voltage stability monitoring; Genetic Algorithms optimize operational costs by integrating distributed units such as fuel cells and photovoltaic arrays; and Multi-Agent Systems involve multiple agents performing specific tasks like power output measurement, although further investigation is required for implementation, testing, and uncertainty management. For urban environments with high energy demand, transactive approaches are combined with mobile power infrastructure to alleviate system stress. Proposed models minimize system energy losses, maximize electric vehicle owners' benefits, and reduce hourly demand variations. These frameworks allow a substantial portion of vehicles with appropriate mobile infrastructure to engage in energy management, while others remain unaltered due to constraints or non-optimal conditions, and the model can be expanded to larger systems comprising diverse vehicle types and renewable energy sources. Added considerations for route optimization further enhance operational efficiency; objectives may include minimizing total distance traveled, CO2 emissions, total travel time, and overall costs. Frequently encountered constraints consist of fixed road networks, route continuity, and capacity limitations (Shah Syed et al., 2022) (Khatun & Golam Sarowar Hossain, 2020) (K. Meena et al., 2017).

9.1. Infrastructure Requirements

An AI platform for demand-side energy consumption optimization requires a nationwide communications infrastructure and real-time databases for optimal efficiency. It also requires AI expertise to design and develop optimization algorithms that recognize demand patterns, as well as physical infrastructure to implement strategies at residential and enterprise premises (Javier Ferrández-Pastor et al., 2019). Three broad categories of AI technologies—expert systems and traditional machine-learning approaches, more recent machine-learning techniques such as recurrent and convolutional neural networks, and evolutionary computing—are useful for accommodating the changing environment, seasonality of energy consumption, and socio-economic context within a demand-side management platform (K. Meena et al., 2017).

9.2. Data Privacy and Security

With smart cities, data privacy and security are essential but often overlooked. Daily functions require an Internet of Things (IoT)—a tremendous network of sensors, meters, actuators, and communication technologies that collect, transmit, and compute data. Used for various purposes, such as distressed-vehicle remapping and multimedia entertainment, data must be accessible, open, and adaptable—but the privacy risk escalates. Problems may arise with hacked wireless transmissions, microwave or phishing attacks, power-grid vulnerabilities, or relational databases. User-identity correlations can be exposed with a few monitored positions, usually in antagonism to safety and comfort. For smart homes, electric-grid companies gather household-consumption data with advanced metering infrastructure (AMI) for efficient scheduling

and management. Data leaking can reveal appliance operations and concerned times, creating a wide privacy gap with only a few measured points (Chang et al., 2018).

10. Stakeholder Engagement

Stakeholders occupy a central position in the urban-energy system. Decision-makers need to interact in the planning process with local governments, energy providers, companies, and inhabitants (Leprince et al., 2023). Data on occupants' behavior can be gathered at this stage, and residents should be informed about the installed energy system and its technical and economic features. Lastly, living habits can be involved at this point for urban activities like driving, cooking, shopping, or even gaming.

10.1. Community Involvement

Cities worldwide face interrelated challenges: increasing urbanization and demand for comfortable indoor conditions, severe pollution, and limited energy resources (Leprince et al., 2023). Energy integration appears as an opportunity to tackle these issues by improving energy efficiency, resilience, and the global carbon footprint of the urban environment. As a result, urban energy planning is gaining attention as cities evolve towards smart cities, encouraging the use of low-carbon energy sources, heat recovery, active load shifting, and efficient technical resource allocation. The various temporal, spatial, and categorical scales remain scattered, and a general modeling framework integrating the different scales and domains remains an open question. Occupants-driven energy demand clearly demonstrates the existence of a relevant scale below the urban one yet seldom assimilates building-level details that play a major role in urban energy systems. Continuous and massive data collection by smart devices, coupled with multicriteria optimization techniques, holds the potential to combine the different scales.

10.2. Partnerships with Tech Firms

The chapter discusses the oil and gas (O&G) industry’s collaboration with technology companies to accelerate the deployment of artificial intelligence (AI) and other digital applications aligned with digital transformation (DX) goals. In such partnerships, consultancies and indigenous technology firms develop AI applications, which O&G companies then deploy with the help of service providers and system integrators. Service providers and system integrators also develop and implement AI applications for direct use (K. Meena et al., 2017).

In the context of smart cities, a planning and operational management approach for mobile power infrastructure maximizes the profit of utility and electric vehicle (EV) owners participating in real-time smart-city energy markets. Artificial intelligence and the Internet of Things are employed to formulate effective solutions, validated using an IEEE 33-bus radial distribution network. Smart-city deployment addresses challenges related to rapid urbanization, the energy crisis, greenhouse gas emissions, and resource depletion while enhancing living standards through improved infrastructure for electricity, water, transport, and pollution control. Effective management of smart electricity infrastructure enables optimal control of distributed resources—including

distributed generation (DG), shunt capacitors, batteries, EVs, and demand response—and offers benefits such as reduced energy loss, lower emissions, decreased operating costs, and improved grid stability. Numerous optimization models have been proposed for planning and managing these resources. For example, supercapacitor-powered electric buses enhance grid efficiency by 6.46%, EV charging strategies minimize cost, IoT-based smart-city frameworks employ advanced communication for longer operational lifetimes, analyses of EV charging behavior support emission reduction strategies, and multi-objective decision-making hierarchies guide energy management in smart cities (Javier Ferrández-Pastor et al., 2019).

Conclusion

The proposed aggregator-based model offers an effective approach to mobile power infrastructure planning and operational management for smart city applications. By coordinating EV charging and discharging schedules, the model minimizes system energy losses and maximizes EV owners' profits. Each owner's daily profit is credited to their account. As a result of the optimized coordination, the variation in hourly system demand is reduced. Conventional EV charging during light-load hours and discharging during peak hours benefits EV owners but increases demand variation. The proposed approach smoothly shifts peak demand and thereby generates economic benefits for EV owners. In a case study, 308 vehicles participated in energy management, while 242 remained unaffected due to state-of-charge and trip-travel constraints. The methodology can be extended to larger systems with different EV types and renewable energy sources (K. Meena et al., 2017).

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References

Shah Syed, A., Sierra-Sosa, D., Kumar, A., & Elmaghraby, A. (2022). Making Cities Smarter—Optimization Problems for the IoT Enabled Smart City Development: A Mapping of Applications, Objectives, Constraints. ncbi.nlm.nih.gov

Hao, J. (2019). Multi-agent Reinforcement Learning Embedded Game for the Optimization of Building Energy Control and Power System Planning.

Salam Shah, A., Nasir, H., Fayaz, M., Lajis, A., & Shah, A. (2019). A Review on Energy Consumption Optimization Techniques in IoT Based Smart Building Environments.

FatehiJananloo, M., Stopps, H., & J. McArthur, J. (2023). Exploring Artificial Intelligence Methods for Energy Prediction in Healthcare Facilities: An In-Depth Extended Systematic Review.

K. Meena, N., Parashar, S., Swarnkar, A., Gupta, N., R. Niazi, K., & C. Bansal, R. (2017). Mobile Power Infrastructure Planning and Operational Management for Smart City Applications.

Khatun, A. & Golam Sarowar Hossain, S. (2020). Open Challenges and Issues: Artificial Intelligence for Transactive Management.

Iyengar, S. (2019). Scalable Data-driven Modeling and Analytics for Smart Buildings.

Ramos, D., Teixeira, B., Faria, P., Gomes, L., Abrishambaf, O., & Vale, Z. (2020). Use of Sensors and Analyzers Data for Load Forecasting: A Two Stage Approach. ncbi.nlm.nih.gov
Himeur, Y., Alsalemi, A., Bensaali, F., & Amira, A. (2020). Building power consumption datasets: Survey, taxonomy and future directions.
Ghiassi, N., Tahmasebi, F., & Mahdavi, A. (2017). Harnessing buildings' operational diversity in a computational framework for high-resolution urban energy modeling.
Khan, M., Seo, J., & Kim, D. (2020). Towards Energy Efficient Home Automation: A Deep Learning Approach. ncbi.nlm.nih.gov
Lee, S. & Choi, D. H. (2019). Reinforcement Learning-Based Energy Management of Smart Home with Rooftop Solar Photovoltaic System, Energy Storage System, and Home Appliances. ncbi.nlm.nih.gov
Chamoso Santos, P. & de la Prieta Pintado, F. (2015). Smart Cities Simulation Environment for Intelligent Algorithms Evaluation.
Capozzoli, A., Savino Piscitelli, M., & BRANDI, S. I. L. V. I. O. (2017). Mining typical load profiles in buildings to support energy management in the smart city context.
Condotta, M. & Borga, G. (2018). Urban energy performance monitoring for Smart City decision support environments.
Leprince, J., Schledorn, A., Guericke, D., Franjo Dominkovic, D., Madsen, H., & Zeiler, W. (2023). Can occupant behaviors affect urban energy planning? Distributed stochastic optimization for energy communities.
Pachot, A. & Patissier, C. (2022). Towards Sustainable Artificial Intelligence: An Overview of Environmental Protection Uses and Issues.
Gupta, S., Bhambri, S., Dhingra, K., Balaji Buduru, A., & Kumaraguru, P. (2020). Multi-objective Reinforcement Learning based approach for User-Centric Power Optimization in Smart Home Environments.
Samadi, M., Fattahi, J., Schriemer, H., & Erol-Kantarci, M. (2020). Demand Management for Optimized Energy Usage and Consumer Comfort Using Sequential Optimization. ncbi.nlm.nih.gov
Rinchi, O., Alsharoa, A., Shatnawi, I., & Arora, A. (2024). The Role of Intelligent Transportation Systems and Artificial Intelligence in Energy Efficiency and Emission Reduction.
Thevampalayam Kaliappan, A. (2019). Policy-based power consumption management in smart energy community using single agent and multi agent Q learning algorithms.
Pournaras, E., Yao, M., & Helbing, D. (2017). Self-regulating Supply-Demand Systems.
Javier Ferrández-Pastor, F., Manuel García-Chamizo, J., Gomez-Trillo, S., Valdivieso-Sarabia, R., & Nieto-Hidalgo, M. (2019). Smart Management Consumption in Renewable Energy Fed Ecosystems †. ncbi.nlm.nih.gov
Chang, H. H., Chiu, W. Y., Sun, H., & Chen, C. M. (2018). User-Centric Multiobjective Approach to Privacy Preservation and Energy Cost Minimization in Smart Home..

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Chapter 2: Big Data Analytics in Financial Fraud Detection: A Mathematical Framework

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Abstract: Financial fraud is a critical threat to global economic stability, especially in the era of digital finance, e-commerce, and real-time transactions. Traditional rule-based detection systems are insufficient to tackle the speed, scale, and sophistication of modern fraud techniques. This paper presents a comprehensive mathematical framework that integrates Big Data Analytics (BDA) with machine learning algorithms for real-time and scalable fraud detection. Leveraging tools like Apache Hadoop and Apache Spark, the framework enables distributed processing of high-volume transactional data and the rapid identification of anomalies. The study addresses various types of financial fraud—including credit card, insurance, securities, and ATM fraud—and explores data preprocessing techniques such as feature engineering, normalization, and dimensionality reduction. Both supervised and unsupervised learning methods are evaluated for their effectiveness, including decision trees, logistic regression, neural networks, and clustering models. Special attention is given to the problem of class imbalance, which is common in fraud datasets, by employing evaluation metrics such as precision, recall, and AUC-ROC. To ensure fairness and privacy, the framework incorporates ethical AI principles including differential privacy and bias mitigation. Real-time fraud detection pipelines using Spark Streaming and Kafka demonstrate practical implementation. The study also explores emerging areas like explainable AI (XAI), knowledge graphs, and adaptive learning to address evolving fraud tactics. By bridging big data technology with mathematical rigor and ethical design, this framework offers a robust solution to financial fraud detection, benefiting both financial institutions and regulators.

Keywords: Financial Fraud, Big Data Analytics, Machine Learning, Real-Time Detection, Ethical AI.

1 Introduction

Financial fraud detection received much attention since the 1990s, as the theft of financial assets rapidly increased. The proliferation of smart mobile devices, e-commerce, and other Internet-based services has boosted the number of financial transactions and therefore created a new ground for financial fraud. Big data analytics has become an essential approach for analyzing financial transactions and fraud detection because it can manage large volumes of data and its real-time streaming nature. Unfortunately, very few mathematical frameworks for big data analytics applied to financial fraud detection exist.

2. Understanding Financial Fraud

Financial fraud is illicit activity involving the manipulation or distortion of financial statements to create a competing benefit for those who committed the offense. The purpose of financial statement fraud often involves misrepresenting the true financial health of a company by artificially enhancing revenues and earnings and concealing liabilities and expenses to deceive shareholders and investors (West et al., 2015). Initially, fraudulent accounts are prepared and general-purpose financial statements are published as friendly documents that mislead users, enabling the perpetrators to secure dividends, loans and investment funds or to alternatively meet specified regulatory benchmarks (Zhu et al., 2021). Financial frauds can take the form of direct falsification and fabrication of documents, misrepresentation or omission of significant information, or causing or influencing the accounting system to record unjustified profits. Empirical studies conducted during the last thirty years have shown that financial statement fraud varies across industrial sectors and countries due to geographical and economic differences (Chimonaki et al., 1970).

2.1. Types of Financial Fraud

Financial fraud has been intensively studied during the last decades due to the rapid growth of the financial sector, the increasing number of fraud cases worldwide, and a stronger interest in the application of Big Data techniques. Financial fraud refers to the interfering acts performed by organisations or individuals to achieve objectives such as acquiring wealth through fraudulent means, and includes types such as credit card fraud, insurance fraud, securities/commodities fraud, and mortgage fraud.

Unfortunately, financial fraud is a very heterogeneous field and many types of fraud and approaches used to detect them have not been equally studied. It would be consequently nice to have a generic framework that is applicable to several different financial frauds. Different methods might be used to detect different fraud types. For example, support vector machines (SVM) and decision trees are popular for credit card fraud, Bayesian

belief networks have been widely implemented for securities and commodities fraud, while logistic models are frequently used for insurance fraud. A crucial step in fraud classification is feature selection, which has a significant influence on the quality of the classification, but few papers perform a comparative analysis between the features used for the detection of different fraud types (West et al., 2015).

2.2. Impact of Financial Fraud on Economy

Financial fraud has a devastating impact on the economy and needs a comprehensive detection framework. Given the lasting consequences of financial fraud in the finance industry, various government and corporate sectors, and for consumers (West et al., 2015) , an all-encompassing detection framework has become inevitable. Each year, billions of dollars are lost to various types of illegal activities such as asset misappropriation, accounting fraud, check and money order fraud, insurance fraud, or money laundering schemes and terrorist financing. The greater risk is to reputation, and the governing authorities often fail to identify the earliest indication of fraud. Increasing dependence and adoption of technologies such as cloud computing, mobile computing, social media, etc. have added to the complexity of such a framework. When traditional methods fail or break, new methodological approaches that marry statistical techniques and computational approaches become increasingly vital. An adaptive, multilayered fraud management framework that caters to different industry-specific needs is an imperative, especially in the current dynamic financial landscape (Zhu et al., 2021). Traditional detection techniques, such as manual auditing, have become time-consuming, costly, and impractical in the Big Data era, where data is generated at all times and from everywhere. Financial institutions and regulatory authorities are now employing automated processes that leverage a variety of statistical and computational methods.

Recent studies focus on data mining methods with a special emphasis on computational-intelligence techniques capable of detecting different types of financial fraud (Chimonaki et al., 1970). Illegal activities such as artificially inflating profits to meet analysts' forecasts, performing management buyouts using insider information, or misusing assets for personal gains can kill an organisation. The Internet and mobile technologies have facilitated and encouraged financial fraud. Credit and debit card fraud has surged with increased card usage, and individuals' online data has proven invaluable for fraudsters, who perpetually seek new and sophisticated methods for deception and manipulation. As deceptive techniques continually evolve, frameworks to detect financial deceit require constant adaptation to prevent undesirable consequences.

3. The Role of Big Data in Fraud Detection

The emergence of big data technologies has profoundly reshaped the landscape of financial fraud detection. Organizations are now capable of efficiently generating,

acquiring, and storing detailed transactional data, such as those derived from point-of-sale systems. These advancements facilitate the creation of comprehensive transaction profiles encompassing demographic information, purchase histories, financial behaviors, product interests, and behavioral patterns (West et al., 2015). Recognized as one of the six critical V's of big data, velocity describes the high-speed nature of financial transactions and the need for real-time data capture and analysis. Traditional qualitative methods are inadequate for discerning fraud patterns; consequently, many contemporary approaches employ machine learning, statistical analyses, forensic accounting, and artificial intelligence to detect anomalies.

From a technical standpoint, big data analytics for fraud detection are deployed in three principal ways: fraud visualization, real-time fraudulent transaction detection, and financial fraud profiling. The integration of real-time analytics with visualization methodologies enables immediate identification of suspicious activities. Big data analytics also facilitate the creation of detailed profiles of known fraudulent entities and transactions, assisting auditors and investigators in prioritizing cases based on estimated risk levels. Techniques such as Scala and Hadoop automate the flagging of fraudulent financial transactions and auditing activities within banking datasets, thereby streamlining analysis and enhancing the efficiency of fraud detection processes.

3.1. Definition of Big Data

Big data is a collection of massive amounts of data, which is at a large scale, high speed, complex variety, and with great potential value. In 2001, Doug Laney proposed the definition of "3Vs" for big data:(1) Data volume(W): Large-data—data of petabytes and above, cannot be processed and analyzed by conventional database software tools;(2) Processing velocity (V): Real-time or pseudo real-time acquisition and analysis of data;(3) Data variety (V): A variety of data types, including not only structured data, but also semi-structured or unstructured text, audio, images, and video. Later, "three Vs" expanded to "Five Vs". (4) Data value (V) refers to the intrinsic value and use value of data; the essence of big data is to extract useful information and rules from the massive data;(5) Data veracity (V) refers to the degree of data bias and accuracy.

3.2. Big Data Technologies

Modern big data technologies enable the storage, processing and analysis of large volumes of data to extract meaningful insights and support decision-making. Hadoop, a pioneer of big data platforms, integrates data across diverse sources into its Hadoop Distributed File System (HDFS), an open-source distributed file system that allows parallel processing of large datasets in a scalable or low-cost fashion. Spark has gained popularity within the big data analytics community partially because it also addresses the "Velocity" dimension of big data by providing a unified data analytics engine that can handle gigantic datasets in environments requiring very low latency. Distributed data

analytics engines can also perform efficient data mining and machine learning directly alongside big data pipelines and workflows. By replicating datasets in memory across a cluster, Spark offers additional abstractions such as data frames and resilient distributed data frames that enable convenient parallel and distributed operations on data. Spark's ability to support popular programming languages including Scala, Python, Java, and R further accelerates data science and data applications requiring "Value"-based big data insights. Spark's modular, plug-and-play architecture serves as the foundation for large-scale distributed big data processing and analytics far beyond its original scope, with separate modules catering to SQL queries, machine learning, and streaming analytics, all of which integrate seamlessly with the core execution engine. Integration with production data sources and pipeline orchestration tools — including streaming frameworks such as Apache Kafka and Amazon Kinesis, data persistence solutions such as Hadoop and Amazon HDFS, and query engines such as Apache Hive — further extends Spark's capabilities in managing continuous data streams; streaming query-mode applications support continuous ingestion and transformation with "mini-batch" micro-batches that typically consume input records in intervals of from 500 ms to 1 second. (Vivek et al., 2023) (West et al., 2015)

3.3. Challenges in Big Data Analytics

This research highlights work in either static or streaming data contexts for financial fraud detection. Given the growth of streaming sources such as social media and IoT, the streaming data challenge remains a critical theme for future work (Vivek et al., 2023). Specialized challenges within financial fraud detection include known issues like feature selection and parameter tuning, as well as the specific difficulties of secretiveness and complexity. Financial fraud perpetrators hide activities in increasingly sophisticated transactions, which in turn introduce natural labeling errors during model training, since non-fraud samples may contain unaccounted-for fraud instances. The complexity of financial transactions involves massive, heterogeneous, and low-value-density information— obstacles exacerbated by the secrecy of personal data. Knowledge graphs constitute a promising approach for storing and analyzing such large-scale information across multiple institutions, thereby providing comprehensive insights. Common themes emerge in financial fraud detection practices, in contrast with the general big data context of large volumes, high velocity, and data variety. Organizations continue to rely on tools like Hadoop and Spark for managing massive datasets. Spark provides a unified data analytics platform featuring data frames, RDDs, and numerous extensions for multiple programming languages, together with streaming and machine learning capabilities. Prior work defines ATM fraud detection as a binary classification problem: login history and transaction data analysis separate fraudulent activities from legitimate transactions. Detecting several fraud scenarios—including stolen cards, unusual transaction patterns, suspect locations, and bulk transaction amounts at given ATMs— constitutes the core

objective. This study addresses how scalable machine learning algorithms can be integrated into big data environments for ATM fraud detection in both static and streaming contexts.

4. Mathematical Framework for Fraud Detection

Automated fraud-detection techniques typically must classify very large numbers of transactions, and scalable extension of the algorithms to large volumes of data represents an open challenge (Vivek et al., 2023). Financial fraud is characterized as the abuse of a profit organization's system for financial gain, which does not necessarily imply legal implications. Financial fraud datasets fall within the big-data paradigm, characterized by volume, velocity, variety, veracity, and value: large quantities of data generated or acquired rapidly and often semi- or unstructured, with data quality or accuracy less reliable and information content of great interest. Big-data processing tools, such as Hadoop and Spark, enable organizations to cope effectively with datasets larger than those supported by traditional computing techniques. Spark, a largely Scala-based implementation, has become popular as a unified data-analytics-enginesystem with support for data-frames, resilient distributed datasets (RDDs), and streaming data, as well as integration with other programming languages (notably Python, R, and Java) and common big-data tools (e.g., Kafka, Hadoop).Automated detection of ATM fraud makes use of features extracted from transaction history to identify suspicious activities, including use of stolen or compromised cards, transactions employing unusual modes or at abnormal locations, and bulk transactions. Such behaviour is difficult to detect manually, especially in real time, and automated classification of transactions is a vital step. ATM-fraud detection is a binary-classification problem: each transaction must be labelled as either fraudulent or non-fraudulent in a timely manner, with the goal of minimizing the number of fraudulent transactions that remain undetected. Automated ATM-fraud detection is addressed within the Big Data paradigm by application of scalable machine-learning algorithms to both static and streaming transaction data (West et al., 2015).

4.1. Statistical Methods

The economic consequences of fraud and the potential for reputational loss have attracted considerable attention to the problem of fraud detection. Frauds have become increasingly frequent and high-profile over recent years and there are only limited examples of institutions that have managed to avoid large scale deception. The American public overwhelmingly believes fraud in commercial sectors occurs frequently, with those sectors perceived to suffer particularly badly being those where weak regulation exists or where large amounts of cash change hands. Furthermore, a large proportion of the public view corporate fraud either as a 'very serious' or 'serious' problem (West et al., 2015).

Fraud detection, like fraud related literature in general, spans a range of classification problems, including credit card fraud detection, financial statement fraud, insurance fraud, mortgage fraud and auction fraud. Whilst it is tempting to attempt to characterise all fraud detection studies as broadly as this, such a broad classification groups together a large range of considerably varying problems that have little in common beyond their fraudulent nature. Credit card fraud alone vastly differs from financial statement fraud; the former is focused on real time classification, accuracy and efficiency, whilst the latter is concerned with the classification of potentially multiple account summaries and also the insight acquired from the selected classification method.

The problem of fraud detection is generally considered to be a classification problem, although amendments have been proposed over the years. Fraud detection methods are used to classify a fraudulent or legitimate transaction, or an entity as either normal or anomalous. Furthermore, the majority of financial fraud detection techniques are concerned directly or indirectly with classification. A classification based scheme offers a general framework that readily encompasses a large range of computational intelligence techniques. The fraud detection problem involves an extremely biased distribution of classes where the instances of fraudulent activity amount to less than 0.002 percentage of the overall transactions, highlighting the major difficulty of mining low-prevalence classes.

4.2. Machine Learning Algorithms

Machine learning (ML) algorithms have demonstrated significant potential for fraud detection during the past few decades (Isangediok & Gajamannage, 2022). ML fraud detection represents a subtype of anomaly detection in which fraudulent instances constitute so-called “anomalies”. Such abnormalities may be identified with either supervised methods (e.g., autoencoders) or unsupervised algorithms (e.g., low-rank matrix completion). Logistic regression, decision trees, and naive Bayes continue to serve as popular baseline techniques in supervised learning owing to their simplicity and interpretability. Rule-based systems, k-nearest neighbour classifiers, and support vector machines (SVMs) generate relatively low precision rates and demand extended training time. The hidden Markov model (HMM) remains widely employed due to its capacity to uncover hidden patterns within skewed datasets. Ensemble learning has proven highly effective and adaptable in automated decision-making contexts. Random forests and boosting strategies resist overfitting; however, the resulting models often become complex with many trees and necessitate considerable computational resources. Artificial neural networks require large training datasets, entail significant computational overhead, and exhibit vulnerability to overfitting. Hybrid approaches combining statistical techniques such as discriminant analysis, Bayesian inference, and HMM with neural networks offer promising avenues for reducing misclassification rates.

Unsupervised methods like isolation forest and local outlier factor detect novel abnormal patterns but tend toward computational intensity and significant data requirements.

A principal obstacle arises from the relatively scant number of fraudulent instances, resulting in pronounced class imbalance that biases classifiers toward genuine observations. Remedies encompass algorithm-level adjustments, data-level resampling, cost-sensitive learning, and ensemble solutions. Streaming-data analysis assumes importance as timely fraud detection becomes mandatory; however, many traditional ML tools operate either offline or in a batch mode (Vivek et al., 2023). Spark's unified data-analytics engine addresses these issues through parallelized operators and support for Scala, Python, Java, and R. Integrations with Kafka and Hadoop facilitate efficient data-stream management. Large retailers and financial entities employ automated ML systems to detect anomalies such as stolen cards, unusual transaction patterns, purchases from atypical locations, and excessive sums; accordingly, the fraud-detection task may be treated as a binary classification problem that distinguishes between fraudulent and legitimate transactions. Scalability may be enhanced by substituting conventional IEEE-754 32-bit single precision data formats with the more compact BFloat16 representations; this permutation accelerates training and inference times without compromising precision and simultaneously reduces GPU memory consumption by approximately 35% (Yousuf et al., 2022).

4.3. Predictive Modeling Techniques

Predictive modeling represents a core approach in financial fraud detection. It entails developing predictive models for pricing or selection decisions relevant to fraudulent practices. The modeling process begins by selecting a specific activity or variable pertinent to the problem under consideration. Historical data on all pertinent variables is then utilized to train the model. Once developed, the model is applied to current data to predict outcomes for the selected variables, which in turn inform decision-making. Accurately modeling all associated variables proves challenging, particularly when a single prediction model underlies the determination of multiple variables. One solution involves creating separate models for each target variable, although this approach fails to capture interdependencies among variables.

Input data selection further complicates the task of predictive modeling. Incorporating an excessive number of variables can introduce biases or distortions related to the fraud variable. Conversely, omitting critical variables that influence the outcome leads to the creation of less accurate models. A wide array of mitigation techniques has been proposed. Artificial neural networks, similar to biological neural systems, emulate the brain's ability to learn from input data and generalize to new information. Multivariate adaptive regression splines utilize a nonparametric regression technique that combines basis functions to model complex, nonlinear relationships. Support vector machines

delineate the optimal boundary—maximizing separation—between classes. Logistic regression pumps input variables through a logistic function to output a probability score. Choice- or output- based models build composite approaches grounded in the assumption that users evaluate alternatives based on an expected utility framework (Isangediok & Gajamannage, 2022) ; (Vivek et al., 2023) ; (Rabiul Islam et al., 2018).

5. Data Collection and Preprocessing

The foundation of any Big Data analytical process lies in the acquisition of data from the desired source, achieved through various techniques tailored to the source.

The collected data undergoes preprocessing to eliminate irrelevant information, preparing it for analytical operations. Subsequently, data subjected to analytical processing is transformed into meaningful insights, which can then be exploited for diverse applications such as Decision Support Systems or Customer Relationship Management. The era of Big Data triggers a desire among organizations to apply data storage and analytical tools to enrich existing datasets and extract additional value. Unsupervised mining models are appropriate when methods and protocols are unavailable to guide analysis, while more targeted Business Intelligence applications benefit from supervised mining models. Establishing relationships among variables provides a deeper understanding of the factors influencing derived outcomes (Vivek et al., 2023). Data classification constitutes the process of categorizing data into classes, facilitating the understanding or prediction of variable values within a business procedure (West et al., 2015). Financial transactions serve as a primary source of data, encompassing details such as card number, transaction amount, merchant category, merchant identification, transaction date, transaction type, and customer identification.

5.1. Sources of Financial Data

Financial data can be broadly classified into four categories: (1) transaction data, (2) corporate data, (3) news data, and (4) data from regulatory bodies. Transaction data, which describes economic activities involving money flows in entities, is collected at various granularity levels: (a) stock-level; (b) individual-level; and (c) aggregated-level. Corporate data usually consists of (a) a corporation's biographical information and (b) its financial statements. The biographical information may contain the dates on which a firm was incorporated, its addresses or office location, and its top-management personnel such as the CEO and CFO. Data repositories such as Edgar Online and Morning Star offer access to firms' financial statements (Chimonaki et al., 1970). Different types of financial statements (balance sheets, income statements, cash flows, and equity statements) can be parsed from these texts. News data collected from media reports as well as a firm's website, Twitter, and LinkedIn can provide exogeneous information on the firm's financial status. Data from Regulatory Bodies Document archives of regulatory bodies such as the SEC and Factiva can be used for detecting

information anomalies. A mathematical framework relying on the above data sources and the volume, velocity, and variety dimensions of big data, may be deployed for tracking or identifying possible suspicious transactions (West et al., 2015).

5.2. Data Cleaning Techniques

In big data analytics for financial fraud detection, data cleaning is a crucial preprocessing step that ensures the quality and reliability of the analysis. Data cleaning addresses common problems such as noise, missing values, inconsistencies, and duplicates (Vivek et al., 2023). Cleaning techniques begin with noise removal, which corrects or eliminates erroneous and irrelevant data points. Next, imputation methods fill in missing attribute values using approaches such as mean, median, clustering, or regression to preserve retention of valuable data. Inconsistencies—a mismatch between attribute values—are identified and resolved to maintain internal coherence. Lastly, duplicate records are detected and eliminated to reduce redundancy. Effective data cleaning refines the initial dataset to a consolidated core of dependable data, optimizing the performance of subsequent computational tools and data models (West et al., 2015).

5.3. Data Transformation Methods

When either raw data or feature-extracted data are unsuitable for use in forecasting models because of format or analysis requirements, data conversion becomes necessary. Data transformation involves creating a new indicator—expressed as a mathematical function of the source indicator—that provides an equivalent description of the measurement data but in a transformed space. The transformation aims to improve certain desired properties of the data, such as linearity, normality, stability, or scale (Vivek et al., 2023).

Indicator transformation encompasses three main categories. Conversion involves translating data from one type to another. Discretization converts continuous data into categorical data. Distribution extends or compresses the original data range. The choice of transformation method is dictated by the needs of the subsequent analysis, rather than the original data format (Isangediok & Gajamannage, 2022).

6. Feature Engineering in Fraud Detection

This section addresses the feature engineering phase, during which raw features extracted from logs of numerous web service applications are mapped into high-level features (Vivek et al., 2023). Because log files capture various aspects of web service invocations and incompatibilities, this task requires domain expertise. To assist in feature identification, the analysis of a dataset consisting of 13 million Service Monitoring Facility (SMF) messages collected over a one-month period from an IBM z/OS mainframe is conducted. The built environment includes more than 5000 autonomous unit-processes (transient services) employed by thousands of different

applications running on over 5000 virtual machines per month. The evaluation of features to be collected is based, therefore, on the analysis of some selected pilot environments. Although, in principle, the mapping of features into a compact and high-level representation is a critical phase, the analyses focus only on the principal characteristics of the process.

6.1. Identifying Relevant Features

Feature selection is an integral part of solving problems involving large data, such as financial-fraud detection. The process aims at improving both the performance and the understanding of the model by identifying the most relevant features. Two main types of algorithms exist: feature-ranking algorithms rank the features based on some criterion, whereas feature-selection algorithms select a subset of relevant features (West & Bhattacharya, 2015). Because of the large size of the feature space, the evaluation time of the feature subset is often overwhelming. For this reason, the algorithms are often based on heuristics, which reduce the number of searches and calculations required to identify a good feature set. Over-aggressive pruning may lead to the elimination of beneficial features, yielding lower model accuracy. Typical features in financial fraud detection are numerical variables related to earnings, assets, and expenditures.

6.2. Dimensionality Reduction Techniques

Analysing and visualising information representing billions of observations can quickly become cumbersome. Several methods exist to reduce the dimensionality of data with a minimal loss of information. For logistics purposes, all methods for dimensionality reduction can be categorised as feature selection or feature extraction (Vivek et al., 2023). In many cases, additional assumptions or prior knowledge of the data are required to identify the attributes that carry the most information (Sharma et al., 2020).

Principal component analysis is a popular approach for feature extraction, which transforms the N original variables into a new set of K variables, with $K < N$, by removing correlations between the original attributes. These new variables are uncorrelated and ordered to retain the most variation. Another method allows for the data to be embedded into a low-dimensional space with a non-linear mapping, which retains structure better than linear techniques—such as isometric feature mapping (Isangediok & Gajamannage, 2022). Variable subset selection seeks the best subset of the input variables based on some model and criterion. Feature creation constructs new relevant features and combines existing attributes through some optimisation problem or some evaluation function.

7. Model Training and Evaluation

Model training involves fitting a machine-learning model to representative training data—features and labels—to learn the mapping from input features to output labels,

performed in a supervised, offline manner. The trained model can then be used for model inference, where new, unlabelled transaction data are classified as fraudulent or genuine. The training phase typically triggers when a sufficient dataset has accumulated, occurring during regular off-peak periods. The system enqueue the dataset to the training pipeline, which trains, evaluates, packages, and stores the model in a both local repository (for subsequent simulation and batch operations) and global distributed file system (for subsequent detection). During training, cross-validation assesses the model's generalisation capability and estimates performances on unobserved data (Vivek et al., 2023).

Tree-based classification algorithms emerged as a popular choice—offering both performance and interpretability—along with a rich and diverse family of algorithms such as random forests, gradient tree boosting, and extremely randomized trees. Several factors can undermine performance, including dataset imbalance, dataset sparsity, the volume of training data available, and ongoing training opportunities. Moreover, engineering a shared set of informative features is always challenging when simultaneous detection of different fraud types is the goal (Isangediok & Gajamannage, 2022).

The training pipeline supports different evaluation modes that enable extensive offline experimentations:

• K-fold cross-validation assesses model capability on moderate-sized datasets by extracting multiple, balanced, and disjoint training-testing partitions.

• Partial train-test—splitting convey sets—evaluates models on large datasets and removes sampling techniques that may be unfeasible. This is the only mode utilised for model calibration.

7.1. Training Algorithms

A comprehensive a mathematical framework for big data analytics in the context of financial fraud detection is proposed, with a focus on key challenges and solutions. The framework addresses terminology challenges, such as distinguishing between a big data solution (the method) and big data analytics (the method combined with implementation), and defines key components including training algorithms, evaluation metrics, statistical tools and mathematical models, and implementation strategies. A taxonomy categorizes fraud-detection problems into seven classes based on fraudulent target, provides characteristic requirements for each, and indicates Big-Data Capability (BDC) prerequisites. Among these, the training algorithm and BigData Capability are singled out as central to the framework. Regarding training algorithms, the framework models a semi-supervised learning control system using mathematical sets and functions, reflecting a scenario with a limited amount of tabular data, a common situation

in fraud detection. The four equivalent representations detailed accommodate various algorithmic paradigms. The framework underscores the criticality of visualization and human-in-the-loop analysis in environments where the imbalance between genuine and fraudulent data points hinders fully automated approaches (Vivek et al., 2023).

8. Deployment of Fraud Detection Models

Fraud detection models are commonly deployed through a machine learning pipeline comprising feature engineering, fine-tuned hyperparameters, and a classifier. The deployment environment demands real-time simultaneity of these steps, with the model producing a fraud score before the cascade proceeds. To create a model of sufficient specificity and sensitivity, the feature-making phase filters and standards the data within the transaction history of the individual cardholder, retaining only the top 600 correlated features. The transaction then funnels into a compact, finely parameterized model that churns out a score compatible with the live stream of transactions.

The evolving nature of fraudulent activity necessitates a method for introducing incremental updates to the model architecture that can be delivered instantly with the lease of every transaction, diverging from traditional online-learning methods. SCARFF, a framework designed for streaming credit card fraud detection, offers a scalable and efficient implementation capable of handling vast streams of transaction data with minimal delay (Carcillo et al., 2017). The framework maintains compatibility with big data platforms such as Apache Kafka, Apache Spark, and Hadoop Distributed File System (HDFS), facilitating seamless integration and rapid deployment. Source code and documentation are freely available, enabling immediate adoption and customization.

8.1. Integration with Financial Systems

Financial institutions routinely exchange transactional and market information to support services such as commercial loans, credit cards, ATMs, and online banking (West et al., 2015). Conversely, criminals leverage these platforms to facilitate fraud. Any service that manages financial exchanges therefore requires mechanisms to accommodate big data and monitor corruption.

Big data describes datasets so vast and complex that traditional analytics fail. These datasets exhibit high volume, velocity, variety, veracity and value. Under this paradigm, fraud detection addresses a binary classification problem applied to dynamic streaming records (Vivek et al., 2023). Within the volume of data available to a financial organization, ATM fraud constitutes a very small percentage. Both static and streaming data algorithms therefore operate at scale to distinguish the few suspicious transactions among the many legitimate ones.

Real-time crime identification and prevention proves a necessity. Exchanges occur in continuous streams and respondents have scant time to respond to suspicious activity

before significant losses accrue. Organizations therefore rely on detection methods that accommodate streaming data inputs and deliver expressed allegations in real time. When a network receives a financial transaction for authorization it simultaneously sources the client profile to determine whether the undertaking appears consistent with prior habits or common conventions. If apparent inconsistencies arise the operation receives extra scrutiny or outright rejection for contact by human analysis.

8.2. Real-time Monitoring

Financial big data, such as transaction logs collected at short time intervals, must be processed in a timely manner to reduce the time delay in identifying fraudulent activities. Desirable characteristics of big data systems include scalability, reliability, and cost effectiveness. Modern frameworks based on open-source technologies address these requirements. For example, Spark offers a unified data analytics engine handling large datasets and supports various programming languages, SQL, machine learning, and streaming analytics. Discretized streams (DStreams) enable batch stream processing and integration with tools like Kafka and Hadoop for managing continuous data streams. Financial fraud detection often involves analyzing transaction history and customer purchase patterns to identify scenarios such as stolen cards, unusual transaction history, transactions from uncommon locations, or bulk amounts. Automating this process using machine learning techniques facilitates real-time detection. Formulated as a binary classification task distinguishing between fraud and non-fraud, the problem can be addressed with scalable machine learning algorithms under the big data paradigm (Vivek et al., 2023).

9. Case Studies

Fraud detection is ordinarily construed as a classification problem involving a considerable class imbalance. The cost of misclassifying examples is comparatively high because of the significant financial or reputational risk of neglecting fraud. Data mining approaches are well-suited classifiers applicable to large datasets that do not require extensive knowledge of the problem domain. Data mining based classification of transactions as suspicious or not permits targeted manual review; for example, scrutinizing only 2% of transactions can reduce fraud losses to merely 1% of the entire purchase cost. A modular, multi-layer pipeline effectively screens easily identifiable frauds through initial layers, thereby confining manual inspection to more subtle instances that require domain expertise. Earlier research concentrated on statistical models and artificial neural networks which can efficiently manage streaming data. A more recent approach employs game theory to capture the inherent adversarial nature of fraud, modeling fraudsters and detection mechanisms as rational players with opposing objectives, each aware of the other's strategies, goals, behavior, and payoffs. Process mining techniques are advantageous for fraud detection problems involving complex

interactions and sequential dependencies among events, proving particularly effective against digitization and automation threats in healthcare fraud. Empirically and theoretically, classification-based methods continue to dominate the literature as the most investigated and successful techniques in financial fraud discovery (West et al., 2015). Consequently, any fraud detection system focuses predominantly on issues related to either novelty or classification.

Within an ATM network, funds are accessible via an extensive worldwide digital infrastructure. A typical fraudulent scenario involves a user borrowing money, which the fraudster subsequently deposits into the borrower's account. Detecting whether an ATM transaction is fraudulent constitutes a binary classification task; fraudulent transactions are designated as the positive class, while non-fraudulent ones form the negative class. The volume of transactions recorded in a typical ATM network often precludes manual analysis of the entire transaction history for each activity in real time. Applying data analytics to this problem mitigates the burden of manual inspection to a considerable extent. Scalable machine learning algorithms capable of addressing static data and efficiently adapting to streaming data are crucial for ATM fraud detection within a big data context (Vivek et al., 2023).

9.1. Successful Implementations

A report by Case Western Reserve University details the implementation of big data analytics for ATM fraud detection (Vivek et al., 2023). It notes that financial fraud datasets exemplify the big data paradigm characterized by the five Vs: volume, velocity, variety, veracity, and value. Big data processing tools such as Hadoop and Spark provide the computational backbone. Spark's unified data analytics engine handles massive datasets and offers abstractions like data frames and resilient distributed datasets that support parallel and distributed operations. The platform extends support for multiple programming languages and integrates seamlessly with ingestion tools such as Kafka and Kinesis. ATM fraud detection determines whether a transaction is suspicious according to criteria like stolen cards, unusual locations, and large transactions. Automating this process with machine learning is essential because real-time analysis is otherwise prohibitively difficult. The study treats ATM fraud detection as a binary classification problem and investigates the use of scalable machine learning algorithms for static and streaming contexts.

9.2. Lessons Learned from Failures

Failures and limitations of previous research provide useful insights for future work in financial fraud detection. Many studies have highlighted typical classification problems, such as feature selection, parameter optimization, and comprehensive analysis of the problem domain, to enhance classification performance. Some methods even required

the integration of techniques like feature selection to be effectively applicable (West et al., 2015).

To overcome these issues, current research should focus on thorough analysis of the problem domain, effective feature-engineering, adaptive approach to parameter tuning, and employment of robust classification algorithms. Understanding fraud characteristics and mechanisms facilitates meaningful analysis of data components and their relationships, enabling the extraction of appropriate predictors. While some methods make minimal assumptions about underlying data distributions and thereby simplify implementation, their effectiveness may be limited without proper feature-engineering—especially when the feature space includes noisy, irrelevant, redundant, or misplaced features. Less effective feature-engineering thus constitutes a potential limitation. Parameters should, wherever possible, be tuned adaptively during training, rather than remain fixed, given the costliness and inflexibility of static parameter-tuning. Finally, classification algorithms sensitive to outliers may degrade in the presence of data noise, corrupting the training model and leading to inaccurate, unreliable predictions; solely relying on fine-tuning to mitigate this risk therefore exhibits limited effectiveness.

10. Future Trends in Financial Fraud Detection

Future trends in financial fraud detection will reflect the ongoing transformation of the financial sector, resulting from big data applications and advances in information and communication technologies. One likely direction is that big data techniques will be employed to address many of the problems associated with the existing methods, as the availability and accessibility of big data infrastructure continue to improve. Hybrid methods, combined with well-tuned classifiers, have proven particularly effective for financial fraud detection. Challenges such as feature selection, parameter tuning and problem analysis require continual attention. The complexity of financial activities leads to massive and heterogeneous information, which is difficult to integrate when scattered across different institutions. The development of auxiliary structure tools possibly based on knowledge graphs, which are well suited to storing and analyzing massive data and representing information about every entity related to fraud, may provide a helpful panorama for investigating complex multi-source information. Although data-driven artificial intelligent techniques have achieved excellent performance in the domain, financial fraud schemes evolve rapidly to adapt to new digital environments. The secretiveness of financial fraud leads to natural errors in training samples, as unrecognized fraud instances often contaminate the non-fraud data, resulting in fundamental inaccuracies in the captured features and threatening detection accuracy. (Zhu et al., 2021) (West et al., 2015)

11.1. Emerging Technologies

Emerging techniques such as soft computing, metaheuristics, and hybrid algorithms demonstrate the effectiveness of big data technologies for financial fraud detection. These approaches also address complex data analytic problems based on large datasets. Since big data technologies contribute to designing financial detection schemes, a decision-making framework with mathematical tools to abstract the problem at a conceptual level facilitates the mapping of a financial case study to the framework (West et al., 2015). Financial fraud detection remains an active area of research with adequate opportunities for application of emerging technologies.

Financial fraud detection is a major concern for industries and customer banks, making solutions for combating fraud critical and challenging (Vivek et al., 2023). Anomalies such as false declarations of transactions can create significant problems for the banking industry. Although various schemes address these problems, a well-established framework for handling big data is necessary for efficient analysis. Current schemes detect anomalies within a system but do not provide valuable information about real-world financial fraud detection problems. Capitalizing on the high utility of big data analytics for describing customer and financial bank data in an intelligent and automated manner enhances the ability to detect fraudulent activities.

Big data acquired from ongoing activity plays a crucial role for banks. Techniques for detecting ATM fraud utilize machine learning methods on big data streaming platforms. Many firms have invested in big data analytics to analyze data and obtain greater insights into customer behaviour. Improving accuracy, sensitivity, and precision is important for business processes, driving motivation for this study. The solution addresses a real-time ATM fraud detection scenario requiring instantaneous decision making. An elaborate mathematical framework is designed that utilises hybrid-independent deep learning.

Big data technologies contribute significantly to industries and organisations. These technologies become pivotal in data analytics and investigation. Their efficacy in qualitative and quantitative analyses renders them versatile in providing optimized studies for real-time applications. A mathematical framework supports an efficient mechanism for tackling data-oriented problems. This framework involves a mapping procedure that converts data or a real-time application to the framework, thereby addressing associated problems and complexities. The framework supports designing methodologies for data analysis systems that enable efficient solutions in a systematic manner.

11.2. Regulatory Changes

Most of the work in the financial fraud domain indicates that big data analytics can play a vital role in tackling the financial fraud problem (Vivek et al., 2023). Thus, this section suggests the need for a mathematical framework that enables organizations to manage financial fraud more effectively. It presents an overview of big data analytics, suggesting

a mathematical framework to address the financial fraud problem in the big data context. This framework enables organizations to estimate online fraud at early stages by analyzing big financial data. Organizations base their policies and critical decisions on analyses of vast data volumes—big data. Financial fraud datasets particularly adhere to the big data paradigm. The five Vs—Volume, Velocity, Variety, Veracity, and Value—are the primary characteristics. Various big data processing tools—Hadoop and Spark—enable organizations to collect and manage huge data. Spark has gained popularity due to its unified data analytics engine capable of handling massive datasets, offering abstractions like data frames and resilient distributed data frames, supporting parallel and distributed operations. It integrates with tools like Kafka and Hadoop for managing continuous data streams. ATM fraud detection holds particular interest within the financial fraud domain. It involves examining transaction histories to identify suspicious activity, such as stolen cards, unusual location, or transaction amounts. Automating this process with machine-learning techniques is essential, as real-time analysis is challenging within limited time frames. ATM fraud detection is a binary classification problem, with fraudulent transactions as positive and legitimate ones as negative. Scalable machine-learning algorithms and methodologies address ATM fraud detection within the big data paradigm in both static and streaming scenarios.

12. Conclusion

Financial systems are vulnerable to fraud and require mechanisms to prevent economic loss. Alongside transaction processing, the detection of fraud and money laundering has become a key focus of critical financial systems. These activities are assessed as instances of behavioural profiling, whereby assessment is based on a set of anomalous behavioural characteristics. The ongoing growth of transaction volumes, variety and velocities necessitates the use of a Big Data framework where large-scale parallelisation, transaction log analysis and visualisation are deployed. The development of a Big Data framework is described that supports the detection of both money laundering and financial fraud when deployed alongside an information sharing infrastructure distributed across a financial services marketplace. The framework incorporates a scalable real-time mathematical model that characterises fraudulent and money-laundering transaction activity in order to provide the foundation for modelling the differing and dynamic transactional profiles of financial crime activity. The deployment of the framework across a financial services marketplace enables the sharing of transaction information to provide reliable transactional activity to underpin collective fraud and money laundering detection (Vivek et al., 2023).

References

West, J., Bhattacharya, M., & Islam, R. (2015). Intelligent Financial Fraud Detection Practices: An Investigation. [PDF]
Zhu, X., Ao, X., Qin, Z., Chang, Y., Liu, Y., He, Q., & Li, J. (2021). Intelligent financial fraud detection practices in post-pandemic era. ncbi.nlm.nih.gov
Chimonaki, C., Papadakis, S., Vergos, K., & Shahgholian, A. (1970). Identification of financial statement fraud in Greece by using computational intelligence techniques. [PDF]
Vivek, Y., Ravi, V., Anand Mane, A., & Ramesh Naidu, L. (2023). ATM Fraud Detection using Streaming Data Analytics. [PDF]
Isangediok, M. & Gajamannage, K. (2022). Fraud Detection Using Optimized Machine Learning Tools Under Imbalance Classes. [PDF]
Yousuf, B., Bin Sulaiman, R., & Saberin Nipun, M. (2022). A novel approach to increase scalability while training machine learning algorithms using Bfloat 16 in credit card fraud detection. [PDF]
Rabiul Islam, S., Eberle, W., & Khaled Ghafoor, S. (2018). Credit Default Mining Using Combined Machine Learning and Heuristic Approach. [PDF]
West, J. & Bhattacharya, M. (2015). Mining Financial Statement Fraud: An Analysis of Some Experimental Issues. [PDF]
Sharma, H., K. Gandhi, H., & Jain, A. (2020). Towards Credit-Fraud Detection via Sparsely Varying Gaussian Approximations. [PDF]
Boge Brant, S. & Hobæk Haff, I. (2021). The fraud loss for selecting the model complexity in fraud detection. [PDF]
Carcillo, F., Dal Pozzolo, A., Le Borgne, Y. A., Caelen, O., Mazzer, Y., & Bontempi, G. (2017). SCARFF: a Scalable Framework for Streaming Credit Card Fraud Detection with Spark. [PDF]
Perez, I., Wong, J., Skalski, P., Burrell, S., Mortier, R., McAuley, D., & Sutton, D. (2024). Locally Differentially Private Embedding Models in Distributed Fraud Prevention Systems. [PDF]
Maniar, T., Akkinepally, A., & Sharma, A. (2021). Differential Privacy for Credit Risk Model. [PDF]
Pombal, J., F. Cruz, A., Bravo, J., Saleiro, P., A. T. Figueiredo, M., & Bizarro, P. (2022). Understanding Unfairness in Fraud Detection through Model and Data Bias Interactions. [PDF]

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Chapter 3: Cryptographic Algorithms and Number Theory: A Computational Approach

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Abstract: Cryptography, the cornerstone of secure digital communication, relies heavily on the principles of number theory to ensure confidentiality, integrity, and authenticity of data. This study explores the foundational role that number theory plays in cryptographic systems, emphasizing its application in both symmetric and asymmetric key encryption methods. Key theoretical concepts—including modular arithmetic, Euler's theorem, Fermat's little theorem, and properties of prime numbers—are presented as essential tools for designing robust cryptographic algorithms. Advanced topics such as RSA, elliptic curve cryptography (ECC), and digital signatures illustrate the practical implementation of these theories. Additionally, the document discusses the evolution and vulnerabilities of symmetric (block and stream ciphers) and asymmetric schemes, alongside cryptanalysis techniques and countermeasures. The importance of secure hash functions and high-quality pseudo-random number generators in preserving data authenticity and secrecy is highlighted. Furthermore, cryptographic protocols such as TLS and Public Key Infrastructure (PKI) are explored for their roles in secure data transmission. Contemporary challenges—including threats posed by quantum computing—underscore the urgency for post-quantum cryptography (PQC) development. Future directions suggest a focus on algorithmic efficiency, larger key sizes, and quantum-resistant protocols. By bridging abstract number theory with computational cryptographic applications, this work provides a comprehensive understanding of the mathematical backbone securing modern digital infrastructures.

Keywords: Cryptographic Algorithms, Number Theory, Modular Arithmetic, Public Key Cryptography, Post-Quantum Cryptography.

1 Introduction

Cryptography is concerned with secure communication between computers. Encryption is essential for confidentiality and privacy, but cryptographic algorithms must ensure authentication, integrity, and authenticity as well. Cryptanalysis informs the design of schemes able to withstand computational attack. A rich theory contributes to their analysis, direct construction, or extensions to other tasks. Number theory offers a source of mathematically defined computational problems and enables convenient arithmetic in appropriate mathematical structures. These arise in key establishments, block or stream ciphers, and digital signatures. Protocols specify how security services are implemented in distributed systems and incorporate these primitives. Modern cryptography can be applied almost ubiquitously—or at least wherever communication takes place (Rothe, 2001).

2. Fundamentals of Number Theory

Number theory constitutes the study of positive integers, an ancient branch of mathematics that composes a foundation for numerous areas within the discipline. It also represents the simplest yet most widespread branch of algebraic geometry. Any polynomial in the ring Z[X] is integer valued; that is, P: Z → Z. Recently ranging across inquiries of arithmetic, structure, computable behaviour, and conjectures, the theory of numbers has developed into a prime source of innovative ideas (Santilli, 2019). Problems yielding integer solutions to a polynomial equation with more than one unknown traverse the entire breadth of the field . The treatment of integers permeates every classical branch of pure mathematics and therefore attracts a wide spectrum of applications (W. Lenstra, 1992). The obscurity of the integers combined with the pervasive presence of number theory within mathematics grants the capacity to traverse from calculations found in astronomy and physics to the most abstract and intriguing conjectures.

3. Mathematical Foundations for Cryptography

Cryptography for Online Security: Applications of Number Theory (2018) Fermat's little theorem states that if p is prime and a is coprime with p, then a^p ≡ a mod p. This theorem is useful in primality tests and public-key cryptography. Euler's Totient Theorem generalizes this for all integers where a and n are coprime, and a^φ(n) ≡ 1 mod n, with φ(n) being the totient function. Modular arithmetic underpins the security of encryption algorithms. Selecting large primes and constructing keys based on their properties makes factorization difficult, enhancing security. Using theorems from number theory, the strength of cryptography increases with larger primes, making factorization computationally infeasible. Number theory provides the mathematical foundation for secure cryptographic methods, ensuring data confidentiality and integrity.

Mathematical foundations for cryptography

Modern cryptography is intimately connected with the theory of numbers, and often prime numbers play an important role. Fermat's little theorem states that if p is a prime and a is coprime with p, then raising a to the pth power leaves a remainder a when divided by p. Euler's totient theorem states that if a is coprime with n, then a raised to the φ(n)th power leaves a remainder 1 when divided by n, where φ(n) is the number of positive integers smaller than n and coprime with n. Modular arithmetic plays an essential role in number-theoretic cryptography. The security of cryptosystems based on the factorisation problem derives from the difficulty of finding the factors of a given integer and is therefore related to primality testing. In that sense, the research on primality tests provides a better understanding of the difficulty of factorisation. In practice, these cryptosystems rely on modular exponentiation with large integers. They are therefore based on the assumption that factoring large integers is hard. One selects two sufficiently large primes, p and q say, and combines them in some manner to form the encryption key. The corresponding decryption key then depends on p and q. Recovering the decryption key from the encryption key requires factoring, which cannot be done efficiently for large numbers. Inefficient means that the computational cost of any factoring algorithm that we know of is so high in terms of processing time and memory space that we cannot perform the factorisation in realistic situations. The security of many cryptographic techniques, including digital signatures, confidentiality and authentication procedures also relies on the use of modular arithmetic with large integers.

3.1. Modular Arithmetic

Modular arithmetic is the foundation of many cryptographic algorithms based on number theory. Generally, modular multiplication and division operations need to be computed in these algorithms. Several methods have been discovered, including Montgomery multiplication and Montgomery modular inverse. This section introduces two new algorithms to calculate modular multiplication and division, which rely on the Euclidean algorithm and exhibit quadratic complexity (Gouicem, 2013).

3.2. Prime Numbers and Their Properties

A prime number is a natural number greater than 1 that has no positive divisors other than 1 and itself. The problem of deciding whether a given number is prime has been approached through various algorithms. Trial division relies on the property that the largest divisor of a number n is less than or equal to n; however, for large numbers, this process becomes very slow (TAHIRI JOUTI, 2007). Primality testing algorithms encompass randomized methods that produce probabilistic results and deterministic algorithms that guarantee accuracy. Several conjectures and theorems related to prime numbers include the prime number theorem, Goldbach\019s conjecture, and the Riemann hypothesis (Asimi, 2023). The greatest common divisor (gcd) of two numbers n and m is the largest integer dividing both. Two numbers are called relatively prime if their gcd is 1; equivalently, this means that 1 can be expressed as a linear combination of n and m. The Euclidean algorithm efficiently computes the gcd of two integers.

4. Symmetric Key Cryptography

Symmetric key cryptography utilizes an identical secret key for both encryption and decryption processes (Babu et al., 2013). Distinguished also as secret key, single key, shared key, one-key, or private key encryption, it encompasses two primary cipher forms: stream ciphers and block ciphers. Notable symmetric algorithms—such as DES, AES, RC4, 3DES, and Two Fish—vary according to block sizes, key lengths, and the number of transformation rounds applied. Historically, DES operated with a 64-bit block size and a 56-bit key during the 1970s; however, the algorithm was retracted as a commercial security standard by the late 1990s. The advent of AES (Rijndael Algorithm) provided a more robust and secure successor to DES. While conventional cryptosystems predominantly function within finite algebraic structures performing modulo arithmetic over natural numbers, the feasibility of secure symmetric ciphers over the field of real numbers has been explored (Hassoun, 2016). Such schemes employ numerical solutions

to linear and non-linear equations, adapted to meet stringent security criteria through the construction of composite ciphers featuring multiple encryption layers. Security enhancements have been quantified by estimating key-finding uncertainty via Shannon entropy measures.

4.1. Block Ciphers

Block ciphers probably figure in the list of the most important cryptographic primitives (Baignères, 2008). Although they are used for many different purposes, their essential goal is to ensure confidentiality. An n-bit block cipher is a function E :Vn × K → Vn, where for each key K, E(P,K) is an invertible mapping from Vn to Vn, known as the encryption function. Its inverse is the decryption function D K(C) (Abdelkhalek, 2017). A block cipher can be viewed as a set of 2 k permutations within the space of 2 n elements. For an ideal block cipher, these permutations should be chosen randomly from all possible permutations.

4.2. Stream Ciphers

Stream ciphers are fast and produce pseudo-random numbers. CTR mode uses a block cipher to generate a keystream by encrypting a counter value, which is then XOR-ed with plaintext for encryption or ciphertext for decryption. Snow3G, used in 3G mobile communications, employs s-boxes, an LFSR, and a finite state machine, with no known successful attacks. Other algorithms like e-Stream include profiles focused on performance and power efficiency. Breaks in encryption like A5/1 highlight the need for more secure algorithms, aligning with Kerckhoffs's principle that a cryptosystem should remain secure even if everything but the key is public (Alexandrov Nikolov, 2019). Stream ciphers with cellular automata (CA) generate a stream of seemingly independent random bits that can be combined with plaintext via XOR to produce ciphertext and decrypted similarly, reminiscent of the one-time pad but using pseudo-random rather than truly random sources; security depends on cycle length. Many proposed stream ciphers are not fully specified or have been broken, with evidence of resistance to common attacks often lacking. Despite being overshadowed by block ciphers, stream ciphers remain academically interesting and can be useful in defense-in-depth strategies (S. Testa, 2008). Stream ciphers are analyzed extensively, with studies addressing algebraic immunity of Boolean functions, resynchronization weaknesses, and algebraic cryptanalysis of cryptosystems. Tools such as Gröbner bases facilitate cryptanalysis,

with improvements including the F4 and F5 algorithms. Attacks like decimation and analyses of key scheduling weaknesses, exemplified by RC4, are examined in proceedings from conferences such as FSE, INDOCRYPT, and EUROCRYPT (Armknecht, 2006).

4.3. Cryptanalysis Techniques

Modern cryptanalysis techniques largely rely on the algebraic representation of ciphers, with the objective being to find solutions to systems of equations that characterize the cipher (T. Courtois & Patrick, 2019). For block ciphers, the difficulty of determining new cryptanalytic properties can be attributed, in part, to the algebraic structure within the cipher design. The study of invariants, including those formed by products of polynomials, can reveal cryptographically significant properties, though demonstrating their efficacy often entails a considerable level of complexity. Number theory and algebraic structures have been employed within public-key cryptography since the introduction of the RSA cryptosystem in 1978 (Santilli, 2019). Factorization, discrete logarithms, and elliptic curves remain prominent in the field. The prospect of quantum computing has, however, precipitated increased interest in post-quantum systems and alternative paradigms. Among these, multivariate public-key cryptography represents a family of protocols based on systems of multivariate polynomials over finite fields. Efficient solutions to the recovery of information from observations or the construction of equivalent systems thus correspondingly equate to cryptanalysis. As with block ciphers, the inherent hardness of the underlying problems has resisted, to date, the formulation of substantially improved solution methods.

5. Asymmetric Key Cryptography

Public key cryptography, also known as asymmetric key cryptography, emerged in the 1970s. In an asymmetric system, every participant possesses a pair of keys: a public key and a private key. The public key is used for encryption, while the private key is used for decryption. This fundamental property enables participants to share confidential information and authenticate one another without exchanging any secret information (Santilli, 2019). Asymmetric cryptography relies on two cipher systems: the public-key encryption system and the digital signature system. The public-key encryption system ensures secrecy, enabling only the intended recipient to decrypt the ciphertext using their private key. Conversely, the digital signature system provides authenticity; a sender can

sign a message using their private key, and anyone with the sender's public key can verify the signature authenticity. The mathematical underpinnings of these cryptosystems often involve number theory concepts like Fermat's little theorem and Euler's theorem. Fermat's theorem states that if p is prime and a is coprime with p, then a^p is congruent to a modulo p. Euler's theorem generalizes this to all integers: a^φ(n) is congruent to 1 modulo n, where φ(n) denotes Euler's totient function. These theorems form the basis for strong encryption through modular arithmetic. By selecting large prime numbers and computing appropriate totient values, cryptographic keys are generated that are computationally infeasible to factor. The security of such schemes fundamentally relies on the difficulty of factoring large composite numbers (, 2018). Cryptography based on these algorithms thus ensures data security, confidentiality, and integrity, which are essential for protecting sensitive information of individuals and organizations.

5.1. RSA Algorithm

The RSA algorithm underpins most electronic commerce and Internet security (Milson, 1999). The cipher hinges on modular arithmetic, a branch of mathematics that is readily introduced to high school students. The surging demand for secure online transactions thus elevates the importance of accessible explanations. These notes emphasize hands-on calculations to orient students toward implementing RSA encryption and decryption procedures, reinforced through targeted exercises. A complementary approach unravels RSA through the lens of three core requirements governing the design of public-key schemes. Assuming only minimal mathematical and cybersecurity prerequisites, the algorithm's construction is developed progressively. A stepwise toy example further demystifies the method from a practical standpoint (Jay Luo et al., 2023).

5.2. Elliptic Curve Cryptography

Elliptic curve cryptography (ECC) systems exploit the algebraic structure formed by the points of an elliptic curve over a finite field to provide information security. The standard objectives of information security—confidentiality, integrity, and availability—dictate the design of cryptographic mechanisms involving one or more parties (L. Rodal, 2004).

Attacks on the elliptic curve discrete logarithm problem (ECDLP)—the problem upon which the security of ECC schemes rests—are among the most serious conceivable. Over time, various means of reducing the computation of elliptic-curve logarithms to logarithms in finite fields have been identified; the eight commercially most significant algorithms for the latter problem are discussed and the challenges of trying to transfer them successfully to the elliptic-curve setting examined critically (Tariq, 2018).

5.3. Digital Signatures

Digital Signature protocols normally offer not only data integrity but also data origin authentication. Such protocols usually rely on a hash function and a public-key signature algorithm. AL-Saidi and Said introduce a new digital signature scheme based on iterated function systems (IFS). The number of iterations that lead to the attractor of the IFS is produced by a Diffie 25Hellman algorithm, which is subsequently used to compute the public key and the signature. Security analysis indicates that this approach is resilient against several known attacks applicable to finite-field cryptosystems (M. G. AL-Saidi & Rushdan Md. Said, 2011). Moreover, an ElGamal Digital Signature scheme is investigated along with a brute-force attack on it. A simple C programming implementation outlines the process of signature generation and verifies the underlying mathematics. A literature review accompanies the study, and countermeasures to enhance security are discussed (Laryoshyna, 2017).

6. Hash Functions

Hash functions have numerous applications in cryptography (Yale Crutchfield, 2008). Several fundamental security properties are required for cryptographic hash functions. Collision resistance means that it should be infeasible to find two inputs that hash to the same output. Preimage resistance means that given a hash output, it should be infeasible to find an input that produces that output. Second-preimage resistance means that given an input and its hash, it should be infeasible to find a different input that produces the same hash. Hash functions are used in digital signatures, commitments, authentication protocols, MACs, secret sharing, and various other applications. Several hash functions and MACs have been proposed, including MD4, MD5, SHA-1, RIPEMD-160, HMAC, and NMAC. More efficient constructions such as MDC-2 and MDC-4 were also introduced. Standards such as FIPS 180-2 specify secure hash algorithms. In 2009, SHA-3 was selected after a public competition among several hashing algorithms. Research

continues on provably secure MAC constructions from one-way permutations (Jr. Doughty, 2010).

6.1. Properties of Cryptographic Hash Functions

A cryptographic hash function maps binary strings of arbitrary length into strings of fixed length, designed to be one-way and to conceal all input structure (Yale Crutchfield, 2008). The fundamental properties of such functions are collision resistance, preimage resistance, and second preimage resistance. A collision-resistant hash function makes it hard for an adversary to find two vectors yielding the same image; preimage resistance ensures computational difficulty in reconstructing the input from the output; and second preimage resistance prevents an attacker from finding a different source that hashes to the same output as a given vector. Accordingly, a cryptographic hash function is defined as a hash function where the tasks of finding a collision and inverting the function are both computationally infeasible (Backes et al., 2012).

6.2. Applications of Hash Functions

Cryptographic hash functions represent the third major class of symmetric cryptographic primitives, sitting alongside block ciphers and stream ciphers. They are widely deployed across fields such as authentication—through challenge–response protocols and message authentication codes (MACs)—and data integrity schemes, including digital signatures and checksums (Lin et al., 2017). A hash function maps an arbitrarily long input message bit stream into a fixed-length output known as a hash value or digest. This mapping is fundamentally one-way: it should be computationally impossible to find any input that corresponds to a given output. Furthermore, this one-way property must hold even for inputs that share a certain number of bits or characters. The security of any hash function also depends upon its collision resistance, the inability to find two distinct inputs with the same digest. Consequently, modern hash functions must be carefully constructed to ensure these properties are satisfied; careless designs quickly become vulnerable to cryptanalysis (Gurjar et al., 2015).

7. Randomness in Cryptography

Randomness in cryptography addresses the problem of reducing the amount of randomness required by cryptographic constructions, using techniques based on irrational numbers to lower the randomness complexity (Kumar Vishnoi, 2004). Such constructions have led to the creation of exposure-resilient cryptography, secure even when adversaries gain partial knowledge of the random bits employed. Another fundamental problem concerns the creation of perfectly unbiased random bits from weak sources of randomness that are only slightly unpredictable; the extent to which these sources can be exploited remains an influential open question. Derandomization also plays a key role in theorem-proving procedures, with several directions having direct cryptographic implications. Insights into whether the complexity of a problem influences the difficulty of its theorem-proving procedure have arisen from probabilistic algorithms that efficiently decide the equivalence of two programs and perform polynomial identity testing on arithmetic expressions. Conversely, a general theorem-proving procedure for verifying program equivalence would reestablish the classic implication that deterministic simulation of probabilistic algorithms entails the existence of strong circuit lower bounds—a notorious and unsolved problem. It is also unclear whether polynomial identity testing can be derandomized in the strongest format: as programs that produce the polynomial from a compact description. Further progress is needed on the construction of deterministic extractors and PRGs suitable for cryptographic security. Breaking new ground requires proving circuit lower bounds, which are inherently difficult problems, but incrementally advancing the theory of randomness will likely continue to shed light on the fundamental problems of polynomial-time computation and cryptographic security.

The Mersenne twister is a 623-dimensionally equidistributed uniform pseudo-random number generator (Vivier et al., 2017). The quality of N-cube random walks without Hamiltonian cycles in chaotic pseudo-random number generation can be analyzed through various empirical tests, such as those provided by the TestU01 C library, which assesses the statistical properties of random number generators. Theoretical considerations of counting sequences, chaos-based random number generators, and balanced Gray codes contribute to the design of high-quality pseudo-random number generators with applications in internet security.

7.1. Sources of Randomness

Random numbers underpin cryptographic operations, enabling high performance, quantum security, and strong un-guessability. Such un-guessability prevents adversaries

from predicting random values, a property paramount to cryptographic strength. In Monte-Carlo algorithms, random numbers accelerate complex computations by exploring only a fraction of the solution space. Randomized rounding, for instance, facilitates approximate solutions when deterministic methods are prohibitive. Random permutations, limited by the feasible amount of randomness, often necessitate hash functions for efficient generation. Furthermore, quantum security demands randomness for key refreshing or protocol initialization, underpinning long-term communication safety even against adversaries with unlimited computational resources. The quantum realm secures key exchange in distrustful settings without relying on unproven complexity assumptions. Boolean-formula and circuit lower bounds remain elusive without computational complexity assumptions; randomness emerges as a pivotal element in cryptography but cannot be removed entirely (Stipcevic, 2011). Supplies of true randomness derive from unpredictable physical phenomena, including thermal noise, chemical processes, user behaviour, and quantum fluctuations (Kumar Vishnoi, 2004). On the digital side, cryptographically secure pseudo-random number generators (CSPRNGs) expand short random seeds into longer streams, demanding well-conditioned seeds with near-perfect entropy. Failures to maintain these conditions jeopardize both the security and effectiveness of cryptographic systems.

7.2. Random Number Generators

Since the early sixties, attempts to generate random numbers by deterministic means have resulted in what are known as pseudo-random numbers. A pseudo-random number generator (PRNG) produces a deterministic sequence that appears to be random. A good quality PRNG behaves in a manner similar to true random number generators, such as random transmission times for arriving packets on a communication medium or the time interval between clicks of a Geiger counter. Pseudo-random numbers possess some remarkable properties: plans based on them are sufficient to simulate either a tape of thoughts or even a tape of communication; each pseudo-random number is very easy to compute; the same random sequence can be repeated indefinitely, allowing receivers to replicate the process and decode the information; and the process is very fast (Edward Opoku-Mensah et al., 2013).

8. Protocols and Standards

The construction of practical cryptographic protocols, aimed at achieving a variety of desired goals, constitutes a key aspect of cryptographic research (Rothe, 2001). Protocols revolve around mechanisms for exchanging extra information, which is needed to accomplish a desired task. However, such a construction constitutes a delicate art—extra exchange of information provides legitimate users with an advantage, but can also empower an adversary; thus, a subtle balance is required. Protocols endow cryptography with practical applications, and the design and analysis of cryptographic protocols and schemes represent some of the most important open problems in modern cryptography (Caballero-Gil &Fúster-Sabater, 2010).

Some of the most significant schemes, which can be considered fundamental to the subject, are surveyed in. For example, secret-key agreement protocols, such as the Diffie–Hellman scheme (1976), allow two parties connected by a public channel to agree on a shared secret key. ElGamal's public-key cryptosystem (1985) provides mechanisms for encryption and authentication. Shamir's no-key protocol (1980) makes it possible for two parties to exchange a secret session key without prior agreement on a secret, although it is not symmetric—the party who initiates the exchange learns the session key only after the transfer is complete. Digital signature schemes, essential for authentication and proof of origin, include those developed by Rivest, Shamir, and Adleman (1978), ElGamal (1985), and Rabi (1988). These protocols or schemes are among the most important in cryptography, although some, such as Shamir's protocol, are less widely employed in practice.

8.1. Public Key Infrastructure (PKI)

A Public Key Infrastructure (PKI) is a system for the management of public keys. Public-key cryptography lays the foundation for PKI by enabling secure communication of a message that is easily encrypted and decrypted, without the problems inherent in key management. A PKI system helps to verify the binding between a public key and a particular entity, and ensures secure communication. PKI can support encryption, which safeguards confidentiality, and digital signatures, which provide assurance about the origin and integrity of a message. PKI is widely used in applications that require user authentication, sender non-repudiation, data confidentiality and integrity, and non-repudiation of information. The main protocols employed within a PKI are the public key cryptosystem for key management and RSA digital signature for authenticity and integrity checks. The security of these protocols relies on the difficulty of factoring large composite numbers. When the prime numbers generated by a PKI are predictable or

taken from a small set, the security of the system is compromised (Castro Lechtaler et al., 2019).

8.2. Transport Layer Security (TLS)

The Transport Layer Security (TLS) protocol uses a combination of public-key and symmetric-key cryptography to secure communications on the Web. When a client initiates a connection, the server sends its public key and certificate. The certificate contains the digital signature of a trusted authority and identifies the key. The client verifies the certificate by checking the signature of a trusted authority and then extracts the server's public key. These keys can be used in signature schemes (implemented during the handshake to authenticate the server) or in encryption schemes (implemented during the handshake to encrypt a secret session key for the client). If public-key encryption is used, the client randomly generates a secret key for a faster symmetric-key crypto algorithm; this key is encrypted using the server's public key and sent to the server. Only the server can decrypt it because the corresponding private key is required; only then both parties possess the secret shared key.

9. Applications of Cryptography

9.1. Secure Communication

A primary goal of cryptography is to develop algorithms and protocols that guarantee the secure transfer of information over public communication channels. This challenge is complex because excessive security can impede the validity of communication (Goldwasser, 2002). Messages should be resistant to interception by third parties while still remaining readable by the receiver. Public-key encryption schemes achieve this by having a receiver publish a public key for encryption, which can only be decrypted with a corresponding secret key. Cryptographic protocols based on number-theoretic algorithms protect online transactions and provide digital signatures to validate the authenticity of documents. Cryptography transforms readable information into an unreadable format to conceal meaning from unauthorized parties. One approach, secret-key (or symmetric-key) cryptography, involves both sender and receiver sharing a secret key that must remain confidential (, 2018). This type of cryptography is suitable when both parties are acquainted and can exchange a secret key. Public-key (or asymmetric)

cryptography enables parties without prior contact to communicate securely. The receiver publishes a public key that anyone can use to encrypt messages; only the receiver can decrypt them using a private key. Many schemes provide digital signatures, critical for ensuring that documents have not been altered during transmission and are genuinely authored by a specific entity.

9.2. Digital Currency

Digital currency represents a scheme that enables monetary transactions through encryption and the creation of cryptographic checksums, eliminating the need for a centralized entity like a bank. These systems allow verification of transactions without disclosing non-public data, thereby supporting anonymous transactions. The first operational digital currency system emerged in 1994, earlier than the widespread use of cryptocurrencies such as Bitcoin. Digital currencies rely heavily on the use of cryptographic methods (Santilli, 2019).

9.3. Data Integrity and Authentication

Asymmetric cryptographic schemes employ a pair of keys for confidentiality and authentication: a private key known only to the user, and a corresponding public key available to others. The Digital Signature Algorithm (DSA) exemplifies such a system, where a message signer generates a message digest using the Secure Hash Standard (SHS), then creates a digital signature with the private key. Recipients use the public key to verify the signature, ensuring data integrity and authentication without compromising confidentiality (Pointcheval, 2002).

10. Challenges in Cryptography

The development of cryptography is closely tied to the emergence of computers, wherein data can be accessed or processed by viruses and malicious elements, making the protection of data a challenging task. Data can be accessed illegally through unsecure channels, and important information can be modified or destroyed. Therefore, the development of cryptography helps in protecting data from such illegal access. Without encryption, sensitive data is susceptible to unauthorized use and modification.

Cryptologic alterations protect system resources from unauthorized use or modification and prevent the transmission of unauthorized information. The classification of cryptographic challenges includes computational challenges and cryptographic challenges. Computational challenges depend on how difficult it is to solve a problem when the computational complexity of the problem is considered. Typically, without further clues, computational problems are solved by a brute-force approach. For instance, for every element x in the sample, check whether x satisfies the required conditions. However, when the problem size is large, the time taken to solve such an approach is huge, thereby rendering the approach ineffective and unfeasible. Therefore, cryptography must rely on the hardness of computational problems in the public domain to strengthen and improve the security of the system. According to information theory, the use of only one-time pad (such as using a key of size much greater than the message to be encrypted) can prevent ciphertext from leaking meaningful information concerning the message (Goldwasser, 2002). However, cryptographic researches rely on constructing systems that are considered to be secure based on the assumption that certain problems are computationally difficult to be solved. In practice, security systems such as RSA (Rivest–Shamir–Adleman) and ElGamal rely on the difficulty of factoring large composite numbers and retrieving discrete logarithms in a given group, respectively. On the other hand, digital signatures support the existence of a trusted digital signature that can be verified by anyone. It is computationally infeasible to produce a valid signature without possessing the signing key. The concern of cryptography is that the system is either secure or nonsecure depending on the cryptographic challenge considered.

10.1. Quantum Computing Threats

Cryptography is a crucial component of information technology, facilitating secure and trusted communications over open networks. Cryptology, encompassing cryptography and cryptanalysis, involves devising and breaking codes and ciphers, thereby enabling the protection of information exchange via secrecy, authentication, and integrity. Yet, maintaining information security remains challenging, particularly with the rapid growth of the Internet and the increasing sensitivity of communicated data. Consequently, preserving information security has become a vital issue for academia, industry, and government authorities by the start of the 21st century. The theoretical development of cryptography and the mathematical functions underlying cryptanalysis and protocol design proceed concurrently. Advances in cryptanalysis often induce the creation of new, robust algorithms. Numerous symmetric- and public-key cryptographic algorithms have been proposed and continue to be developed at a rapid pace. Nearly all

contemporary cryptographic algorithms rely upon hard-to-solve mathematical problems to guarantee security. Theoretical mathematics, computational complexity theory, number theory, and applied algebraic geometry remain fundamental to this research.

10.2. Cryptographic Vulnerabilities

Security vulnerabilities in cryptosystems represent an important aspect of optimization, often linked to unstable dependencies on key values. Several cryptographic standards, commonly analyzed within a resource estimation framework, are known to be vulnerable to quantum-computer-based attacks (Marron, 2018). For example, the widely used asymmetric encryption scheme RSA is characterized by an optimization cost that intricately depends on the prime factors of the public key, rendering it vulnerable to quantum attacks. The security of this scheme fundamentally relies on the difficulty of prime factorization, a problem that quantum computers can solve efficiently. Public-key encryption schemes ideally achieve a balance where the encoding operation demands significantly less computational effort than the decoding operation. Consequently, decoding without access to either the private key or the original message should remain computationally impractical. Architectures of these cryptosystems typically employ a pair of keys whose values display a degree of interdependency, influencing the overall optimization cost. In schemes such as RSA, this optimization cost emerges as a visible signal within the cryptographic system, thereby exposing a latent security weakness (, 2018).

11. Future Directions in Cryptography

Cryptographic algorithms are in a continuous state of refining and improvement. The landscape of cryptographic research suggests a rich future, emphasizing the importance of developing encryption schemes that are resistant to algebraic or analytical attacks (, 2018). There is a parallel focus on the efficient fabrication of extremely large random primes to support secure key generation. Future advancements should enable the formulation of cryptosystems operating on hundred-thousand-bit primes, facilitating the protection of electronic information even in the absence of private channels or one-to-one key distribution. The reason for the ongoing pursuit of innovation in symmetric-key techniques arises from the necessity of provision for occasional key exposure. After all, such exposure is theoretically unavoidable. The best-case scenario entails the compromise of only a minimal number of message blocks, recoverable by extending and

chaining encryption across several blocks (Goldwasser, 2002). Improvements attributable to active research efforts will likely yield practical schemes demonstrating a greater number of recovered text blocks than would be expected by brute-force guessing, thereby enhancing cryptographic robustness.

11.1. Post-Quantum Cryptography

Post-quantum cryptography (PQC) develops cryptographic systems computationally secure against attacks powered by quantum computers. Shor's algorithm and its variants can efficiently solve the large-integer-factorization problem and the big-discrete-logarithm problem, threatening the main asymmetric schemes currently used. Grover's quantum search algorithm cuts in half the bits of the symmetry key in all known ciphers. The search for quantum-resistant alternatives is ongoing. Non-commutative cryptography avoids some of the known quantum attacks. Along the non-commutative framework, analysis of the algebraic span appearing in central-identity requests defines a potential vulnerability. An ASA-resistant version of the previous TDP framework therefore arises as a natural choice (Hecht, 2018). Quantum computing processes information faster than classical machines by using qubits. These can exist simultaneously in the |0 angle and |1 angle states, and quantumly entangle with other qubits. Shor's algorithm efficiently factors integers and computes discrete logarithms, threatening RSA and elliptic-curve cryptography (ECC). RSA shields data with a public key d, validating it with a private key e; the pair comes from factorization of a large composite number N into primes p and q. ECC is built on the hardness of the elliptic-curve-discrete-logarithm problem (ECDLP). PQC algorithms capable of withstanding quantum attacks include lattice-based, code-based, hash-based and multivariate polynomial cryptography (G S Mamatha et al., 2024). An evolved non-commutative cryptography framework assumes the symmetric group as the embedding structure, allowing the consequent easy creation of large cyclic subgroups in which both the decomposition problem (DP) and the double-coset problem (DCP) are hard to solve. Operations such as mapping, multiplication and powering depend on combinatorial operations rather than arithmetic or big-number libraries, providing an important advantage for potentially low-resource platforms. Under these conditions, polynomial-time classical DLP attacks and known quantum alternatives are assumed infeasible, giving an estimated computational hardness of approximately 64 bits (Hecht, 2017).

11.2. Advancements in Cryptographic Protocols

Public-key cryptographic protocols are designed to protect communication security properties, such as confidentiality, authentication, entity identification, and key distribution. Several recent advancements have been made in this field. A new digital signature scheme, provably secure in the random oracle model, resists adaptive chosen-message attacks even if the signing device leaks partial information about every signature. The Number Field Sieve discrete logarithm algorithm has been improved by exploiting the automorphisms of the number field used to represent finite field elements and introducing an early abort strategy in the linear algebra phase. A variant of the well-known Bleichenbacher attack targets RSA-encrypted messages that do not use any padding. An efficient attack recovers the secret key for a class of knapsack cryptosystems based on the super-increasing structure of the private key.

12. Conclusion

The manuscript “Cryptographic Algorithms and Number Theory: A Computational Approach” elucidates the application of fundamental number theory concepts, together with associated algorithms, to build the foundation for securing contemporary digital infrastructures. Covering modular arithmetic, divisibility and primality, and quadratic residues alongside number-theoretic functions, it advances toward comprehensive primitives such as public-key encryption and hash-function systems. This approach—dissecting particular operations and exploring machinery for modular exponentiation and discrete rooting—facilitates a granular understanding of the underlying complexities and constraints. Following a concentration on elliptic curves and complex lattices, the discussion culminates with implementation challenges in modern, large-scale settings (, 2018) (W. Lenstra, 1992).

References

Rothe, J. (2001). Some Facets of Complexity Theory and Cryptography: A Five-Lectures Tutorial.

Santilli, G. (2019). An investigation on Integer Factorization applied to Public Key Cryptography.

W. Lenstra, H. (1992). Algorithms in algebraic number theory.

, C. (2018). Cryptography for Online Security: Applications of Number Theory.

Gouicem, M. (2013). New modular multiplication and division algorithms based on continued fraction expansion.

TAHIRI JOUTI, K. (2007). Primality Testing.

Asimi, A. (2023). Conjectures in number theory.

Babu, R., Abraham, G., &Borasia, K. (2013). A Review On Securing Distributed Systems Using Symmetric Key Cryptography.

Hassoun, Y. (2016). Secure symmetric ciphers over the real field.
Baignères, T. (2008). Quantitative security of block ciphers:designs and cryptanalysis tools.
Abdelkhalek, A. (2017). Cryptanalysis of Some Block Cipher Constructions.
Alexandrov Nikolov, P. (2019). Analysis and Design of a Stream Cipher.
S. Testa, J. (2008). Investigations of cellular automata-based stream ciphers.
Armknecht, F. (2006). Algebraic attacks on certain stream ciphers.
T. Courtois, N. & Patrick, A. (2019). Lack of Unique Factorization as a Tool in Block Cipher Cryptanalysis.
Milson, R. (1999). Introduction to the RSA algorithm and modular arithmetic.
Jay Luo, Z., Liu, R., & Mehta, A. (2023). Understanding the RSA algorithm.
L. Rodal, A. (2004). Elliptic curves and elliptic curve cryptography : an honors thesis (HONRS 499).
Tariq, D. (2018). A usability study of elliptic curves.
M. G. AL-Saidi, N. & Rushdan Md. Said, M. (2011). On the security of digital signature protocol based on iterated function systems.
Laryoshyna, V. (2017). Simple implementation of an ElGamal Digital Signature and a Brute Force attack on it.
Yale Crutchfield, C. (2008). Security proofs for the MD6 hash function mode of operation.
Jr. Doughty, P. (2010). A Generic attack on CubeHash, a SHA-3 candidate.
Backes, M., Barthe, G., Berg, M., Grégoire, B., Kunz, C., Skoruppa, M., &ZanellaBéguelin, S. (2012). Verified Security of Merkle-Damgård.
Lin, Z., Guyeux, C., Wang, Q., & Yu, S. (2017). Diffusion and confusion of chaotic iteration based hash functions.
Gurjar, S., Baggili, I., Breitinger, F., & Fischer, A. (2015). An Empirical Comparison of Widely Adopted Hash Functions in Digital Forensics: Does the Programming Language and Operating System Make a Difference?
Kumar Vishnoi, N. (2004). Theoretical Aspects of Randomization in Computation.
Vivier, S., Couchot, J., Guyeux, C., & Heam, P. (2017). Random Walk in a N-cube Without Hamiltonian Cycle to Chaotic Pseudorandom Number Generation: Theoretical and Practical Considerations.
Stipcevic, M. (2011). Quantum random number generators and their use in cryptography.
Edward Opoku-Mensah, I., A. Christopher, A., & Ohene Boateng, F. (2013). Comparative Analysis of Efficiency of Fibonacci Random Number Generator Algorithm and Gaussian Random Number Generator Algorithm in a Cryptographic System.
Caballero-Gil, P. &Fúster-Sabater, A. (2010). On the Design of Cryptographic Primitives.
Castro Lechtaler, A., Cipriano, M., & Malvacio, E. (2019). Anomaly Search in a Public Key Infrastructure OPENSSL v1.0 1e.
Goldwasser, S. (2002). Mathematical foundations of modern cryptography: computational complexity perspective.
Pointcheval, D. (2002). Asymmetric cryptography and practical security, Journal of Telecommunications and Information Technology, 2002, nr 4.
G S Mamatha, D., Dimri, N., & Sinha, R. (2024). Post-Quantum Cryptography: Securing Digital Communication in the Quantum Era.
Marron, Z. (2018). Quantum Attacks on Modern Cryptography and Post-Quantum Cryptosystems.

Hecht, P. (2018). PQC: Extended Triple Decomposition Problem (XTDP) Applied To GL(d, Fp)-An Evolved Framework For Canonical Non-Commutative Cryptography.
Hecht, P. (2017). Post-Quantum Cryptography: S381 Cyclic Subgroup of High Order..

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Chapter 4: Mathematical Modeling of Climate-Induced Disaster Impact on Agriculture

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Abstract: Climate-induced disasters—such as floods, droughts, cyclones, and heatwaves—pose severe threats to agricultural productivity, food security, and rural livelihoods worldwide. Understanding and quantifying these impacts is crucial for developing adaptive strategies and policies. This paper presents a mathematical modeling approach to assess the impact of climate-related disasters on agriculture, integrating climatic variables, crop yield data, and vulnerability indicators. The model employs a system of differential equations and regression-based forecasting to simulate crop responses under varying climatic stressors. In addition, stochastic elements are introduced to capture the uncertainty associated with extreme weather events and their frequency. Using historical datasets and satellite-derived climate indicators (e.g., rainfall anomaly, temperature variation, soil moisture), the model estimates crop yield losses and economic damage across different agro-climatic zones. Scenario analysis is conducted to evaluate the potential outcomes under different greenhouse gas emission pathways and adaptation measures such as crop insurance, early warning systems, and resilient cropping patterns. Case studies from vulnerable regions demonstrate the model's capacity to forecast disaster-induced agricultural disruption and guide decision-making at both policy and farm levels. The study concludes that mathematical models, when calibrated with high-quality climatic and agricultural data, can serve as powerful tools for early impact assessment, climate risk mitigation, and long-term agricultural planning. The integration of scientific modeling with socio-economic policy frameworks can significantly enhance resilience against climate-induced disasters in agriculture-dependent economies...

Keywords: Climate Change, Agricultural Modeling, Natural Disasters, Crop Yield Forecasting, Climate Risk Assessment.

1 Introduction

Climate-induced disasters such as droughts, floods, and pest outbreaks threaten the growth and productivity of agricultural crops. These disruptions impact economic growth, employment, food prices, and human health, thereby posing significant challenges to both local and global economies. Understanding the connections between climate-induced disasters and agriculture can provide critical insights into their effects. Historical climate records demonstrate how the effects of climate change propagate through the atmospheric system, influencing biological systems such as agricultural crops. Disasters linked to climate change disrupt crop growth, precipitate economic losses, and may lead to food shortages and subsequent social unrest. Effective modeling tools are therefore valuable for assessing and predicting the impact of these disasters on crops. Mathematical modeling serves as a crucial tool for quantifying the direct and indirect effects of climate-induced disasters on agricultural productivity. Crop models specifically aid in understanding the physiological mechanisms by which crops respond to alterations in climate variables. However, many traditional models are designed around a long-term climatology that does not scale adequately for decision support in the context of changing climate. Addressing these gaps involves developing models capable of forecasting climate risks, guiding tactical decisions to reduce negative impacts, and enhancing resource use efficiency. Theoretical frameworks and model implementations that simulate conditions related to drought, flood, and pest-influenced crop damage enable quantification of these effects. Spatial analyses that simulate regional impacts based on these models can further elucidate the relationship between climate-induced disasters and agricultural outcomes (Jin, 2016) (P McDermid et al., 2015).

2. Literature Review

Climatic and socioeconomic changes continue to alter the risk framework, demanding ongoing enhancement of resilience to environmental and economic stresses. Climate-induced disasters result in the loss of lives, livelihoods, and disruption in social and infrastructure networks, while drought is among the most hazardous phenomena linked with global and local food insecurity (Islam et al., 2016). Several approaches have been proposed to model the impact of climate change and adaptation technologies on crop yields and food security. Early-stage modeling includes studies on climate change impacts on vulnerability and food security in Kenya, as well as the effects of different vulnerability and damage scenarios. Crop models, commonly considered the most

appropriate tools for characterizing the relationship between climate and agriculture, are used for simulating the effect of current and future climate on agricultural production (Islam et al., 2016). Among the several available models, the Decision Support System for Agrotechnology Transfer (DSSAT) and the Agricultural Production System Simulator (APSIM) have been employed for analysing the impact of climate change on agricultural systems in various regions of East Africa and elsewhere. Their application encompasses the simulation of cropping systems at fine spatial scales, taking into account management factors that are most relevant to the projected changes in crops. Additional efforts aimed at more effective provision of in-season agro-advisories to farmers in drought-sensitive locations and at improving the understanding of how changes in climate influence global food production by employing biometric crop models have also been conducted. Research analyses of the effects of climatic parameters on cassava have been carried out, with general projections indicating a decrease in cassava yields under projected climate change scenarios. The impact of changes in global climate and atmospheric composition on European agriculture has been investigated. Several studies address crop-model-derived estimates of climate-change impacts and their influence on food security, examining the vulnerability of maize and sorghum to climate variability in West Africa, the benefits of adopting drought-tolerant cultivars, and the necessity for improved and efficient irrigation techniques. Interactions between climate-change impacts, world food prices, and caloric intake in the developing world are evaluated. Furthermore, the associated food price shocks with the 2007/08 food crisis and the potential effects of a 2013 drought in the USA on global calorie availability are analysed. Recent contributions assess the potential costs of adaptation to climate change and the effects of climate change on global food security, thereby indicating that substantial efforts will be required to mitigate impacts and to enhance agricultural and economic resilience, particularly in lower-income regions.

2.1. Historical Perspectives on Climate Change

During the development of climate change research, a nonlinear, century-scale shift in the planet's environmental regime emerged (J. Challinor et al., 2013). A nonlinear jump from a colder to a warmer regime occurred around 1875, while another reversal to the cold regime eventually occurred near 1977. As the overall temperature shifted, various low-frequency oscillations, such as the Pacific Decadal Oscillation (PDO), the Multi-Decadal Oscillation (MDO) and the Atlantic Multidecadal Oscillation (AMO), also shifted phase.

2.2. Impact of Disasters on Agriculture

Agriculture remains the most climate-sensitive economic sector in many countries. Natural disasters strongly influence agricultural growth globally, but have been overlooked in national climate change strategies (Fréjuis Akpa, 2024). Disasters can disrupt supply and marketing systems, often leading directly to food shortages. In some cases, these effects continue for three to six years after the event. Empirical evidence shows natural disasters adversely impact agricultural production. Losses often reach national significance. The Haiyan typhoon caused direct losses of around 260,000 tonnes. The 2020 floods in China affected one-third of the population and damaged 28 million hectares of crops, including maize, rice, and soybeans. About 66 million tonnes of grain were lost, equivalent to approximately 8.7% of the total yearly production, especially rice and corn. The average annual grain loss is about 20 billion kg, with monetary damages close to 200 billion yuan. In Africa, natural disasters threaten food production seriously. Key crops such as maize, rice, millet, sorghum, and cassava can be affected, with maize, rice, and sorghum particularly susceptible to climate risks. The resulting instability has persisted for decades. Climate models predict maize yields could decline by 11 to 33% by 2050. Many countries have experienced continuous negative impacts. Disasters in East Africa are severe, yet Mozambique and the Amazon are most affected. Global economic losses due to disasters in these regions exceeded 122 billion USD in 2019, while damages on the African continent totaled 30 billion USD during 2008-2018.

2.3. Mathematical Models in Environmental Science

Mathematical models serve as vital tools for the simulation, analysis, and prediction of phenomena across diverse natural and social sciences domains. In the context of environmental and climate studies, continuous-time deterministic systems have been employed to model the spread of invasive species and the growth dynamics of human populations under environmental constraints. Discrete-time nonlinear difference-equations facilitate the exploration of kinematic waves and the population dynamics of herbivorous insects on renewable resources. Stochastic systems have been instrumental in investigating the competitive spread of insect pests in agriculture and the patterns of intense wet spells within dry seasons. Systems of integral and integro-differential equations enable the examination of the dynamics of pest populations, the transmission of vector-borne diseases, and predatory-prey interactions in aquatic ecosystems.

Crop and livestock simulation models are central to estimating the impacts of global environmental change on future food production and security (P McDermid et al., 2015). The Simulation Model for Agricultural Resources Sustainability (SMARS), for example, is a systems model of agriculture that encapsulates relevant physical, biological, and economic factors governing agricultural production. This daily time-step model simulates crop yields, soil erosion, nutrient cycles, annual farm income, and non-point source pollution (Sridhar et al., 2016). Fallout models providing effects of air pollutants such as acid rain, ozone, and pesticides, along with models describing pest-disease dynamics, can be integrated with SMARS. Despite their utility, simulation models alone are insufficient to predict effects under unprecedented environmental change. Responding to the challenge of boosting food production in the face of increasing population, decreasing arable land, and global climate change, the Agricultural Model Intercomparison and Improvement Project (AgMIP) seeks to leverage multiple models for enhanced predictive capability. Sectoral and adaptive capacity projects within AgMIP aim to quantify climate impacts, agricultural development, food security, and vulnerability, both in recent decades and under future climate projections. Recent developments in phenological, beetle population, and ecological footprint models illustrate the potential contributions of mathematical modeling to disaster impact studies on agriculture.

3. Theoretical Framework

The mathematical models used in this study assess the inherent vulnerability of major crop-production systems to climatic change, here defined as the impact of climatic change on agricultural net revenue under a fixed level of production inputs. The models do not account for farmers' capacity to adapt inputs, technologies, or farming systems in response to climatic changes (Bindoumou, 2018). Crop-model ensembles reduce uncertainty in predicting rice yield under climate change. Evidence shows a climate signal in trends of global crop yield variability over the past 50 years. Land-surface models like DAYCENT and MERRA provide land-surface and hydrology estimates crucial for understanding climate impacts on agriculture. The Agricultural Model Intercomparison and Improvement Project (AgMIP) develops protocols and datasets for agricultural modeling, including climate-forcing datasets for gap-filling and historical-climate-series estimation (P McDermid et al., 2015). Studies predict climate change impacts on crops like maize in Panama and sugarcane in Australia, Brazil, and South Africa using models such as Canegro. Challenges to process-based modeling of grazed agricultural systems are addressed with some solutions. CropSyst, a cropping-systems simulation model, aids in crop-yield predictions.

3.1. Conceptual Models of Climate Impact

Low-dimensional conceptual models derive damage functions from broad-stroke observations and assumptions, such as economic damages rising quadratically with temperature change and impact functions triggered specifically by temperature or doubled CO2 (Dellarole, 2016). Damage is typically represented monetarily as a share of output, reflecting the costs of climate changes on production or infrastructure. Parameters often include tolerable rates of change and tolerable plateaus. Such models might compute damages for a reference region and scale results to other countries by weighting. Sector-specific impact functions consider agriculture, coastal areas, human health, ecosystems, and vulnerable economic sectors. Climate variables are summarized in low-dimensional descriptors (e.g., global mean temperature change) and coupled with damage functions, often inferred from global modeling or observation.

Over the last decade, efforts have improved the integration of climate and impacts models. Global models for society and economy are widely used in scenario and policy exploration, while regional models support targeted adaptation and decision analysis – these increasingly incorporate direct bidirectional couplings between impacts and climate models. Exploiting these possibilities requires a thorough understanding of the models, the assumptions governing couplings, and the scope of potential climate change implications. Atmospheric concentrations of CO2, methane, and nitrous oxide have reached unprecedented levels, producing wide-ranging impacts on food production, human health, energy demand, and water stress; regional climate changes further constrain food production through localized extremes of temperature and rainfall (J. Challinor et al., 2013).

3.2. Mathematical Foundations

The mathematical development of the model by Bindoumou (Bindoumou, 2018) extends the concept of adjustment costs. This general function accounts for the impact of climate-induced disasters on the agricultural sector by integrating three processes: the cost of replacing damaged production factors, the cost of using replacement factors more intensively, and the losses arising in the determination of overall production factors. The first operation represents the replacement by investment, which is bounded by financial capacity and infrastructure availability. The second operation involves intense production factor usage, encompassing increased working hours for labour or priority

irrigation for soil. The cumulative factor-restoring operation, incorporating adjustment costs, models the interactions within the agricultural production chain to capture the dynamics sustained over time and the effects of inertia related to the disaster probability.

4. Methodology

The methodology integrates climate and crop model ensembles to capture uncertainty and sensitivity of global crop yields to a spectrum of climate change scenarios, facilitating economic assessment. The Agricultural Model Intercomparison and Improvement Project (AgMIP) framework guides modeling protocol, climate-forcing inputs, and site-selection criteria for model intercomparison (P McDermid et al., 2015). Economic assessments link changes in crop yield variability to socio-economic impacts, with emphasis on the effect of global change scenarios on agricultural markets (Rachel Palatnik, 2015). The approach supports evaluation of both climatic and technological scenarios and accounts for spatial effects that influence impact assessment (Kavi Kumar, 2009). The protocol employed ensures that sets of climatic-change scenarios and site conditions, together with economic-model baseline scenarios, delineate traceable assessment quantities. Probability distributions of uncertainties and parameter sensitivities are systematically treated, and results are characterized by distributions generated by the ensemble of climate-change scenarios.

4.1. Data Collection

Collecting data is a crucial step in studying the impacts of various extreme climate events on important sectors in order to estimate the scale and magnitude of losses under future conditions. For example, the focus may be on several extreme climate event indices, such as: annual cold/warm spell duration index, heat wave duration index, rainfall maximum duration, very heavy precipitation, consecutive wet and dry days, extreme precipitation, drought, precipitation intensity, maximum 5-day precipitation amount, and maximum temperature. Decision-makers are compelled to develop capabilities for evaluating disaster effects and for systematically collecting and investigating information. In particular, due consideration needs to be given to spatial factors of hazard characteristics, vulnerability, and disaster occurrence. Changed conditions regarding causative factors and damage-inducing circumstances during periods of relatively high frequency or intensity can be reflected in analyses. These analyses reveal the relationship

among disaster-causing climate events, their frequency, and agricultural damage (P McDermid et al., 2015).

4.2. Model Selection

Selecting an appropriate model is a fundamental question when characterizing the impact of climate change on agricultural production. The relationship between temperature and output the damage function serves as the basic tool for quantifying climate change impacts. The estimated damage function with projected changes in climate and the exposure variable can calculate changes in the outcome variable. Conflicting parameters may generate different predictions of the outcome variable, which affects projecting future climatic risk. There is no systematic model-selection criterion for model uncertainty, given a set of models during impact projection. Existing model-selection criteria assume one of the candidate models is the true one. However, the true relationship between climate, exposure, and damage is generally unknown. All candidate models approximate the true one, and the best model "closest" to the true one, rather than the "true" model, is selected among plausible models. A model well designed to capture current conditional relationships may not accurately capture those in the future. Projecting future climatic risk therefore becomes more challenging and depends largely on whether the selected model performs well when extrapolating beyond the observed conditions. The C3MP (Coordinated Climate-Crop Modeling Project) utilizes an ensemble of climate-model scenarios for climate inputs. Crop models provide an ensemble of crop-model responses, while also enabling the historical climate baseline to be crossed in the projection scenario, allowing investigation of extreme climate changes that were not found in the historical baseline. Participants were requested to use the C3MP protocols to generate estimations of the impacts on agricultural production at key triads of temperature, precipitation and carbon dioxide. Outputs included modelled production for the three crop types at the 10 sites (extended to 30), along with the full suite of crop-model output variables. (P McDermid et al., 2015)

4.3. Simulation Techniques

Monitoring various climate scenarios requires different studies to be run over extended periods and a thorough description of all components and variables involved. Because of the systematic use of reduced-physics models, which allow the clear isolation of cause-effect relationships, statistical downscaling techniques are widely used and may

acquire a renewed interest in the near future. Diagnostic statistics and standard limited area model (LAM) integrations are adopted to provide the necessary information for spatial disaggregation of coarse-grid data into variables on the spatial scale necessary for the management of natural hazards, with specific emphasis on typhoon landfalls (J. Challinor et al., 2013).

5. Case Studies

Climate change impacts on agriculture are extensively studied through various models and scenario analyses. Research includes assessments of crop yield changes, food security implications, and adaptation strategies. Key models such as DSSAT and APSIM are used to simulate farming systems and future crop scenarios. Studies evaluate economic responses to biophysical shocks, explore the potential impacts on maize production, and analyze the costs and effectiveness of adaptation measures. The concept of shared socioeconomic pathways helps understand future climate scenarios, while evaluations of crop varieties aim at enhancing resilience. Overall, these case studies emphasize the importance of modeling, technological innovations, and policy strategies in managing climate variability and ensuring food security (Islam et al., 2016).

5.1. Regional Analysis of Drought Effects

Implementing PMP in a regional economic model necessitates constructing a regional CPTP model that accurately captures drought-induced impacts in that region. The regional drought strategy model is thus formulated using a linear complementary programming approach to investigate the effects of climate-induced natural disasters, such as drought, on agricultural commodity production capacity and the utilization of natural resources (Ghaffari et al., 2022). Regional and subregional framed drought intensities are the primary determinants of drought severity assessments (Wu & A. Wilhite, 2004). Overall, drought is defined as occurring at state and regional levels when the value of the drought indicator exceeds the region's regular value. Drought severity is described in terms of moderate, severe, and extreme levels. The model is implemented at the state level using regionalized drought intensities from the Palmer Hydrological Drought Index (PHDI) for selected stations, as calculated by the Climate Prediction Center (CPC). Drought intensity mapped at the state scale constitutes the first spatial layer. Regions with moderate drought intensities, such as Kansas, Missouri, and North Dakota, rank tenth among almost 200 stations governed by pmp_drought. Those

experiencing extremes—specifically Alaska, New Mexico, and Wyoming—rank between thirty-four and seventy-five. The remaining states with normal PHDI values occupy the first to ninth and seventeenth places. This ranking system is employed to ascertain the annual drought index of all drought-impacted states, linking intensities and regions. Subsequently, to construct the annual drought index, the stations within each state are averaged according to their annual ranks and weights, as provided by pmp_drought. The resulting drought intensity coefficients serve as vital inputs for the regional agricultural drought strategy model.

5.2. Flood Impact Assessment

Flood events constitute an extreme form of natural disaster that significantly threatens agricultural income in many regions of the world. In this context, climate exerts a substantial influence on agricultural production, with direct and lag effects linked to soil fertility, farm labor availability, capital, investment, revenue, and related aspects. Flood occurrences can result in soil leaching, elevating the rates of nutrient loss and decreasing soil fertility. Experts rely on these reports to determine the necessary assistance for farming households in flood-prone areas. Floods also corrupt planting materials, causing reduced yields; farm obstructions by floodwater decrease harvest and plant protection activities; the destruction of houses resulting from these events diminishes domestic labor availability; and transportation and trading activities are curtailed by flood-induced disruptions. Consequently, yields tend to fall. Furthermore, floods damage several assets, including land, household structures, stored seeds and grains, fowls, and equipment. Flood impacts represent a crucial indicator capturing various aspects of climate change (W. Arnell & N. Gosling, 2016). Thus, the total exposure to flooding for crop production is calculated by combining data on the area of all crops in each grid cell with information on flood impacts under different climate projections (the maximum exposed area for any of the individual irrigation types is used rather than the sum to avoid double counting) (Fréjuis Akpa, 2024).

5.3. Pest Outbreaks and Climate Change

Climate change can directly and indirectly alter the risk of pest outbreaks through modified climatic suitability, and indirect changes in the types of crops that can be cultivated or crop quality. Pest ranges are known to be shifting in response to climate change, with evidence suggesting distinct poleward range extensions for plant viruses,

bacteria and fungi (Garrett et al., 2009). Along with hypothesized direct effects of phenology, experimental and modelling studies also consistently find that climate change can alter the magnitude of pest outbreaks, sometimes considerably. Severity of outbreaks in some cropping systems is projected to increase; a multi-pest study for Europe found that several currently economically important pests would have higher damage potential under future climate change. This is in part due to decoupling of phenology between pest species and natural enemies. Certain pathogens like powdery mildew and sugar beet rust are also expected to extend both range and severity, and several models of insect damage suggest a larger potential for crop loss due to insect pests.

6. Results

Many studies of disasters focus on slow-onset, large-scale events such as droughts or more rapid-onset events such as riverine flooding that create two distinct zones—a region impacted by a disaster and a region unaffected by that disaster. These events are large enough to be considered independently of other disasters and there is little or no confounding interaction between different types of disaster outside of a tightly defined watershed. The consideration of a lightning strike presumably occurs on a far smaller spatial scale than these events, and the size of an impact is typically limited to a zone well within a single agricultural production region. Additionally, multiple types of disasters could happen simultaneously or in rapid sequence; however, no disasters are permitted to impact the same spatial area at the same time. When this is the case, natural disasters cause damage to only the asset raised by the cheapest means. Each agricultural commodity has a different replacement value and is distinguished in several different ways. Finding an agricultural hit is the logical starting point once a disaster is generated because the economic incidence of the damage depends on the affected region's crop production composition.

6.1. Model Outputs

The combination of a weather generator and crop simulation models such as DSSAT and APSIM developed for the Tropical Western Pacific, plus sequence modeling to pipe together the short-sequence outputs into a whole-of-season simulation that represents the implications of the altered rainfall sequences, shows promise to be a useful approach in the absence of long-sequence rainfall generators. In the case of the Island Climate

Update (ICU) scenarios, the altered rainfall distribution produces a greater average crop yield for coconuts but a decrease for other crops in the base-case setting. For crops with multiple sowing windows, the provision of additional sowing opportunities in the rainy season is likely to improve yields. Crop yields from the base case scenario, under the various ICU scenarios, show a general trend of decreasing yields with increasing temperatures, consistent with model outputs across latitudes (Rachel Palatnik, 2015). Grain yields for maize and rice tend to reduce because the temperature increase causes shorter crop growth periods and hence lower biomass accumulation; the reduction in yield for yam is caused by the decrease in rainfall in the island scenarios (P McDermid et al., 2015).

6.2. Statistical Analysis

Our study examines the impact of climate on agriculture. A conditional dependence model for multivariate extreme values is adopted to examine the dependence structure between extreme weather events and crop yield losses. Because climate and agriculture are highly debated, the study focuses on the relation between climate and agriculture, which remains a matter of debate. Many studies discuss the impact of weather variables on food production. Temperature affects yields, whereas precipitation influences inter-annual production changes. Traditional analyses employ linear regression, focusing on mean effects. The relation between climate and agriculture appears non-linear. Previous work shows that production peaks roughly at an average temperature of 13 °C and then declines at higher temperatures. Hence, warming is expected to reduce productivity in hotter regions.

Extreme weather events—such as heatwaves, droughts, and floods—represent significant impacts on crop yields and quality. The frequency and severity of these events are expected to increase with climate change. These extreme conditions damage crop production worldwide, with indirect effects occurring through pests and soil processes. The analysis assumes that extreme weather events relate to substantial crop losses. Two related hypotheses are tested: (i) weather variable tails associate with crop yield tails and (ii) the strength of this association varies across countries and crops. The conditional extreme dependence of yield losses is modeled for four weather variables across Asia, Africa, and Latin America.

Because aggregating across spatial and temporal dimensions leads to information losses that determine the magnitude and direction of climate change impacts on agricultural markets and land-use patterns, the study focuses on disaggregated patterns rather than aggregate measures (Rachel Palatnik, 2015). Aggregation is performed across steep gradients from low to high impacts or from increases to decreases. Global production of individual crops is projected to decrease by 10–38 % under these climate change scenarios. However, large uncertainties remain in spatial patterns, which derive from climate projection uncertainties and impact model choices. This uncertainty regarding climate impact on crop productivity is noted (Marmai et al., 2022).

7. Discussion

These approaches enable the comparative assessment of damage and recovery across the full range of modelled variables, as GLOFRIS models outputs of expected flood damage (risk) and system resilience based on the broad set of modules. Comparison of the modelled economic risk and resilience between the climate scenarios shows how climate change is projected to make the impact of river flooding on European agriculture significantly more damaging and at the same time the affected systems are projected to become less resilient. Figure 3 shows three illustrative cases supporting these findings. When analysed in greater detail, the multiple modules and simulated variables of GLOFRIS can provide insight into the causes behind these changes, such as the decrease in soil water retention capacity that leads to increased hydrological soil stress and generates a projected reduction in the resilience of most agricultural systems.

7.1. Interpretation of Results

Certain crops, such as maize, wheat, soybeans, groundnuts, and sorghum, exhibit yield responses to temperature and precipitation that are sub-linear. This pattern can be approximated by Cobb-Douglas production functions with exponents smaller than 1 for precipitation and temperature, a commonly used formulation in empirical studies of agricultural yield response to climate change (Kavi Kumar, 2009). Linear damage functions therefore tend to overstate both positive and negative impacts of temperature, implying that constant elasticity models provide a more appropriate representation for these crops. The estimation exercises also generate quantitative results that can be directly interpreted. Representative values for the sensitivities required to calibrate a parsimonious agricultural damage function are 1–2% of gross output per degree Celsius

for temperature and –7– –15% of gross output per 10% increase in precipitation. These sensitivities correspond to elasticities of roughly 0.05–0.30 with respect to precipitation and 0.01–0.02 with respect to temperature. Such elasticities offer rigorous guidance for studies that must adopt damage functions, without the benefit of crop-level yield respecifications (P McDermid et al., 2015).

7.2. Implications for Policy

Climate-induced disasters threaten sustainable development goals and human security, especially in villages and hamlets dependent on crops, livestock, and fisheries. Projects to diversify economic activities benefit resilience but require critical infrastructure, resources, and skills not yet widespread. Trained satellite imagery can produce sub-kilometer crop maps for near-real-time loss estimation, but data needs and regional capacity remain significant challenges. Disaster risk management and climate change adaptation can be integrated through scenario planning, participatory workshops, and qualitative and quantitative analysis. Input-output tables for sectors such as rice, wheat, and maize provide data for assessing impacts and vulnerability (Dellarole, 2016). Climate change already affects the frequency and intensity of tropical storms, elevating danger globally (Anríquez & Toledo, 2019).

8. Limitations of the Study

The present study exhibits a number of limitations that offer opportunities for further improvement. Among these, the following stand out: (a) restrictions on the variables under analysis, as a result of unavailability of long homogeneous records of the monthly rainfall at finer spatial scales; (b) limitations inherent to the use of a single model, induced by the construction methods and model parameterization; (c) the fixed spatial scale of application imposed by the resolution of the spatial climatic data used in the model. The scarcity of data concerning the relationships among rainfall and rice production variables in the world remains a common problem faced by investigators. These relationships are crucial for the performance of models for decision support and prediction (J. Challinor et al., 2013). An approach to decision support in the agricultural sector consists of the use of climate scenarios obtained from the information in the climate models. In this case, climate data from 15 General Circulation Models (GCMs), under four different Representative Concentration Pathways (RCPs) defined in the fourth IPCC6 report, are used instead of the observed climate data, as input to the

statistical model. Since the first method cannot be replicated to other regions, the historical meteorological time series could play the role of input data. The SDSM model is implemented once for every rain gauge location or intermediate station on the grid where modelled climatic data are to be produced. The model is subsequently used with limited modifications for simulating the corresponding climatic variables under local climate change scenarios for the selected stations. The approach adopted in the calibration of SDSM assumes that the basic predictor-predictand relationships remain valid in the changed climate. Therefore, the method can be accepted only for projections under scenarios that have relatively minor changes in atmospheric circulation patterns (P McDermid et al., 2015). Application of the modeling approach to other basins would provide a valuable tool to the basin authorities for planning command area irrigation strategies by selecting appropriate crops with higher net incomes to optimize water use. Similarly, the methodology can be adopted by planners and policy makers for risk assessment and development of contingency plans associated with climate-related hazards and major linked outbreaks such as rice blast and brown planthopper. Nevertheless, the proposed methodology is generally applicable and can be adapted to manage any other climate- and non-climate-related hazards affecting the production of any agricultural commodity.

9. Future Research Directions

Characterizing the impacts of climate-induced disasters on a complex agricultural production system requires a comprehensive understanding of the whole system. Although considerable research has addressed the direct impact of weather conditions on crop yield, a comprehensive representation encompassing logistics infrastructure, agricultural cooperatives, and weather conditions has been largely unexplored. A system dynamics model was developed to simulate the impact of different types of climate-induced disasters on agricultural productivity. The model was validated with data from the 2018 Japan Floods and the computation results for the 2020 Kyushu floods in Japan were discussed. The results suggest that the impact of disasters on agricultural productivity can be mitigated by preparing sufficient storage capacity in agricultural cooperatives. Future research should focus on further development of disaster modules, considering the gradual return of farming activity and including indirect impacts such as crop and wood shortages. A more integrated modeling of the interregional flow of agricultural products and supply chains is needed, and the risk of simultaneous disasters may have to be considered. While flood routing and road network models were not included, existing studies offer suitable methods and can be included in the model. The spatial resolution can be improved by considering the precise distribution of crops and

agricultural cooperatives within each municipality. Implementing these improvements will facilitate a better understanding of the impact of climate-induced disasters on agriculture.

9.1. Innovative Modeling Approaches

Innovative modeling approaches provide insights into how climate change and extreme climatic events affect agriculture, enabling the development of effective adaptation strategies. Climate change and agricultural vulnerability have been widely studied using various models and scenarios, including decision support systems such as DSSAT and APSIM, to assess impacts on crop yields and food security. Modeling approaches also evaluate adaptation strategies, incorporating variables such as drought-tolerant crop varieties and efficient irrigation methods. Frameworks like shared socioeconomic pathways help manage uncertainties in climate change research, emphasizing the importance of integrated modeling to inform policy decisions and develop resilient agricultural systems (Islam et al., 2016). Cropping system models facilitate understanding of physiological mechanisms under changing climate factors. Advances in data science support platforms that integrate real-time weather, satellite data, and cropping system modeling to assist stakeholders in forecasting crop yields and making decisions. Nonetheless, current crop models often cannot accurately reproduce field conditions across spatial scales, and a robust framework linking geoscience and information technology remains underdeveloped. Traditional models, relying on long-term average climate data and exhibiting limited scalability, are therefore constrained in their utility for decision support and risk management. Addressing these challenges offers practical benefits beyond scientific novelty. Cropping system models aim to predict climate risk, optimize management strategies, and improve efficiency (Jin, 2016). A Crop Modeling Coordinated Climate-Crop Modeling Project (C3MP) supports agricultural decision-making by assessing crop-specific climate impacts and adaptation across multiple models and global gridded scenarios. C3MP methodologies encompass simulations based on international climate-change scenarios and experiments articulating yield sensitivities to probabilistic climate forcing, utilizing numerous crop models and distributed scenarios (P McDermid et al., 2015).

9.2. Longitudinal Studies

Previous studies have used longitudinal observations of crop yields and climate variables for estimating the impact of climate changes on crop yields. Cline regressed the annual wheat, rice, and maize yield on the climate variables controlling for country-fixed effects and concludes that if global mean temperature increases by 2.5–3.0 °C, the global food production is estimated to decline by 3.0–12.0%. Longitudinal observations often span a short period and correspond to a narrow range of climate change, which limits their use of learning about climate change effects. Figure 9.3 shows historical annual mean temperatures data of Nakasaki prefecture in Japan for the period of 1900–2010. Such longitudinal data often vary within a narrow range (circa 1 °C) and these data alone provide limited information for estimating the impact of future hypothetical climate change. Because longitudinal data vary only within a narrow range, temperature coefficients estimated from the longitudinal data capture the effects of weather or climate shocks but cannot characterize the temperature impacts under substantial climate change. The common method for overcoming this problem is to make assumptions about the functional form of temperature effects and then estimate the parameters of the function from longitudinal data. The damage functions proposed by Chen and McCarl and Mall et al. are adopted in numerical experiments presented here. Examples in the literature have assumed a quadratic or polynomial relationship between crop yields and the temperature and specified the damage function using either one or multiple temperature measures. The approach taken here is to evaluate the harm formula using Swiss data on farm income.

10. Conclusion

The simulation of agricultural ecosystems integrates biophysical, socioeconomic, and climatic variables to enhance the forecasting of climate change impacts on crops, farming systems, economies, and sectors (Islam et al., 2016). There is considerable interest in mathematical methods that can systematically address the diverse variables, parameters, constraints, and uncertainties involved with such simulations, thereby improving the accuracy of extreme event forecasting and the social consequences of climate-induced disasters (Jin, 2016).

Multivariate models have gained attention for their ability to incorporate the effects of multiple climate phenomena on agricultural disasters, particularly through the use of statistical techniques that capture dependencies among various types of extreme events. Recognizing the interconnected nature of crop-impact disasters and climate extremes, these models offer a pathway to more comprehensive and reliable assessments. By

framing agricultural disasters as a hierarchy of related multivariate extremes, it becomes possible to leverage the relationships among different event types. Copulas, which construct multivariate distributions from specified dependence structures and marginal distributions, serve as an effective tool to characterize the complexity of such dependencies. Given a set of crop-impact disasters, the associated climate extremes can be viewed as multivariate covariates; the hierarchical framework thus exploits these covariates to enhance the modeling of multivariate crop-impact disasters. This approach reduces the risk of underestimation and supports more accurate disaster assessments.

References

Jin, Z. (2016). Crop modeling for assessing and mitigating the impacts of extreme climatic events on the US agriculture system. [PDF]

Islam, S., Cenacchi, N., Sulser, T. B., Gbegbelegbe, S., Hareau, G., Kleinwechter, U., Mason-D'Croz, D., Nedumaran, S., Robertson, R., Robinson, S., & Wiebe, K. (2016). Structural approaches to modeling the impact of climate change and adaptation technologies on crop yields and food security. [PDF]

Islam, S., Cenacchi, N., B Sulser, T., Gbegbelegbe, S., Hareau, G., Kleinwechter, U., Mason-D'Croz, D., Nedumaran, S., Robertson, R., Robinson, S., & Wiebe, K. (2016). Structural approaches to modeling the impact of climate change and adaptation technologies on crop yields and food security. [PDF]

J. Challinor, A., M. Osborne, T., Shaffrey, L., Weller, H., Morse, A., Wheeler, T., & Luigi Vidale, P. (2013). Methods and resources for climate impacts research. [PDF]

Fréjuis Akpa, A. (2024). The effects of climate extreme events on selected food crop yields in Sub-Saharan Africa. ncbi.nlm.nih.gov

Sridhar, G., Wheeler, T., Osborne, T., & Turner, A. (2016). Addressing the uncertainties associated in assessing the impacts of climate change on agricultural crop production using model simulations. [PDF]

Bindoumou, M. (2018). Climate Change and Dynamic Adjustment in Agriculture: The Case in Cameroon. [PDF]

Dellarole, A. (2016). ESSAYS ON ECONOMIC MODELLING OF CLIMATE CHANGE IMPACTS AND ENVIRONMENTAL POLICIES. [PDF]

Rachel Palatnik, R. (2015). Climate-dependent yields. [PDF]

Kavi Kumar, K. S. (2009). Climate sensitivity of Indian agriculture : do spatial effects matter?. [PDF]

Ghaffari, A., Nasseri, M., & Pasebani Someeh, A. (2022). Assessing the economic effects of drought using Positive Mathematical Planning model under climate change scenarios. ncbi.nlm.nih.gov

Wu, H. & A. Wilhite, D. (2004). An Operational Agricultural Drought Risk Assessment Model for Nebraska, USA. [PDF]

W. Arnell, N. & N. Gosling, S. (2016). The impacts of climate change on river flood risk at the global scale. [PDF]
Garrett, K., Forbes, G., Pande, S., Savary, S., Sparks, A., Valdivia, C., V Cruz, C., & Willocquet, L. (2009). Anticipating and responding to biological complexity in the effects of climate change on agriculture. [PDF]
Marmai, N., Franco Villoria, M., & Guerzoni, M. (2022). How the Black Swan damages the harvest: Extreme weather events and the fragility of agriculture in development countries. ncbi.nlm.nih.gov
Anríquez, G. & Toledo, G. (2019). De-climatizing food security: Lessons from climate change micro-simulations in Peru. ncbi.nlm.nih.gov

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Chapter 5: Modeling Financial Market Volatility Using Stochastic Differential Equations

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Abstract: Volatility modeling is a central theme in quantitative finance due to its significant role in asset pricing, risk management, and derivative valuation. Financial market volatility exhibits complex statistical properties—such as clustering, mean reversion, heavy tails, and asymmetric responses to market shocks—that challenge classical modeling approaches. Stochastic differential equations (SDEs) offer a powerful mathematical framework for capturing these dynamic features in continuous time. This paper explores the theoretical foundations and practical applications of SDEs in modeling volatility, starting from geometric Brownian motion and evolving toward more realistic stochastic volatility models, including the Heston and jump-diffusion models. These advanced formulations incorporate time-varying, non-constant volatility and allow for sudden jumps, addressing empirical discrepancies in financial data and enhancing option pricing accuracy. Key concepts such as Itô calculus and mean-reverting stochastic processes underpin the mathematical rigor behind these models. Additionally, we examine calibration methods and model performance using historical market data. The integration of volatility risk, implied volatility surfaces, and risk-neutral valuation aligns model behavior with observed market dynamics. Applications extend to exotic derivatives, path-dependent options, and foreign exchange markets. The paper emphasizes the importance of aligning mathematical sophistication with empirical robustness to navigate the stochastic nature of modern financial systems effectively.

Keywords: Stochastic Differential Equations (SDEs), Financial Market Volatility, Stochastic Volatility Models, Option Pricing, Itô Calculus.

1 Introduction

The study of financial market volatility constitutes a fundamental research task within the field of quantitative finance. Over the past forty years, considerable progress has been made toward obtaining reliable characterizations of volatility dynamics for companies traded on the main US Stock Exchange, as well as for reference market indexes. Volatility models play a central role in a large number of financial applications, from asset pricing to risk management and portfolio optimization. At the same time, stochastic processes have become instrumental in quantitative finance, particularly since the availability of a rigorous and self-contained mathematical framework for their analysis allowed meaningful applications in several areas of the financial industry. Several authors analyze the main stylized facts of market volatility and illustrate the implications for stochastic models of financial markets. Financial market volatility fluctuates rapidly in time, is persistent and highly autocorrelated; exhibits mean-reverting behavior; volatility shocks tend to cluster; extreme events lead to extreme volatility; volatility is highly sensitive to jumps in price; and negative returns tend to generate larger volatility than positive returns. Volatility is therefore a very complex quantity with no identical object in other areas of science (Di Persio & Gugole, 2018). Financial markets, at a first approximation, can be viewed as continuous systems subject to infinitesimal random fluctuations. The most suitable tool for modeling such systems are stochastic differential equations (SDE). This link between financial volatility and stochastic differential equations indicates that the main features of stochastic volatility can be accounted for within the framework of SDE's and, conversely, that SDE's constitute a natural starting point for the modeling of volatility maps (shen, 2009).

2. Theoretical Foundations

The process of modeling financial market volatility has been the subject of extensive research. Constructing asset pricing frameworks in continuous time inherently involves stochastic differential equations (shen, 2009). Such models focus exclusively on the price and volatility of the underlying asset, omitting other factors. The most rudimentary representation of an asset price is captured by geometric Brownian motion, recognized as a market-complete and arbitrage-free model. Nonetheless, real-world observation of market data reveals a plethora of phenomena that geometric Brownian motion fails to replicate effectively (A. Londoño & Sandoval, 2015). As a result, more versatile models have emerged from the foundational geometric Brownian structure, enabling a broader spectrum of behavior to be captured. Typically applied to stock price simulation, such

models also find frequent utility in the pricing of derivative instruments. The Black–Scholes framework, predicated on the geometric Brownian assumption, faltered following the 1987 market crash, catalyzing the development of stochastic-volatility formulations that account for volatility clustering. These models bridge the gap between econometric analyses of the market and the formulation of pricing methodologies (Di Persio & Gugole, 2018).

2.1. Differential Equations

The definition of differential equations is of primary importance. Consider a function y(y0 itself) subject to continuous-time change, and a function f:$\mathbb{R}2\rightarrow\mathbb{R}$ determining the local derivative around y0. Then the ordinary differential equation of y with the initial condition y0 with the initial condition y0 is described by $dy(t)/dt=f(y(t),t)$, $y(0)=y0$, for $t\geq0$. Most of the financial modeling interprets $dy(t)/dt$ as the local rate of change of y, and when the function $f(\cdot,\cdot)$ is a linear function with constant coefficients, this kind of differential equations has explicit solution formulas that facilitate modeling. In addition to these standard differential equations, such that time is regarded as a variable and y(t) is described as $y(t+\Delta t)$, where the increment of t, Δt, is fixed. Furthermore one of the remarkable type of the continuous time change processes can be expressed by the stochastic time differential equations (SDEs)

223. Volatility in Financial Markets

A comprehensive description of market volatility must incorporate key empirical characteristics, such as heavy-tailed distributions for daily and intraday returns (Di Persio & Gugole, 2018). Financial markets undergo continuous shifts among periods of varying volatility, creating long memory effects and clusters of extreme events. These features necessitate a time-varying, model-sensitive definition of volatility (shen, 2009). Market fluctuations reflect the complex interplay between rational economic decisions, market imperfections, psychological influences, and imperfect information dissemination. Volatility is commonly assessed by the standard deviation of asset returns, a measure that naturally emerges from the fundamental law of large numbers (S. Lima, 2019). The first approach to modeling asset price dynamics in an uncertain environment was Brownian motion, introduced by Bachelier. As stochastic calculus has advanced, mathematical modeling of uncertainty has become richer and more versatile, establishing itself as a well-tested foundation for numerous applications.

3. Stochastic Differential Equations (SDEs)

The Black–Scholes formula, first published in 1973 by Black, Scholes (1973) and Merton (1973), describes a theoretical framework for option pricing based on geometric Brownian motion. It has been extensively used in academia and the derivatives industry as the foundation for estimating risk-neutral densities implied by option prices. Modeling the stochastic process of the underlying asset under the risk-neutral measure remains an active research area (A. Londoño & Sandoval, 2015). Numerous extensions to Black–Scholes have emerged over time, including local volatility, stochastic volatility, and jump–diffusion models (Wang, 2016). Present-day focus has shifted from option pricing formulae towards using stochastic differential equations (SDEs) to characterize the underlying risk-neutral stochastic process. This approach allows for modeling fundamental risk drivers—such as underlying asset price, stochastic volatility, interest rate, and stochastic convenience yield—directly instead of an aggregate measure. Consequently, SDE-based models can provide a more detailed and comprehensive representation of market dynamics and options prices.

3.1. Definition and Properties

Stochastic volatility models capture the dynamics of volatility, a key risk factor in financial markets that influences asset prices and derivative valuations such as options. Beginning with the geometric Brownian motion model of Merton (1973), which gives constant volatility in the Black–Scholes framework, the stochastic differential equation (SDE) for the log-price process $X(t)$ is $dX(t) = \mu\, dt + \sigma\, dW1(t)$. Here μ and σ are constants, assumed deterministic, and $W1(t)$ denotes a Wiener process. Implied volatility recovered by inverting the Black–Scholes formula is not constant, however, and exhibits several statistical stylized facts. Volatility clustering is one such fact: large movements of a market index are followed by large movements of either sign, whereas small movements are followed by small movements. Stochastic volatility models generalize the standard framework by assuming that σ itself evolves stochastically according to another SDE driven, for example, by a Wiener process $W2(t)$ correlated (or not) with $W1(t)$, allowing for non-constant volatility and a richer modeling capability. The literature includes the Hull and White model , the Scott model , and the discrete versions of Taylor (1986) and Harvey et al. (1994). A special class of stochastic volatility features algebraic mean reversion. Consider a non-negative volatility variable $y(t)$ described by $dy = F(y)\, dt + G(y)\, dZ(t)$, where $Z(t)$ is a Wiener process (possibly correlated with $W1(t)$) determining the noise term, and $F(y)$ is a nonlinear drift that drives y towards the long-

term average <y>. If the mean reversion is algebraic, then a fictitious potential V(y) with force F(y) = -dV(y)/dy can be constructed and contains quartic terms growing as y^4. Taking G(y) proportional to y^2 the result is a stochastic Cauchy oscillator. We use the measured time series of a financial market during the period 1995–2003 to calibrate the four free parameters and test the quality of this specification.

3.2. Ito's Lemma

Consider X_t as an n-dimensional diffusion Itô process, a solution of the stochastic differential equation:

(1) $dX_t = b(t,X_t)\,dt + \sigma(t,X_t)\,dB_t$, $t \in [0,T]$ where B is an m-dimensional Brownian motion, $1 \leq m \leq n$ and the coefficients satisfy "usual" conditions for existence and uniqueness of strong solutions (S. Lima, 2019). Let $f:[0,T] \times \mathbb{R}^n \to \mathbb{R}$ be a twice continuously differentiable function. The process f(t,X_t) is also an Itô process that satisfies (El-Khatib, 2006)

(2) $df(t,X_t) = (\partial f/\partial t + \nabla_x f\, b + \tfrac{1}{2} \mathrm{Tr}(\sigma \sigma^* H_x f))(t,X_t)\,dt + (\nabla_x f\, \sigma)(t,X_t)\,dB_t$

where "*" the transposition of the matrix,

$\nabla_x f = (\partial f/\partial x_i)_{1 \leq i \leq n}$ is the gradient and $H_x f = (\partial^2 f/\partial x_i\, \partial x_j)_{1 \leq i, j \leq n}$ is the Hessian matrix with respect to the space variable x.

3.3. Applications of SDEs in Finance

SDEs are capable of identifying the values or prices of financial integrals, even for path-dependent forms such as Asian options and Barrier options. The financial sector continues to explore SDE applications to illustrate the underlying stochasticity in modeling stock prices, interest rates, domestic exchange rates, international foreign exchange rates, inflation rates, and financial volatility (Mohammed Alzughaibi, 2018). They further assist in evaluating quantitative and qualitative outcomes for investors or

stakeholders when purchasing financial derivatives. Pricing options and calculating volatility are intricately related problems with profound influences on one another. The unavailability of closed-form solutions for these problems necessitates numerical approximations. In mathematical finance, derivatives serve as tools to reduce risk and pursue high yields, making accurate pricing and risk measurement crucial. Louis Bachelier's 1900 dissertation introduced a probabilistic description of price fluctuations using stochastic analysis, which inspired significant models like the Capital Asset Pricing Model (CAPM) of 1965 and the Monte Carlo method of 1977. Unlike convergent scientific methods, financial modeling often follows divergent approaches for prediction. The Black-Scholes model provides a widely-used European option pricing formula based on arbitrage-free assumptions and normal distributions. Backward Stochastic Differential Equations (BSDEs), introduced by Bismut and extended by Pardoux and Peng, have gained importance for pricing complex derivatives, including American and Asian options; compared to the Black-Scholes model, BSDEs exhibit greater robustness in the presence of uncertain probability models and have been adapted to various contingent claims (Wang, 2016).

4. Modeling Approaches

In the context of stochastic volatility modeling, several approaches have been proposed that are both coherent and tractable. One class is the local volatility framework, where the volatility function is deterministic, depends only on the current stock price and time, and is derived so as to exactly fit the observed market prices of plain-vanilla options. Models of this type include the pioneering ones of Dupire (1994), Derman and Kani (1994), and Rubinstein (1994). Their motivation has been to develop pricing frameworks within which existing calibration methodologies could be justified, and to overcome some of the practical difficulties associated with early volatility models (Mitra, 2009). Local volatility models yield complete markets and therefore unique arbitrage-free prices. Moreover, they preclude the possibility of asset-price jumps . The introduction of stochastic volatility accommodates such jumps as an additional source of risk.

4.1. Heston Model

The Heston model, introduced in Heston (1993), is a widely known stochastic volatility (SV) model. It assumes that the volatility process follows a Cox–Ingersoll–Ross (CIR) dynamic, where λ denotes the long-term mean and represents the speed of mean

reversion. By modeling the random fluctuations in volatility, the Heston framework addresses limitations of constant volatility models, which are inconsistent with observed option prices and implied volatility surfaces. The pricing equation is derived by considering a portfolio that hedges the option with the underlying asset and a volatility-related instrument. Under the risk-neutral measure, the partial differential equation (PDE) incorporates the market price of volatility risk θ in its coefficients. European option prices can be computed using a fast, quasi-closed-form solution, enabling efficient calibration to market data by minimizing discrepancies between theoretical and observed prices (Di Persio & Gugole, 2018).

The volatility process is nonnegative and mean-reverting, consistent with empirical observations. The availability of a computationally efficient, semi-analytical solution for European options constitutes the greatest advantage of the Heston model over competing SV frameworks, facilitating calibration to market quotes (Janek et al., 2010). It was among the first models to explain the volatility smile while allowing practical implementation and the valuation of exotic derivatives at prices more consistent with the market than those generated by the Black–Scholes formula. The instantaneous variance evolves as a mean-reverting square-root (CIR) process, specified by parameters such as the long-run variance, the speed of mean reversion, and the volatility of variance. The model's properties include the characterization of marginal distributions and tail behavior. An adaptation for foreign exchange (FX) markets successfully accounts for the volatility smile. Different volatility structures observed in various markets—for example, the asymmetric skew typical of equity returns—have also been incorporated. The departure from geometric Brownian motion is pronounced. For option pricing, the value function of a contingent claim satisfies a PDE that reflects the correlation between asset returns and volatility, as well as the market price of volatility risk.

4.2. Jump-Diffusion Models

Geometric Brownian motion assumes price changes with a normal distribution, yielding an empirically inadequate log-normal distribution for returns. Jump-diffusion processes incorporate price jumps while preserving continuous diffusion and the Itô Markov property (S. Lima, 2019). The Black–Scholes–Merton framework arose from the need to estimate option values and concluded that asset prices evolved according to geometric Brownian motion. Merton later introduced a jump process to extend the Black–Scholes–Merton model, leading to geometric jump-diffusion dynamics (El-Khatib, 2006). Incorporating jump components throughout the option's life, even in the very short term,

improves the fit to actual option prices. Jump-diffusion models augment the standard continuous asset dynamics with a jump process, capturing continuous Gaussian shocks through a Wiener process and discontinuous jump shocks via a Poisson process. The jump component follows a lognormal distribution to ensure strictly positive stock prices (Di Persio & Jovic, 2016). The model can be described by an SDE of the form

4.3 Stochastic Volatility Models

Early financial theories, such as the Black-Scholes model, assumed constant volatility and normally distributed returns. These assumptions are often violated in practice, leading to more complex models where volatility varies randomly over time. Stochastic volatility (SV) models are financial models that allow volatility to evolve according to a predetermined stochastic process (Mitra, 2009). The correlated stochastic volatility models generalize the Black and Scholes-Merton framework by modeling volatility as a stochastic process correlated with the log-return of prices. Various models differ in the dynamics of volatility; Vasicek, Heston, and exponential Ornstein-Uhlenbeck have received recent attention. Theoretical properties of these models, such as the volatility and return distributions and higher-order moments, can be evaluated through numerical simulations to assess their predictive ability. Implementations of the models confirm that their characteristics can be maintained in practice, supporting their use in market risk management and option pricing. Analyses of Italian stock-market data indicate that the exponential Ornstein-Uhlenbeck model captures the main statistical properties of both volatility and log-returns (Cisana et al., 2007).

A significant class of SV models includes those of Johnson and Shanno, Scott, Hull-White, Stein and Stein, and Heston. The principal distinction between local and stochastic volatility is that local volatility responds directly to the asset price; it has no independent random component. In contrast, SV models have their own source of randomness. SV models tend to be less analytically tractable and rarely admit closed-form option pricing solutions, necessitating simulation. Many incorporate a mean-reverting process, often Ornstein-Uhlenbeck, causing volatility to fluctuate randomly around a long-term mean. Mean reversion controls the degree of volatility clustering or burstiness observed in many markets.

5. Estimation Techniques

Quantitative modelling of product and service demand has direct applications in supply chain design and marketing, among other fields. This paper operationalizes a recently proposed method for quantifying the structural parameters and model coefficient functions of a stochastic differential equation (SDE) driven by a seasonal Ornstein–Uhlenbeck covariance structure. Employing a combination of maximum likelihood estimation and least-squares fitting, this approach offers an alternative to the semiparametric kernel-based technique of . Implementing the method in Python, an application to the sales of a major US-based consumer packaged goods company is presented.

Since their introduction into economics by Mandelbrot (1963), stochastic volatility (SV) models have flourished and are now standard tools for describing the evolution of volatility measured by financial returns. A central goal of SV models has been to reproduce the volatility persistence observed in empirical data. It is commonly accepted that some financial data exhibit long-range dependence, while others show intermediate or short-range dependence; continuous-time fractional stochastic volatility models enable representing these forms of persistence. An estimation procedure, based on a continuous-time version of the Gauss–Whittle objective function, provides estimates by minimizing the discrepancy between the spectral density and the data periodogram. Applied to fractional stochastic volatility models, it yields estimates of the drift, standard deviation, and memory parameters of the volatility processes, facilitating the analysis of indices such as the Dow Jones, S&P 500, CAC 40, DAX 30, FTSE 100, and NIKKEI 225. Stochastic volatility models, which capture the latent and intermittent behavior of volatility, have addressed the challenges present in early approaches that modeled the logarithm of volatility via an Ornstein–Uhlenbeck process, where estimation often relied on the maximization of intractable likelihood functions (Casas & Gao, 2006).

5.1. Method of Moments

The classical method of moments has been frequently applied to estimate the parameters of the stochastic volatility (SV) model. In financial markets, the vector of observed data often contains prices of options and underlying stock prices or their logarithms (Di Persio & Gugole, 2018). The state vector consists of the stock price together with one or more additional unobserved variables. Parameter estimation methods first use the observed

option prices to reconstruct the unobserved state vector, often by computing option prices as a function of the observed variables or employing implied volatility as a proxy for the instantaneous unknown volatility. The exact likelihood function is usually not available in closed form, but a variety of approximations exist that make it possible to write the joint likelihood in a form suitable for estimation through the classical method of moments. When proxies such as implied volatility are used, the computation of the likelihood becomes even simpler. Estimates obtained using the method of moments are consistent with those derived via auxiliary likelihoods as well as with econometric estimates available in the literature (Franke & Westerhoff, 2011).

5.2. Bayesian Methods

Bayesian estimation represents a natural approach to analyzing stochastic differential equation (SDE) models, given their hierarchical structure (Bertschinger et al., 2018) ; (Griffin & F.J. Steel, 2008). Griffin and Steel consider Bayesian inference for models in which the instantaneous volatility is represented by a continuous superposition of Ornstein-Uhlenbeck (OU) processes. Continuous-time stochastic volatility models have demonstrated considerable success in modelling financial time series such as stock prices and exchange rates. Desirable properties for such models include consistency across different sampling frequencies and the potential to derive option pricing formulae. Stanton (1997) introduces the standard model, wherein the asset price S(t) satisfies the stochastic differential equation

$$dS(t) = \mu\, dt + \sqrt{\upsilon(t)}\, dW_1(t)$$

with instantaneous volatility $\upsilon(t)$. Although most work presumes that $\upsilon(t)$ is a Brownian motion, alternative specifications are of interest. Griffin and Steel replace the Brownian motion by a continuous superposition of OU processes and argue that Gamma-mixture specifications may exhibit long memory properties. During the investigation of such continuous-time models, Griffin and Steel develop efficient Bayesian computational algorithms, concentrated on estimating stochastic volatility and leverage effects. The authors propose Markov chain Monte Carlo (MCMC) methods that are more straightforward to implement and faster to converge than traditional approaches. Bertschinger et al. analyze simplified versions of agent-based market models and demonstrate the feasibility of Bayesian parameter estimation. Both the Vikram Sinha and the Franke Westerhoff models comply with a state-space formulation. Consequently,

latent states can be integrated into the MCMC procedure, enabling the simulation and estimation of latent state dynamics. The Vikram Sinha model considers a market of N traders submitting buy, sell, or inactive orders at each time step. The valence of an order is independent and identically distributed with mean zero and variance σ_{max}^2. Prior to submitting an order, each trader decides whether to trade, with a probability that increases with perceived mispricing. Perceived mispricing is defined as the logarithmic deviation of the current price p_t from the exponentially weighted moving average of past prices p_t^*,

6. Numerical Methods

6.1. Milstein Method

Because the stochastic volatility model is the general form of SDEs, the Milstein scheme can be applied to it and therefore is worthy of being studied and more deeply analyzed. The Milstein method constitutes a powerful alternative to the Euler scheme by offering improved convergence properties: it achieves strong convergence order 1.0 compared to Euler's 0.5; and it enables larger timesteps without the severe loss of accuracy that Euler can exhibit (shen, 2009). In the general case, however, implementing the Milstein scheme entails simulating iterated Brownian integrals, a challenging task except under a restrictive commutativity condition that is unlikely to hold for the stochastic volatility model (Jourdain & Sbai, 2009). This limitation curtails the direct applicability of the Milstein method in practice unless specific model properties are exploited.

6.2. Monte Carlo Simulations

Monte Carlo methods generate random numbers to simulate sampling from processes that follow certain distributions, providing solutions to otherwise intractable problems like modeling the financial system in stock markets and option pricing (Wang, 2016). Market volatility and option pricing are modeled by stochastic differential equations through the derivation of the Black-Scholes model and Monte Carlo simulations, using a real dataset from the S&P 500 index over a two-year period as illustration. Diverse stochastic volatility models reflect the evident randomness of volatility: a key factor in option prices, they are essential to reproducing important stylized facts such as the volatility smile (Schmitz Abe, 2008). While exact solutions to the process are known for

some models, others require numerical methods like partial differential equations and Monte Carlo simulations to determine prices, which become particularly useful toolboxes when dealing with high dimensional problems or exotic derivatives.

7. Empirical Analysis

The study of volatility has attracted attention since the financial crisis due to the possibility of explaining price fluctuations of securities and indices. Financial markets exhibit multiple stylized facts, including heavy-tailed return distributions and volatility clustering. In particular, the distribution of volatility itself is a key observ able for a better characterization of market dynamics (Di Persio & Gugole, 2018). According to the Efficient Market Hypothesis (EMH), price fluctuations follow a memory-less random walk; however, this is inconsistent with empirical findings. Stochastic volatility models reproduce the essential stylized facts observed at different temporal scales, reflecting the variety of economic agents acting in the market. Several stochastic volatility models exist in the literature, commonly formulated as coupled stochastic differential equations in the Itô interpretation. Two model formulations are available for estimating volatility: one assumes that volatility evolves according to a specific stochastic process, and the other assumes that price changes derive from a given volatility process. A visible market price can be interpreted as a result of different and competing forces, such as fundamental price, trend followers, contrarians, and technical traders (S. Lima, 2019). When economic agents focus on long-term price accuracy, the system behaves almost randomly; otherwise, the system becomes deterministic and should be able to model switching occurring in market phases, e.g., to high or low volatility levels (Bertschinger et al., 2018).

7.1. Data Collection and Preprocessing

The financial data employed for modeling are public and sourced from platforms such as Yahoo Finance. Collected information includes the opening and closing prices, daily highest and lowest prices, and trading volume for specific stocks. For the analysis presented in this chapter, daily closing prices constitute the primary dataset. Historical prices and trading volumes are an inherent reflection of firms' performances. Given the impracticality of accounting for all variables influencing stock price dynamics, precise forecasting of future prices remains elusive. However, to derive volatility indicators, prior curation of the stock price data is essential. The logarithmic returns of the raw stock

price series are utilized to inform volatility models. Since everyday price fluctuations are relatively minor, the logarithmic returns approximate the percentage returns. This formulation facilitates the deployment of stochastic differential equations with time-dependent drift and diffusion coefficients.

7.2. Model Calibration

A dedicated component is required for calibration, as the fractional Ornstein–Uhlenbeck process follows a precise specification and cannot be modified (A. Londoño & Sandoval, 2015). The front-end calibration operates on parameters that determine a new spot variance, Sigma; the variance mean reversion, alpha; and the term structure of the instantaneous variance (Hakala, 2019). Moreover, stochastic sampling algorithms for stochastic differential equations are typically considered as specification and simulation tools, instead of calibration or direct estimation devices. Accordingly, a remarkable advantage of the calibrated model is that it maintains a structure closed to the original fractional framework; thus, it can integrate the Hurst parameter as an additional calibration variable, extending the classical specification. This is particularly relevant because the parameter H is not constant a priori and can exhibit index spikes.

7.3. Backtesting Results

The backtesting of the available models provides an estimate of the expected performance of the differential stochastic-equation approach when applied on longer time horizons (Cisana et al., 2007). The models are tested over two distinct elapsed time-intervals of the data, and two predictive horizons are considered. The length of the first elapsed time-interval is 225 days, which corresponds roughly to a 1-year trading period; the second interval corresponds to roughly 1.5 years of trading (or 361 data points). The starting point for each elapsed interval is January 1990 (A. Londoño & Sandoval, 2015). Predictive horizons of 25 days and 30 days are used, which correspond roughly to one month of trading data, for reasons of estimation convergence. The models are also back-tested versus two different financial signals: the VIX and the VDAX indexes, respectively for the SPX and the DAX. In the following, back-testing results are presented for the models separately.

8. Risk Management Implications

Financial volatility remains highly variable and difficult to predict. In the future, extreme events such as financial crises and market crashes are likely to continue challenging efforts to model or forecast volatility accurately. The models presented above do not provide a means for quantifying the risk of a given investment portfolio, nor do they permit the construction of risk-minimizing portfolios. Methods that serve these functions are described in (Xu, 2014).

8.1. Value at Risk (VaR)

VaR is a key measure of risk in a portfolio of assets, representing a high quantile of loss distribution for a particular horizon. Traditionally, historical simulation and the variance-covariance approach have been used to estimate VaR, but both methods fall short under actual market conditions. Historical simulation assumes constant volatility and fails to account for volatility clustering, leading to underestimation during high volatility periods. The variance-covariance approach assumes normally distributed returns, which underestimates VaR for fat-tailed and leptokurtic distributions (Bhattacharyya & Madhav R, 2012). Dynamic VaR models integrate an ARMA (1, 1)-GARCH (1, 1) framework to capture autocorrelation and time-varying volatility, while fat-tailed behaviour is modelled using distributions such as Pearson Type IV, Johnson SU, Manly's exponential transformation, and both normal and t-distributions. These approaches better represent characteristics like volatility clustering and leptokurtosis, providing more accurate risk assessments.

8.2. Stress Testing

It is relevant to the financial domain when considering stress testing. The inability of classical models to capture fat-tails and clustered volatility induces the definition of a new scheme to stress the model. The flexibility provided by the continuous-time framework and infinitely many possible diversification outcomes allows for a realistic representation of extreme events while maintaining a high degree of confidence in the results.

8.3. Portfolio Optimization

Optimal portfolio choices represent a critical issue in mathematical finance. The dynamic portfolio selection problem has been analyzed extensively under classical utility maximization criteria (Lin & SenGupta, 2021). Emerging financial products often display nonlinear features in various payoff functions, making option pricing and managing portfolio problems based on traditional linear or quadratic models no longer suitable. Optimal portfolio selection problems under nonclassical utility functions are more realistic and demanding at both theoretical and practical levels (Omidi Firouzi & Luong, 2014). A generalized model starts from the classical utility maximization criterion; a general utility function depending on wealth is applied as the objective function in a market with stochastic volatility. The general utility maximization problem for an incomplete market with stochastic volatility using a backward programming principle method is discussed, followed by the portfolio optimization problem considered for a specific class of general utility functions within a stochastic-volatility market model under the incompleteness assumption. Explicit solutions for the value functions and the optimal strategies are determined in two examples—power and logarithmic utilities (Wang, 2016).

9. Comparative Analysis of Models

Three models provide a starting point in different ways. Vasicek provides an exogenous source of stochastic volatility for equity prices but is insufficient in a financial factor-structure framework. The Heston model is the standard in financial data modelling owing to its elegant closed-form PDE solution for option pricing and ability to reproduce several stylized facts, but it leads to an incomplete market, introducing arbitrarily chosen risk premia and potentially destroying the uniqueness of the underlying term structure (A. Londoño & Sandoval, 2015). The exponential Ornstein-Uhlenbeck (exp-OU) model exhibits a wider range of stylized features that are widely reproduced by universities and central banks, such as excess kurtosis and a realistic volatility distribution, and tends to be more parsimonious and stable when estimating market risk. Its single-factor exponential dynamics can be linked to a two-factor linear model for fundamentals. A simple explanatory framework illustrates the meaning of these three informational sources. Historical volatility can be considered a “bottom-up” measure that derives from asset prices and acknowledges information aggregation as a necessary feature of data regularities. Implied volatility embodies a “top-down” component that foresees market patterns and “predicts the future” more precisely than a bottom-up proxy. The VIX and

VXO indexes represent a final quantitative point where information is aggregated and subjected to experts' revisions derived from available economic theories. Concurrent sources of information frequently signal convergence towards one coherent narrative or indicate stronger areas of concern (Cisana et al., 2007).

9.1. Model Performance Metrics

The accuracy and precision of numerical schemes for the mean-reverting CEV SDE (3.3) were compared using relative errors in the L2 norm with Euler–Maruyama and Milstein schemes for small powers of the diffusion coefficient. The two numerical methods were also examined on their ability to maintain boundary conditions, with the CEV SDE preserving non-negativity much more robustly than the CIR SDE (3.2) for similar parameters. In an application to option pricing, the new model was compared against Heston's (1993) model, with parameters optimized by simulated annealing to minimize the difference between model and observed option prices. Both models performed similarly under normal market conditions, with the new model slightly outperforming Heston's during the 2008 financial crisis in terms of RMSE. Lagrange's interpolation revealed that the new model better captured the volatility surface, squared log-returns exhibited autocorrelation, and the volatility-return correlation was negative—stylized facts not simultaneously matched by Heston's model (A. Londoño & Sandoval, 2015).

9.2. Case Studies

We analyze a model with better empirical properties than Heston's model. Our model has a precise economic meaning, is simple to calibrate, and has reduced run times due to few parameters. It captures most stylized facts observed in the market and performs similarly to Heston's model at regular times in terms of RMSE. The model performs better during times of high volatility and uncertainty, such as during the 2008 financial crisis, and shows better dynamics of the volatility surface, evidence of autocorrelation in square log-returns, and a negative correlation between volatility and price levels. The simplest model for equity prices is a geometric Brownian motion, which has market completeness and no arbitrage opportunities but suffers from known issues like volatility smile and clustering effects. To address these shortcomings, extended models have been proposed, including those by Merton, Derman and Kani, Dupire, Hobson and Rogers, Hull and White, and Heston. Some of these models violate market completeness, leading

to non-unique prices. The models studied in this paper allow for a pricing theory based on results that do not impose constraints on the eigenvalues of the volatility matrix.

10. Future Directions

As volatility clustering has just recently been introduced to simplify basic pricing and estimation problems, the main area of exploration will be to build upon existing works. Application of such models will be performed on historical values from indices such as S&P 500 and NASDAQ. Future work includes developing numerical methods for solving backward stochastic differential equations (BSDEs). Black Monday, October 19, 1987, marked the largest one-day percentage decline in stock market history when markets around the world crashed. Many stock market hypotheses and assumptions of the economy were put into question but no definite conclusions were ever reached. Information surrounding this event seems to contradict the standard Black-Scholes equation for option pricing. It is after this event that stochastic volatility models became popular for hedging and derivative pricing. Any new model built on Black-Scholes can only be changed in key places that can be refined. Therefore, the main focus will be to change the volatility factor and manipulate several assumptions. As Black-Scholes is based upon historical data, this procedure will utilize the fact that the market is incomplete and will select a unique derivative pricing measure which reflects concerns of the economy from a sequence of measures.

10.1. Integration with Machine Learning

The increased availability of large financial datasets enables the utilization of more complex models for volatility projection. Convolutional network structures offer a natural fit for inhomogeneous and textured data. Single-source market models of each asset possess multiple drawbacks, the most important of which include the losses of market-wide feedback and cross-asset correlations — a crucial phenomenon (S. Lima, 2019). Construction of multi-source market models for major market indices and sectors significantly improves the accuracy of volatility series indics, which confirms the influential role of cross-asset correlations in the financial system. The main traditional stochastic volatility models are based on diffusion processes—often referred to as continuous-time models—and assume that the logarithm of the volatility follows an Ornstein–Uhlenbeck process, a geometry Brownian motion, or a Cox–Ingersoll–Ross process (Ramos-Pérez et al., 2020). These types of models allow closed-form solutions

to the pricing problem in several cases, and it is worth pointing out that, despite their simplifying assumptions, they are often able to reproduce stylized facts on future market volatility. Unfortunately, traditional stochastic volatility models cannot reproduce important characteristics observed for the ex-post volatility measured from market data, and the key point is usually identified with the presence of jumps. Machine learning techniques such as Gradient Descent Boosting, Random Forest, Support Vector Machine, and Artificial Neural Network can improve the prediction of volatility for indices such as SP500.

10.2. High-Frequency Data Analysis

In the last decade, the availability of high-frequency data recorded at very fine time scales has increased the emphasis in financial applications on the modelisation of short time dynamics. Differently from deterministic chaotic systems, which may be considered deterministic, complex financial systems obey stochastic dynamics, a consequence of the collective behavior of multiple interacting agents (1982- Hua, 2018). The characterization of the stochastic processes underlying financial markets remains so far an open problem, and attempts have been made to identify them by the proper analysis of relevant time series. Frequent assumptions on the short time dynamics of the logarithm of the price were (in the limit of long time intervals) the well-known Black-Scholes model of geometric Brownian motion, based on the premise that, automatically over long time intervals, financial time series obey Normal statistics. Empirical whitish noise properties of financial time are quite well verified in the frequency spectrum, and it has been observed that they become even more realized when returns are computed over time intervals of the order of a few minutes (Di Persio & Gugole, 2018). Available high-frequency time series span various markets over different periods: transaction price and transaction volume time series investigated at the level of a single trade. Statistical characterizations of the so-called waiting times between consecutive trades have been proposed, and a number of studies attempted to investigate their spectral density. Stochastic volatility models focus on the latent nature of volatility giving a natural view of observed clustering (shen, 2009).

11. Conclusion

Stochastic differential equations provide a mathematical framework for modeling continuous-time evolution of dynamical systems subject to random disturbances. In

finance, these equations are often utilized to capture the behavior of asset prices, interest rates, and other key financial variables influenced by inherent market uncertainty (Di Persio & Gugole, 2018). When employing stochastic differential equations to describe asset prices, the random disturbances are typically represented using the concept of Brownian motion. Brownian motion, originally named after botanist Robert Brown, is a continuous-time stochastic process, often called a continuous-time random walk. This mathematical abstraction is instrumental in representing random fluctuations observed in diverse natural and financial phenomena.

The Black–Scholes–Merton model treats stock or foreign exchange prices as following a geometric Brownian motion with constant drift and volatility, enabling the derivation of closed-form solutions for European-style option prices. Many empirical studies on the price of local (intraday) and daily volatility have been carried out. These studies often compare parametric versus nonparametric modeling strategies or rely on realized volatility using data sampled with fixed time intervals or tick time. Previous works have focused on the price of volatility risk for daily volatility, supporting the view of modeling the volatility process using a function of quadratic variation.

References

Di Persio, L. & Gugole, N. (2018). Volatility of prices of financial assets. [PDF]
shen, karl (2009). A Preliminary View of Calculating Call Option Prices Utilizing Stochastic Volatility Models. [PDF]
A. Londoño, J. & Sandoval, J. (2015). A new logistic-type model for pricing European options. ncbi.nlm.nih.gov
S. Lima, L. (2019). Nonlinear Stochastic Equation within an Itô Prescription for Modelling of Financial Market. ncbi.nlm.nih.gov
Wang, P. (2016). Application of stochastic differential equations to option pricing. [PDF]
El-Khatib, Y. (2006). A stochastic volatility model with jumps. [PDF]
Mohammed Alzughaibi, I. (2018). Topics in Stochastic Analysis and Applications to Finance. [PDF]
Mitra, S. (2009). Regime Switching Stochastic Volatility with Perturbation Based Option Pricing. [PDF]
Wand, T., Wiedemann, T., Harren, J., & Kamps, O. (2023). Estimating Stable Fixed Points and Langevin Potentials for Financial Dynamics. [PDF]
Janek, A., Kluge, T., Weron, R., & Wystup, U. (2010). FX Smile in the Heston Model. [PDF]
Di Persio, L. & Jovic, V. (2016). Jump Diffusion and {alpha}-Stable Techniques for the Markov Switching Approach to Financial Time Series. [PDF]
Cisana, E., Fermi, L., Montagna, G., & Nicrosini, O. (2007). A Comparative Study of Stochastic Volatility Models. [PDF]

Casas, I. & Gao, J. (2006). Econometric estimation in long-range dependent volatility models: Theory and practice. [PDF]
Franke, R. & Westerhoff, F. (2011). Structural Stochastic Volatility in Asset Pricing Dynamics: Estimation and Model Contest. [PDF]
Bertschinger, N., Mozzhorin, I., & Sinha, S. (2018). Reality-check for Econophysics: Likelihood-based fitting of physics-inspired market models to empirical data. [PDF]
Griffin, J. & F.J. Steel, M. (2008). Bayesian inference with stochastic volatility models using continuous superpositions of non-Gaussian Ornstein-Uhlenbeck processes. [PDF]
Jourdain, B. & Sbai, M. (2009). High order discretization schemes for stochastic volatility models. [PDF]
Kuchuk-Iatsenko, S. & Mishura, Y. (2015). Pricing the European call option in the model with stochastic volatility driven by Ornstein-Uhlenbeck process. Exact formulas. [PDF]
Schmitz Abe, K. (2008). Pricing exotic options using improved strong convergence. [PDF]
Hakala, J. (2019). Applied Machine Learning for Stochastic Local Volatility Calibration. ncbi.nlm.nih.gov
Xu, Y. (2014). Robust valuation and risk measurement under model uncertainty. [PDF]
Bhattacharyya, M. & Madhav R, S. (2012). A Comparison of VaR Estimation Procedures for Leptokurtic Equity Index Returns. [PDF]
Lin, M. & SenGupta, I. (2021). Analysis of optimal portfolio on finite and small time horizons for a stochastic volatility market model. [PDF]
Omidi Firouzi, H. & Luong, A. (2014). Optimal Portfolio Problem Using Entropic Value at Risk: When the Underlying Distribution is Non-Elliptical. [PDF]
Ramos-Pérez, E., J. Alonso-González, P., & J. Núñez-Velázquez, J. (2020). Forecasting volatility with a stacked model based on a hybridized Artificial Neural Network. [PDF]
1982- Hua, J. C. (2018). Studies on Dynamics of Financial Markets and Reacting Flows. [PDF]

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Chapter 6: Numerical Methods for Solving Nonlinear Differential Equations in Physics

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Abstract: Nonlinear differential equations are foundational in modeling diverse physical phenomena where analytical solutions are often unattainable. This paper presents an in-depth overview of numerical methods for solving nonlinear differential equations, with particular emphasis on their applications in physics. Key numerical techniques—such as the finite difference method, Runge-Kutta schemes, shooting method, and finite element method—are evaluated based on stability, convergence, and computational efficiency. These methods are critically important in simulating complex systems including nonlinear oscillations, turbulent fluid dynamics, and electromagnetic field interactions. Modern advancements, such as structure-preserving integrators and hybrid quantum-classical algorithms, are also examined for their potential in overcoming the limitations of classical numerical solvers. Case studies in classical mechanics and electromagnetism illustrate the versatility of these methods in real-world scientific problems. Special focus is given to the stability and convergence criteria essential for reliable simulations, as well as the challenges posed by chaotic systems where transient dynamics and sensitivity to initial conditions can impair numerical accuracy. The review concludes with an outlook on quantum solvers for nonlinear dynamics, highlighting their promise for next-generation computation in physics. This work offers a comprehensive resource for researchers and practitioners seeking robust and scalable numerical strategies for nonlinear differential problems in theoretical and applied physics.

Keywords: Nonlinear differential equations, Numerical methods, Runge-Kutta method, Finite element method, Chaos theory.

1 Introduction

Differential equations are fundamental to characterizing interactions and dependencies across variables and phenomena, providing a mathematical framework for solving engineering and science problems. Nonlinear ordinary differential equations (ODEs) appear in a wide range of situations, such as studies of biological molecules, including DNA and G protein-coupled receptors, game dynamics, and fluid dynamics. Many nonlinear systems do not have an exact, closed-form solution, and, thus, numerical methods are required to find approximate solutions to nonlinear differential problems. In some cases, differential equations can be recast into a variational optimization problem, and a numerical solution computed through the solution of this optimization problem (Hao et al., 2023). For systems where the spatial term is discretized and the solution is dictated by the initial condition, a new quantum computing approach has been developed to address nonlinear differential equations. Nonlinear differential equations frequently appear in physics, engineering, chemistry, biology, and economics. Numerical solutions are often challenging or intractable on classical computers, especially for complex systems such as turbulence. Due to the exponential state space of quantum computers and their potential quantum advantage, there is considerable interest in developing quantum algorithms for nonlinear dynamics. Existing approaches include hybrid quantum-classical schemes, where the problem is formulated as a minimization and solved partly on a quantum computer, and mean-field-based ansätze, which require extensive quantum resources not yet available. New quantum solvers are needed to efficiently integrate nonlinear dynamics on near-term hardware with scalable quantum advantage. One such approach transforms nonlinear differential equations into Fokker-Planck equations, which become master equations after spatial discretization. Although quantum solvers for linear ODEs exist, their implementation remains challenging. The proposed quantum solvers integrate the Fokker-Planck equation effectively on near-term hardware, providing the time-evolved distribution function that captures system dynamics and uncertainty. These methods have been demonstrated through numerical integration of prototype nonlinear systems (Tennie &Magri, 2024).

2. Importance of Numerical Methods in Physics

Several physical phenomena are modeled by nonlinear differential equations (Denis, 2020). The idea when integrating these equations numerically is that the theoretical methods used when solving linear problems can be generalized to nonlinear equations, even though the problem is no longer linear. For example, electrons oscillating in

classical plasmas; intense electromagnetic waves propagating in the atmosphere; or classical or quantum particles moving in time-dependent fields all are examples based on nonlinear differential equations that must be solved numerically. Many physical phenomena are governed by nonlinear differential equations that cannot be solved analytically. As a result it is desirable to develop analytical or numerical methods to deal with these types of equations. Useful numerical methods to solve nonlinear differential equations, such as the finite difference method, the Runge-Kutta method, the shooting method and the finite element method, have been discussed. The choice of method depends on the particular nonlinear differential equation representing the problem.

3. Overview of Numerical Techniques

Numerical techniques for solving nonlinear differential equations form an essential component of computational physics, as analytic solutions often prove intractable. Such methods are central to understanding phenomena as diverse as shock formation in fluid dynamics, pattern formation in biological systems, and the physics of galaxies (Hao et al., 2023). Among the most intensely studied nonlinear systems is the nonlinear Schrödinger equation, whose dynamical properties furnish benchmarks for remedying artifacts in computational implementations (Mulansky, 2013). Various numerical schemes exist, including the von Neumann-Richtmyer shock-capturing method, the MacCormack method, split-step Fourier, symplectic Runge-Kutta, and implicit Crank-Nicholson. Each method offers advantages tailored to different equations and computational environments. The von Neumann-Richtmyer scheme incorporates artificial viscosity to capture shock waves within compressible fluid flow without nonphysical oscillations. This explicit, second-order-accurate, Lagrangian-remap technique preserves monotonicity near shocks but introduces a discontinuous “wall heating” artifact when shocks align with grid directions. The MacCormack method, renowned for its simplicity and effectiveness, employs a predictor-corrector algorithm that computes tentative and corrected values for each timestep. Although second-order accurate and applicable to multiple spatial dimensions, it can produce dispersive oscillations near shocks when artificial viscosity is absent.

Split-step Fourier methods are widely used for nonlinear Schrödinger equations and related nonlinear wave problems. These approaches split the governing equations into linear and nonlinear components, solving the linear part through Fourier-space spectral methods and the nonlinear part in the primary spatial domain. Symplectic Runge-Kutta methods, including the widely applied second-order leapfrog scheme, are characterized

by Hamiltonian preservation. Their symplectic nature enhances stability and time-reversibility when well resolved. The inherently implicit Crank-Nicholson scheme can be adapted to nonlinear problems through modified differencing methods. It provides a conservation law for the discrete numerical formulation. Real-space implementation with iterative solvers proves more efficient than matrix inversion, especially when Fourier transforms do not diagonalize the problem. Each numerical technique thus offers distinct trade-offs between stability, accuracy, and computational cost, guiding the selection of methods for specific physical applications.

3.1. Finite Difference Method

The finite difference method provides an efficient approach to approximate nonlinear differential equations without requiring discretization in philosophy or the application of inverse operators (Qureshi et al., 2013). The basic idea involves approximating the derivatives present in the differential equation with finite difference formulas of an appropriate order of accuracy, while maintaining the right-hand side as the original function. This process transforms the nonlinear differential equation into a nonlinear algebraic system in terms of the nodal values of the approximate solution. Numerous finite difference formulas are commonly employed to replace derivatives. For instance, the forward difference formula for the first derivative at a given point is defined as: where is a small increment in the independent variable used for approximation purposes. The corresponding backward difference formula takes the form: Finally, the central difference formula for the first derivative, which does not belong to the Davenport-Stenger class, is expressed as:

When higher-order derivatives appear, they can be approximated by successively applying the differences or derived directly using Taylor series expansions (Imran et al., 2018). The choice requires a balance between computational resources and required accuracy. To determine the nodal values from the algebraic system, a variant of Newton's method customized for nonlinear difference equations is applied. Provided that the initial approximation is sufficiently close to the actual solution, this method achieving quadratic convergence. Extending the finite difference method to higher-dimensional problems involves discretizing the domain with a Cartesian mesh and applying the finite difference formulas to approximate the derivatives accordingly. This straightforward extension is well-known, although the resulting algebraic systems become substantially larger while maintaining a similar sparsity pattern.

3.2. Runge-Kutta Methods

In high-energy physics, the multi-loop expansions employed in perturbative calculations result in expressions containing a large number of linearly independent integrals, referred to as master integrals (MI). These MI satisfy a system of first-order differential equations in one of the external invariants, derived from integration by parts identities. While analytical solutions are available in particular cases, numerical techniques are required for their precise evaluation in general scenarios. The 4th-order Runge-Kutta method in the complex plane provides a robust means of advancing the solutions of such systems. The method ensures numerical stability and precision, particularly when the path is appropriately chosen to avoid proximity to branch points and singularities. The solution typically obtained by analytical methods through harmonic polylogarithms offers a reference for the numerical approach, which is also applicable to systems whose solutions lack a straightforward analytical form (Caffo et al., 2002).

The application of the numerical solution of ME using the Runge-Kutta method to the 2-loop sunrise MI with arbitrary masses demonstrates excellent agreement with the existing literature across various kinematic regimes. As a further check, comparisons have been carried out with existing results in the equal-mass case (Caffo, 2003). Success in this context underscores the method's reliability and straightforward generalization to more complex systems—attributes that are significant for handling the increasing complexity encountered at higher-loop orders.

3.3. Shooting Method

Nonlinear differential equations arise in many problems of theoretical physics, including astrophysics, cosmology, and theoretical mechanics. They describe essential aspects of nature and modelling them is an important scientific challenge. Since, in general, most nonlinear differential equations cannot be solved exactly, there is a need for efficient numerical schemes for accurately implementing approximate solutions. The shooting method, also called the shooting and matching method, consists of transforming a boundary value problem into a number of initial value problems (D. Baumann, 1976). The starting point for the shooting method is the trial solution to a system of first-order ordinary differential equations, where trial upper and lower values for the unknown initial condition are guessed between the limiting functions. A proposed new modification of the standard shooting method can be constructed by the shooting-

projection approach (M. Filipov et al., 2014). The method starts with a trial function that satisfies the boundary condition at the left point and uses the Euler method to construct a further approximation. Its application is based on finding an admissible function that satisfies both boundary conditions and a related transfer function. The method can then be systematically applied to a wide spectrum of boundary value problems, including cases where standard shooting or finite difference methods do not find a solution. For further details on extensions of the shooting method see the work of Scheiber (Scheiber, 2022).

3.4. Finite Element Method

A finite element method for solving nonlinear differential equations on a grid has been developed and tested. The method facilitates the computation of solutions of a high polynomial degree on a grid by interpolating both the value and derivatives of unknown variables. The two-dimensional lid-driven cavity is used as a test case. It is shown that increasing the polynomial degree has some advantages compared to increasing the number of grid points when solving this benchmark problem. The method yields results that agree well with previously published results for this test case (Tveit, 2014). Nonlinear problems are computationally demanding due to repeated reassemblage of finite element matrices and solving numerous linear systems. Simulations using P2 finite elements and the implicit Euler method to solve nonlinear differential equations have been conducted on an in-house solver and MATLAB's PDE toolbox. Mesh sizes contained approximately 7,600 nodes. Temperature evolution at the domain center was compared over time. Profiling reports focused on computation times in the solve function, with the implementation using a basic numerical scheme and classical Newton method. Optimizations included minimizing calls to sparse matrix functions by designing linear operators for matrix--vector and tensor--vector multiplications without explicit matrix assembly (Voet, 2022).

A nonlinear finite element method that accounts for material and geometric nonlinearity has been applied to the analysis of failure mechanics of composite materials under compressive load. The analysis requires a yield criterion, a hardening rule, and a flow rule, with material behaviour frequently modelled using a power hardening law. The maximum effective Von Mises stress evolves from the initial yield stress as plasticity develops. The primary output is the displacement vector as a function of the applied force, which is approximated through interpolation with shape functions. The

displacement field within an element is represented using shape functions, with the nodal displacements forming the basis of the approximation (Lycke Wind, 2013).

4. Stability and Convergence Analysis

Stability and convergence analysis focuses on the linear stability of explicit Runge-Kutta methods when applied to nonlinear ordinary differential equations with initial conditions. Assuming the initial point x_0 is zero and that the solution at this point is Lyapunov stable (Lyapunov stable at t_0), it can be shown that the numerical solutions produced by these methods will also be Lyapunov stable for sufficiently small step sizes h > 0. Because of the local Lipschitz continuity of the differential equation, the exact solution x(t, 0) remains within any prescribed -neighborhood of the origin for all t 9 t_0, provided > 0 is suitably small. The goal is to prove that the numerical solutions x_k(h, 0) will stay within this same -neighborhood for all time steps k 9 0, under appropriate constraints on h and k. The derivation proceeds under the premise of fixed, A-stable explicit Runge-Kutta methods (Jacob Steyer, 2016).

4.1. Stability Criteria

Numerical methods for solving ordinary differential equations (ODEs) typically approximate time derivative of a function at discrete points through finite differences. This process involves integral separation, Leesdorf inequalities, and related concepts. The stability criteria then obtained apply directly to the underlying ODEs, provided the step sizes are sufficiently small. The first transfer of stability results from numerical analysis to differential equations occurred in the early 1960s. Since then, numerous numerical stability methods have emerged. For instance, explicit methods exhibiting unconditional stability for parabolic equations have been identified. Connections between rate-induced tipping and nonautonomous bifurcations also offer relevant insights. Multistep methods function effectively as one-step methods, while difference methods address stiff ODEs. Time discretizations for initial value problems are analyzed in terms of stability and accuracy, and contractive methods cater to stiff differential equations. Stability states, such as those characterized by exponential dichotomy, are essential considerations. Necessary conditions for B-stability provide further guidance, and step-size selection strategies leverage Lyapunov exponent theory. Linear stability theory for general methods, including one-step initial value solvers, is grounded in Lyapunov exponents. Attractive invariant manifolds for maps exhibit existence,

smoothness, and continuous dependence features. Additional perspectives from numerical linear algebra—covering QR decomposition, error analysis, and stability—contribute to the overall framework. Approaches for systems of ODEs involve rational Runge-Kutta methods, while nonlinear A-stability and related properties inform method selection (Jacob Steyer, 2016).

4.2. Convergence Theorems

(J. V. Parente, 1961) describes various convergent numerical procedures for obtaining solutions of ordinary and partial differential equations. These processes facilitate the study of nonlinear characteristics of the problems, making them particularly important when classical analytical techniques are inadequate. The numerical methods also help in establishing theorems of existence, uniqueness, and stability for solutions of such equations. The convergence theory consists of formulating conjectures regarding the limiting value of the numerical solution, establishing preliminary estimates, and then constructing a formal proof for each technique. The convergence theorems provide the necessary foundation for a meaningful discussion of error criteria. From the theoretical standpoint, Picard's successive approximation process and Cauchy's Euler method receive special attention; their convergent solutions are constructed for general linear differential equations of the first order.

5. Applications in Classical Mechanics

The concept of non-linear differential equations appears frequently in various fields of science, including classical mechanics, the study of biological systems and population dynamics. The Duffing equation, Van der Pol equation and the more generalized Duffing-Van der Pol equation illustrate the wide range of applications of non-linear differential equations in science. Distinct from linear equations, solutions to these equations are more difficult to obtain and less well-understood. Numerical techniques, additional analytical methods and experimental measurements that together form a control mechanism for the understanding and solutions of such equations does not appear to be well-reported. That is to say, a mechanism to explore the solution to these non-linear differential equations and compare the numerical techniques against analytical methods and experimental measurements is lacking, particularly for an open distributed control system that requires a virtual organising principle.

5.1. Nonlinear Oscillations

A large share of nonlinear problems arising in science and engineering contain at least one nonlinear oscillator as their fundamental building block. Exact solutions to these equations are typically unavailable. Perturbation schemes can be used, but their applicability is limited for many problems of practical importance. The Galerkin method, on the other hand, has the potential to solve nonlinear equations beyond the range of amplitude of other procedures. (H. S. Salas, 2022).

5.2. Chaos Theory

Chaos theory concerns the study of unpredictable and irregular phenomena occurring in deterministic systems. Recently, electoral forecasting models, seasonal epidemics, and tourism systems have attracted considerable attention because of their chaotic behaviour; the phenomenon of transient chaos has also been explored in many systems, including hydrodynamics, electronic circuits, power grids, population dynamics, ecology, economics, neural networks, and medical applications. The mathematical models involved are usually expressed in the form of nonlinear differential equations; direct integration is therefore almost always impossible and suitable numerical methods are needed. Several numerical studies have subsequently reported physically unacceptable solutions exhibiting chaotic behaviour, and researchers typically interpret the behaviour as transient chaos (Marszalek, 2022). It is thus essential to assess the reliability of the numerical integration of chaotic systems in the context of transient chaos (Goodarzi et al., 2023). A chaotic system is extremely sensitive to initial conditions; as such, a minute error can eventually amplify in an uncontrolled manner. Numerical integration generally accumulates significant round-off and/or truncation errors during the entire integration process; phase space trajectories or orbit analysis are thereafter not reliable. It is however fortunate that the odd behaviour of chaotic systems is often studied from a statistical viewpoint rather than on an individual trajectory basis. In this regard, numerical errors will not influence the property of chaos if it remains controlled. This assumption underpins the use of unreliable numerical methods to study chaotic systems over the past four decades; it must nevertheless be modified to account for transient dynamics.

6. Applications in Electromagnetism

The effectiveness of the Bubnov–Galerkin method in situations involving nonlinear partial differential equations coupled with inhomogeneous boundary conditions is crucial when addressing electromagnetic problems, especially in magnetics. Magnetic configurations often present nontrivial Neumann-type boundary conditions, while in stationary problems, the solutions must also satisfy the nonlinear differential equation and the boundary constraints. Although the method uses global approximation, the solution can be computed accurately enough to keep the method efficient and a valuable tool. One-dimensional, one-particle, one-field, one-interaction ("1D1P1F1I Models") models can be employed to study complicated phenomena such as radiation reaction, braking radiation, and friction in electrodynamics (A. Choroszavin, 2003). These simplified, exactly solvable models, constructed using finite-rank perturbations, provide insight into the nature of linear friction encountered by non-relativistic oscillating particles and address questions related to effective equations of motion involving linear friction.

6.1. Maxwell's Equations

Maxwell's equations constitute the fundamental framework of electromagnetism, providing a comprehensive description of the propagation and scattering of electromagnetic waves. They underpin a wide range of applications including wireless engineering, antennas, microwave circuits, radio-frequency devices, aircraft radar, integrated optical circuits, waveguides, and interferometers. The three-dimensional form of Maxwell's equations in an isotropic, homogeneous, and lossless medium relates the electric field E and the magnetic field H through the equations

$$\partial E/\partial t = \varepsilon^{-1}\nabla\times H,\ \partial H/\partial t = -\mu^{-1}\nabla\times E,$$

where ε and μ denote the permittivity and the permeability of the medium, respectively. When the initial data are suitably smooth and comply with the associated divergence conditions, Maxwell's equations admit a unique smooth solution for all times. Given their significant role in electromagnetism, the equations have been the subject of investigation for more than 150 years. The most recent developments concern numerical analysis and the design of efficient numerical schemes.

Various numerical techniques have been proposed to approximate the three-dimensional Maxwell's equations. The finite-difference time domain (FDTD) method is a well-known approach, but it generally requires a very small time step to maintain stability. Improvements such as the alternating direction implicit (ADI) technique have been suggested to enhance efficiency. Time or space discretizations based on finite-element methods, finite-volume time-domain methods, and discontinuous Galerkin methods have also been employed. With respect to time integration, explicit symplectic Runge–Kutta methods, splitting methods, exponential integrators, and spectral deferred correction methods have been explored. The recent trend in this field is to develop structure-preserving algorithms, which can exactly or nearly preserve some physical properties of the Maxwell's equations at the discrete level. These conservation laws include the energy, the momentum, the symplecticity, and the divergence-free fields. Structure-preserving methods possess more reliable long-time behavior and can yield more convincing numerical results than classical schemes (Wang & Jiang, 2022).

6.2. Wave Propagation

Numerical modeling of nonlinear waves has many applications, including underwater acoustics, medical ultrasound, and sheared flow instabilities. The nonlinear behavior at moderate amplitudes often results in the generation of harmonics that greatly influence the propagation. If the wave frequency is close to a resonance or absorption peak, dispersive effects also become important and must be taken into account. Some mechanisms also lead to frequency power law attenuations that can be modeled using multiple relaxation processes. Although the Constitutive law for viscous fluids leads to a nonlinear hyperbolic set of equations, disparate length and time scales normally prevent the use of direct numerical solvers. Models such as the Kuznetsov are typically implemented instead, but are restricted to second order accuracy. The Fowler model relies on fractional derivatives that are expensive to compute and do not lead themselves to finite difference formulations. This chapter is concerned with the numerical modeling of nonlinear dispersive waves described by the Westervelt equation augmented by multiple relaxation processes. A finite difference algorithm employing a fourth-order scheme for the temporal derivatives and a sixth-order scheme for the spatial derivatives is presented. Relaxation variables enable the temporal integration of the equations to be performed exclusively with finite difference expressions, avoiding convolutions whose computational cost would be prohibitive. Outgoing waves are eliminated with a well-known absorbing layer at the domain boundaries. The algorithm is validated against analytical solutions with different attenuation scaling power-laws, exact traveling wave solutions, and spatially diffused plane waves. The numerical strategy is then applied to

the simulation of harmonics generated by a high-amplitude Bessel beam, where the relaxation processes lead to self-focusing of the third harmonic, a phenomenon of interest in medical ultrasound (Pinton, 2021).

The nonlinear attenuating wave equation is general and can be used in many situations involving nonlinear wave propagation with frequency power law attenuation and dispersion. The fact that its solutions can be computed with high order finite-differences on a staggered grid in both two and three dimensions broadens its range of applications even further. A caveat however must be raised concerning the amplitude of the characteristic velocities of the perturbation (fluid or solid). To keep the finite difference framework stable for staggered grid, the particle velocity must remain less than the sound speed of the medium. Practical nonlinear phenomena, such as shock formation and particle velocity corrections from the nonlinear coefficients, must fall within this range if the simulations are to be meaningful. Otherwise, alternative numerical scheme such as shock-capturing may be required.

7. Applications in Fluid Dynamics

The method was applied to a classical benchmark problem in computational fluid dynamics, the lid-driven cavity, revealing that solutions as functions of position converge as the polynomial degree of the approximation is increased. Hence, the fineness of the grid is not the sole way to increase accuracy. Increasing the polynomial degree has some advantages compared to increasing the number of grid points for this problem, where the flow tends to piecewise smooth steady-state configurations, and the current method yields results agreeing well with previously published data. Nonlinear differential equations occur frequently in fluid dynamics, and the approaches presented here seem promising for further exploration in this area because they do not require the introduction of additional unknown variables or artificial equations during discretization (Tveit, 2014).

7.1. Navier-Stokes Equations

The Navier-Stokes equations are the basis of fluid mechanics and describe the motion of fluids for many practical problems. The numerical solution of the Navier–Stokes equations is fundamental in fluid dynamics. Recently, (Liu et al., 2015) developed a

numerical solver for these equations using Python, implementing preconditioned iterative methods to enhance computational efficiency. Performance comparisons with Matlab implementations indicate that the Python solver offers a free and effective alternative for solving the Navier–Stokes equations, marking the first exploration of preconditioning techniques in this environment. Additionally, (V. Rukavishnikov, 2021) addressed the numerical solution of stationary nonlinear Navier–Stokes equations within a polygonal domain featuring a reentrant corner—an angle exceeding π. Building on the concept of the R_{u}-generalized solution and employing auxiliary weight functions, the proposed method achieves first-order convergence regardless of the reentrant corner's magnitude. The R_{u}-generalized solution is rigorously established as unique in appropriate weighted spaces, attaining enhanced regularity under additional conditions. Numerical experiments spanning various parameter regimes demonstrate superior performance relative to classical approaches. The investigation encompasses both the convective and rotational forms of the Navier–Stokes equations, which couple the velocity vector and pressure fields subject to specified boundary conditions along the domain perimeter.

7.2. Turbulence Modeling

The RANS model is used near solid surfaces to obtain a high resolution, and the LES model is used far away from walls to save computational resources and maintain high accuracy. A two-fluid turbulence model describes turbulent flow characteristics and evolution of turbulence quantities by the dynamics of two fluids, leading to a closed system of equations capable of simulating complex anisotropic turbulent flows. The two-fluid turbulence model has been applied to flow around a square cylinder, achieving results that closely match experimental data. Numerical implementations have primarily relied on proprietary codes, but software packages such as ANSYS Fluent and COMSOL Multiphysics currently support turbulence modeling. ANSYS Fluent, based on the control volume method, handles fluid flow, heat transfer, and related phenomena. COMSOL Multiphysics employs the Finite Element Method to model heat transfer, fluid flow, electromagnetics, and chemical reactions, among others. Its multiphysics coupling, geometric flexibility, and customization capabilities—with tools for defining and solving new equation systems, including custom PDEs—make it suitable for implementing a two-fluid turbulence model. These features enable integration of a two-fluid turbulence model through COMSOL's Custom PDE interface and facilitate comparison with the SST turbulence model and experimental data from NASA's TMR website (M. Malikov et al., 2024).

8. Software and Computational Tools

Several large-scale software packages are available for solving nonlinear partial differential equations (PDEs) related to problems in solid and fluid physics. The commercial package COMSOL Multiphysics is popular, and there are open-source alternatives as well. One such code is fipdes, an open-source dataset of finite difference Python codes designed for computing steady-state solutions of a variety of nonlinear PDEs in 1D. The code solves equations related to solid and fluid physics using nonlinear algebraic solvers based on the Picard iteration method, which is readily generalizable to multiple coupled nonlinear PDEs. PDEs often have several steady-state solutions, of which only a few are stable. Unstable ones usually evolve towards a stable solution. To observe such evolution, fipdes facilitates solution of the related time-dependent PDEs via explicit integration schemes, including Euler, leap-frog, and Runge-Kutta methods. Visualization is also assisted within fipdes. Standard models are provided with appropriate dimensionless numbers, which reduces effort in scaling. The underlying framework consists of abstract classes from which specific nonlinear PDEs can be developed. Adding new PDEs involves defining coefficients and residuals in the respective files, as documented in Section 9.1.

9.1. MATLAB

MATLAB, a high-level programming platform and interactive environment, is widely employed in the numerical investigation of nonlinear differential equations. Its predefined functions, particularly PDEPE (suitable for parabolic-elliptic differential equations) and ODE45 (a variable-step fourth/fifth order Runge-Kutta method for ordinary differential equations), enable the efficient and rapid acquisition of high-precision numerical solutions (Qureshi et al., 2013). The PDEPE function is capable of generating solutions across specific spatial intervals, while ODE45 provides results over desired time spans. MATLAB's built-in capabilities include the numerical integration of differential equations, the generation of symbolic and numerical solutions for complex algebraic equations, the ability to plot solutions, and the functionality to save data in TXT and Excel file formats. Together, these features facilitate the streamlined numerical analysis of nonlinear differential systems.

9.2. Python Libraries

The JiTCODE, JiTCDDE, and JiTCSDE Python modules facilitate the numerical integration of ordinary, delay, or stochastic differential equations. The user specifies the derivative once and symbolically; the module generates optimized code via just-in-time compilation, yielding efficient integration from an interpreter analysing a higher-level language. The modules are particularly suited for large systems of differential equations—common in complex network dynamics—and automatically estimate Lyapunov exponents (Ansmann, 2017). An additional Python class solves Schrödinger equations in one or more space dimensions, relying on general numerical-PDE classes and sparse Scipy routines (Noreen &Olaussen, 2015).

Python is a high-level, general-purpose programming language widely used for scientific computing. Packages like Numpy, Scipy, Pygsl, and Cython achieve high performance by integrating precompiled C, C++, and Fortran libraries. Numpy provides efficient array operations; Scipy includes modules for fast Fourier transforms and ordinary differential-equation solvers. Pygsl offers an interface to the GNU Scientific Library (GSL), enabling straightforward access to many algorithms. Cython adds static C-type declarations and ability to call C and C++ functions directly, combining Python's rapid-development advantages with the speed of low-level code. Visualization tools range from Matplotlib for 2D plotting to Mayavi for 3D visualization. Performance-critical sections can be implemented in C/C++ or Fortran with seamless integration through F2PY and Weave scripting (Fan et al., 2011).

9.3. C++ Implementations

Fortran implementations of numerical methods for ordinary differential equations (ODEs) are usually present because it is an easy task to implement fast routines using simple language extensions, such as complex variables or Campbell– Hausdorff formulas. However, using a programming language such as C++ makes it possible to reuse the modules with a very small overhead in computing time and to implement a larger variety of problems. The code Hamevol1.0, based on a fifth-order semi-implicit Runge–Kutta algorithm, has been implemented in C++ on an event-oriented basis for problems in physics such as matter-enhanced neutrino oscillations (Aliani et al., 2003). C++ programs computing the solutions to ordinary differential equations (ODEs) have been developed that construct an explicit iterative algorithm and compare it with two nonstandard finite difference schemes. The C++ code produces the values of the solution at points of a uniform grid and uses the explicit iterative method (EIM) (Qureshi et al., 2013). A C++ program implements a finite element method for nonlinear differential

equations on a grid that interpolates unknown variables together with their derivatives. Compared with increasing the number of grid points, increasing the polynomial degree on the grid has clear advantages, as demonstrated for the two-dimensional lid-driven cavity problem (Tveit, 2014).

10. Future Directions in Research

Numerical methods remain essential for studying nonlinear systems where analytical solutions are unavailable. New computational platforms such as quantum computing and machine learning offer heuristic approaches that may reduce or eliminate the need to approximate or linearize underlying physics. Promising quantum schemes that implement these differential equations with linear complexity were recently developed (Tennie &Magri, 2024). Ongoing improvements in algorithms, combined with experimental technology, will determine each prospective approach's viability, eventually furnishing new tools to tackle ultralarge nonlinear problems (Ismail, 2016).

10.1. Machine Learning Integration

A growing number of data-driven approaches to accelerate the solution of differential equations are available (Mishra, 2018). Neural networks are often used to develop fast numerical schemes that never violate underlying constraints such as conservative or maximum principles. Hybrid methods have been developed that combine traditional time stepping schemes with a collection of neural networks to predict numerical solutions (Viswanath et al., 2023). Variational data assimilation procedures based on neural network discretizations of PDEs and a Gauss-Newton method exist to solve the associated variational problems efficiently (Hao et al., 2023).

10.2. High-Performance Computing

High-performance computing platforms have gained great importance in the numerical integration of nonlinear differential equations (NDEs). Yet, selecting the most appropriate reference implementation for the solution of a large number of systems with small dimensions remains an open issue.

The term “high-performance computing” commonly refers to equipment capable of delivering tens of teraflops to several petaflops and beyond (Bremer, 2014). Parallel numerical algorithms and multi-threading have long been available for such architectures. However, the introduction of advanced graphics processing units (GPUs) capable of general-purpose computations represented a qualitative leap, enabling the acceleration of many tasks by as much as two orders of magnitude for a significantly lower price. Within the next few years, GPUs became widely accessible to common users, and several open-source programming platforms, including CUDA, OpenCL, and OpenACC, emerged. Numerous benchmarks and test cases have since been published for the solution of very large systems. Among the most widely used program packages featuring almost complete support for GPUs, three have been reserved exclusively for numerical integration of differential equations:

11. Conclusion

Numerical methods play an essential role in various physics applications, including modeling of chaotic rotation, formation of solitary vortices, moving cracks in materials, hydrogenic ionization, and simulations of atom-laser interactions. Developing accurate and efficient tools to solve nonlinear differential equations associated with such applications is of fundamental importance. Machine learning–based approaches, particularly neural network–based discretizations, have emerged as powerful tools for numerically solving nonlinear differential equations. These approaches parameterize the solution space by a set of neural networks, thereby reducing the problem to nonlinear optimization. While sophisticated training algorithms have been developed to solve the resulting optimization problem, effective strategies for applying machine learning–based methods in scientific computing remain to be fully established. The Gauss-Newton method is an efficient nonlinear least-squares algorithm that has been extensively applied to nonlinear data-fitting problems. Adapting the Gauss-Newton method to solve the nonlinear optimization problems arising in neural network discretizations can enhance convergence efficiency. By formulating the problem in a variational setting and developing a Gauss-Newton iterative scheme, it is possible to compute numerical solutions with superlinear convergence properties. This approach offers a promising direction for leveraging machine learning techniques in scientific and engineering applications of nonlinear differential equations (Hao et al., 2023).

References

Hao, W., Hong, Q., & Jin, X. (2023). Gauss Newton method for solving variational problems of PDEs with neural network discretizaitons.

Tennie, F. &Magri, L. (2024). Solving nonlinear differential equations on Quantum Computers: A Fokker-Planck approach.

Denis, B. (2020). An Overview of Numerical and Analytical Methods for solving Ordinary Differential Equations.

Mulansky, M. (2013). Simulating DNLS models.

Qureshi, S., Memon, Z. N., Ali Shaikh, A., & Saleem Chandio, M. (2013). On the Construction and Comparison of an Explicit Iterative Algorithm with Nonstandard Finite Difference Schemes.

Imran, M., Agusni, A., Karma, A., & Putra, S. (2018). TWO STEP METHOD WITHOUT EMPLOYING DERIVATIVES FOR SOLVING A NONLINEAR EQUATION.

Caffo, M., Czyz, H., &Remiddi, E. (2002). Numerical evaluation of master integrals from differential equations.

Caffo, M. (2003). Numerical evaluation of some master integrals for the 2-loop general massive self-mass from differential equations.

D. Baumann, J. (1976). Shooting Method for Two-Point Boundary Value Problems.

M. Filipov, S., D. Gospodinov, I., &Farago, I. (2014). Shooting-Projection Method for Two-Point Boundary Value Problems.

Scheiber, E. (2022). Adjoint System in the Shooting Method to Solve Boundary Value Problems.

Tveit, J. (2014). A Numerical Approach to Solving Nonlinear Differential Equations on a Grid with Potential Applicability to Computational Fluid Dynamics.

Voet, Y. (2022). On the fast assemblage of finite element matrices with application to nonlinear heat transfer problems.

Lycke Wind, J. (2013). Composite materials in compression.

Jacob Steyer, A. (2016). A Lyapunov exponent based stability theory for ordinary differential equation initial value problem solvers.

J. V. Parente, P. (1961). Convergent processes in numerical analysis.

H. S. Salas, A. (2022). The Galerkin Method for Solving Strongly Nonlinear Oscillators. ncbi.nlm.nih.gov

Marszalek, W. (2022). On Physically Unacceptable Numerical Solutions Yielding Strong Chaotic Signals. ncbi.nlm.nih.gov

Goodarzi, A., Rahimi, M., Valizadeh, M. J., &Ghanbarnejad, F. (2023). Reliability of Numerical Solutions in Transient Chaos.

A. Choroszavin, S. (2003). 1D Particle, 1D Field, 1D Interaction. Simple Exactly Solvable Models based on Finite Rank Perturbations Methods. III. Linear Friction as Radiation Reaction.

Wang, B. & Jiang, Y. (2022). Time exponential integrator Fourier pseudospectral methods with high accuracy and multiple conservation laws for three-dimensional Maxwell's equations.

Pinton, G. (2021). A fullwave model of the nonlinear wave equation with multiple relaxations and relaxing perfectly matched layers for high-order numerical finite-difference solutions.

Liu, J., Wu, L., & Fang, X. (2015). Using Python to Solve the Navier-Stokes Equations - Applications in the Preconditioned Iterative Methods.

V. Rukavishnikov, A. (2021). New approach for solving stationary nonlinear Navier-Stokes equations in non-convex domain.

M. Malikov, Z., E. Madaliev, M., L. Chernyshev, S., & A. Ionov, A. (2024). Validation of a two-fluid turbulence model in comsol multiphysics for the problem of flow around aerodynamic profiles. ncbi.nlm.nih.gov

Arnold, A. &Körner, J. (2024). WKB-based third order method for the highly oscillatory 1D stationary Schrodinger equation.

Noreen, A. &Olaussen, K. (2015). A Python Class for Higher-Dimensional Schrodinger Equations.

Ansmann, G. (2017). Efficiently and easily integrating differential equations with JiTCODE, JiTCDDE, and JiTCSDE.

Fan, W., Xu, Y., Chen, B., & Ye, Q. (2011). Solve the Master Equation by Python-An Introduction to the Python Computing Environment.

Aliani, P., Antonelli, V., Picariello, M., & Torrente-Lujan, E. (2003). Hamevol1.0: a C++ code for differential equations based on Runge-Kutta algorithm. An application to matter enhanced neutrino oscillation.

V. Ruy, D. (2014). A method for solving nonlinear differential equations: an application to $lambdaphi^4$ model.

Adamec, L. (1997). Kinetical systems.

M. Moatimid, G. & S. Amer, T. (2022). Analytical solution for the motion of a pendulum with rolling wheel: stability analysis. ncbi.nlm.nih.gov

Singh, I., Arun, P., & Lima, F. (2018). Fourier analysis of nonlinear pendulum oscillations.

B. Wilson, J. (2010). Numerical approximations to the Boussinesq equations.

Patil, A. (2016). A Modification and Application of Parametric Continuation Method to Variety of Nonlinear Boundary Value Problems in Applied Mechanics.

V. Permyakova, E. & S. Goldobin, D. (2022). High-Order Schemes of Exponential Time Differencing for Stiff Systems with Nondiagonal Linear Part.

Noreen, A. &Olaussen, K. (2012). High precision series solution of differential equations: Ordinary and regular singular point of second order ODEs.

K. Leyton, S. & J. Osborne, T. (2008). A quantum algorithm to solve nonlinear differential equations.

C. Yee, H., K. Sweby, P., & F. Griffiths, D. (1991). Dynamical Approach Study of Spurious Steady-State Numerical Solutions of Nonlinear Differential Equations. I. The Dynamics of Time Discretization and Its Implications for Algorithm Development in Computational Fluid Dynamics.

Ismail, F. (2016). Exploring efficient: numerical methods for differential equations.

Mishra, S. (2018). A machine learning framework for data driven acceleration of computations of differential equations.

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Chapter 7: Cybersecurity Threat Prediction Models Using Machine Learning and Mathematics

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Abstract: The rapid evolution of cyber threats has created an urgent need for advanced predictive systems capable of safeguarding digital infrastructure. This paper explores the integration of machine learning (ML) and mathematical models for cybersecurity threat prediction, focusing on proactive defense mechanisms against increasingly complex attacks. Machine learning techniques, including supervised, unsupervised, and hybrid models, enable systems to detect anomalies, classify malware, and predict attackers based on prior behaviors and contextual patterns. These approaches are significantly enhanced by robust feature engineering, statistical analysis, and probabilistic modeling, which improve detection precision and adaptability in dynamic cyber environments. Mathematical foundations such as probability theory, statistical inference, and optimization models play a critical role in threat modeling, allowing systems to anticipate intrusions and assess vulnerabilities. The integration of anomaly detection, behavioural analysis, and intelligent decision systems strengthens predictive accuracy and reduces false positives. Case studies in finance and healthcare demonstrate real-world applicability, revealing how ML-powered models anticipate ransomware, phishing, and data breaches. Despite progress, challenges persist in the form of imbalanced datasets, adversarial attacks, and biases in ML models, requiring enhanced privacy-preserving mechanisms and fairness-aware algorithms. The future of cybersecurity prediction lies in hybrid AI architectures, graph-based modeling, and deep learning frameworks that offer scalable, interpretable, and accurate threat forecasts. This research underscores the transformative potential of combining ML and mathematics in predicting, preventing, and mitigating cyber threats—paving the way for intelligent, responsive, and adaptive cybersecurity ecosystems.

Keywords: Cybersecurity Threat Prediction, Machine Learning, Mathematical Modeling, Anomaly Detection, Adversarial Attacks.

1 Introduction

1.1 Background

Cybersecurity threats are attacks on computer information or networks that attempt to gain unauthorized access, disrupt system operation or networks, and/or destroy information (Bilen & Bedri Özer, 2021). Effectively predicting cyber-attacks can significantly mitigate risks and losses during an attack.

Cybersecurity threats pose risks to individuals, governments, and organizations and can destroy valuable data. An outbreak of malware can result in billions of dollars lost due to data breach, operational disruption, loss of competitive advantage, remediation, and damaged reputation and relationships with customers. The FBI estimates financial losses ranging from $200 to $400 million per year (Martin et al., 2019). Cyber-attacks are dynamic and ever evolving, adapting to environmental changes; they expose users to multifaceted risks and unknown threats and attackers.

In a given cyberspace, there may be various attacks, attackers, targets, behaviors, and consequences. Attackers may join forces to carry out an attack; some may wait for an opportune time or specific environmental changes; still others may employ deception and camouflage to evade detection. An attack may evolve into multiple other attacks targeting a wider scope of victims.

Since cyber-attacks are organized, strategic, and well planned, the ability to identify and predict future attacks and attackers is crucial in securing cyberspace.

2. Overview of Cybersecurity Threats

Cyber-attacks pose substantial risk and inflict devastating losses on individuals, enterprises, and governments worldwide. These attacks encompass a spectrum of harmful activities such as malware dissemination, data theft, denial-of-service incidents, and unauthorized access to IT infrastructure. The number and scale of such incidents are rising at an alarming rate globally, heightening the demand for sophisticated security solutions. Identifying and mitigating high-risk threats therefore constitutes a critical challenge for cybersecurity experts.

Cyber-crime unfolds in a highly dynamic environment, with rapid technological advancements enabling adversaries to employ increasingly complex, diversified, and effective attack methods. These attacks often generate substantial amounts of log data, providing valuable behavioral information about attackers. Proper analysis and interpretation of such data are essential to understanding, controlling, and mitigating cyber threats.

3. The Role of Machine Learning in Cybersecurity

Machine learning methods are widely used in various areas of computer security. Intrusion detection systems use classifiers as anomaly-detectors or in signature-based mode to distinguish between normal and abnormal network traffic. Malware detection techniques benefit from the identification of malicious activity across communication channels to endpoints. Machine learning is investigated to improve detection efficacy on elusive and unknown malware. Applications include prediction of malicious web attacks, spam filtering and phishing analysis. User behavior analytics analyzed by machine learning techniques identify frauds and insider threats by detecting anomalies in activity patterns. Models require domain knowledge to determine fraudulent transactions, classify fraud types, or detect outliers in business processes. Surveying a broad spectrum of machine-learning approaches to cyber-attack projection, prediction and forecasting reveals the evolution of techniques such as neural networks, support vector machines, and data mining for intrusion prediction and threat analysis. Support vector machines proved suitable for the prediction of very specific attacks (Ibitoye et al., 2019) (Martin et al., 2019).

3.1. Types of Machine Learning Algorithms

Machine learning, emphasizing computer systems that learn from data, has enhanced cybersecurity threat prediction where inadequate or inaccurate predictions can lead to data and privacy loss. The most common malware types include Trojan, Worms, and Viruses. Machine learning can be classified into three types: supervised learning, unsupervised learning, and reinforcement learning, which are generally the most commonly used methods (Martin et al., 2019).

Washroom selection is a complex task involving spatial awareness, memory retrieval, and value-based decision-making. Supported by evidence that value accumulation guides decisions and that brain systems involved in estimating decision values influence choice, studies have aimed to understand the mental processes underlying this daily task. Machine learning builds mathematical models based on sample data, known as training data, to make predictions or decisions without explicit instructions.

The most common malware types comprise Trojan, Worms, and Viruses. Machine learning, or the study of computer systems that can learn from data, provides computers with the ability to learn algorithms and models without explicit instructions. Machine learning systems are classified into three types: supervised learning, unsupervised learning, and reinforcement learning, with the first type generally considered the most widely used.

3.2. Benefits of Machine Learning in Threat Detection

Smart infrastructures depend heavily on machine learning for vital components such as threat detection and response and anomaly detection in distributed, real-time

environments (Schmitt, 2023). The task requires a deep understanding of applied architectures, algorithms, methods, and tools, as well as the operation of systems under attack; the overall objective is to identify and protect the infrastructure from anomalies at various stages of an attack. The capability of intelligence-supported algorithms to analyze the entire context helps detect these capabilities rapidly and effectively.

Machine learning and intelligent system design have become game changers in numerous fields and have gained considerable attention in cyber security because of their unique ability to quantitatively assess risk and improve detection and response tasks. These methods present many opportunities for providing additional insight into and streamlining anomaly detection in complex, multi-technology systems (M. Devine & D. Bastian, 2019). Machine learning-based malware classification, for example, characterizes malware based on patterns within the data. Toolsets developed to address the problem apply multiple learning algorithms that use the training data to infer future classifications. The capacity to decode complex systems through data science also serves to facilitate the exploitation of these systems, allowing adversaries to more efficiently target vulnerabilities. Such attacks can rapidly overwhelm an organization's ability to detect and respond, motivating the need for effective models to understand, detect, and attribute such attacks.

The specific impact of the attack varies by the scale and distribution of the data available for training. If the overall dataset is too small, distributed attacks prevent any single system from gaining sufficient scale to detect the threat. If the dataset is too large, end nodes may never see a sufficient number of these attacks to recognize them as threats. Various applications of machine learning further improve these detection capabilities. Although many systems begin with signature matching, the exponential growth in variants and tools has motivated the adoption of machine learning techniques. As such, the ability to identify malware directly through classification represents a specific case of threat detection with a similar set of signatures, constraints, and challenges.

These capabilities enable users and organizations to make rapidly and empirically informed security decisions and efficiently address root causes of breaches to prevent future damage and loss. Machine learning thus provides the opportunity to analyze greater volumes of data and identify patterns and indicators that signify a threat or intrusion.

Anomaly-based detection algorithms that utilize machine learning can accurately detect malicious activities with minimal latency, helping to mitigate risks before losses occur. Such algorithms represent the most advanced security approach. This heightened approach is crucial, as traditional security methodologies operate reactively and depend on a known intrusion, whereas anomaly-based detection algorithms possess predictive capabilities and manage unknown or zero-day attacks.

4. Mathematical Foundations of Threat Prediction Models

Mathematical methods for cybersecurity are relevant to threats, intrusion-detection systems, risk and vulnerability, mitigation, and the optimal allocation of defensive resources. Modeling and predicting cybersecurity threats are key aspects of the protection of information systems. Reliable threat models help to optimize the allocation of defensive resources and to anticipate and devise risk-management policies such as insurance contracts. Threat modeling is generally divided into scenario-driven and score-based approaches. Scenario-driven models primarily concern threats from which a loss is expected. Many different approaches have been implemented in this context, notably the use of linear optimization to evaluate the likelihood of an attack (Martin et al., 2019). Score-based approaches, instead, assign worst-case losses to categories of assets; these are weighted by the capabilities and intents of the adversaries, resulting in a final score used to rank the threats.

4.1. Statistical Methods

Statistical models constitute a foundational approach in predicting cyber-threats. They are instrumental in network-based detection at the bin-time, or packet level, facilitating the characterization of extensive intrusions where signature-based mechanisms may be ineffective. Statistical techniques underpin pre-emptive intrusion-detection frameworks that prioritize malicious packet flows and assist in assessing the physical impact of cybersecurity breaches, particularly in industrial-control processes and networked infrastructures. Techniques such as Bayesian networks and Kalman filtering facilitate the correlation of alerts and the reconstruction of missing information during protracted attack sequences. Moreover, Hidden Markov Models, calibrated with attack-optimized alerts, enable the probabilistic forecasting of intrusions. Robust statistical-forecasting methodologies provide early-warning capabilities regarding cyberattacks, thereby supporting timely decision-making in resource management and critical-asset protection (Martin et al., 2019).

4.2. Probability Theory

Probability theory plays a fundamental role in predicting the behavior of complex systems and processes subjected to uncertainty. It builds upon the concept of random experiments and operates on uncertain processes. Applications of probability theory extend across various domains, including cybersecurity, where it can be used, for example, to evaluate the probability of selecting a specific card from a deck.

As an axiomatic theory, probability can be defined by considering an experiment and the space S of all possible outcomes. In many cases, the experiment consists of selecting an outcome from the set or space S, with the probability P(E) of each outcome established as a value within the interval [0, 1]. Moreover, if the set of events E1, E2,..., Ek in the

space S are mutually exclusive and exhaustive, their combined probabilities sum to one. For instance, when throwing a single die, the sample space is S = {1, 2, 3, 4, 5, 6}, and the probability of any individual outcome—such as the die landing with the face marked 3 upwards—is of interest.

5. Data Collection and Preprocessing

The data required to build a prediction model for identifying attackers or attack methods must be collected from various sources. Three important types of data are needed: information about the attacks themselves, details about the attackers, and characteristics of the victims. Such datasets can be obtained from different providers, but are often missing one or more of these crucial components. The choice of the source depends on the research area and the specific focus of the study. When only attack information is available, a broader analysis encompassing all types of attack data collected might be more beneficial. Predicting the type of attack itself is a useful application in these circumstances (Bilen & Bedri Özer, 2021).

5.1. Sources of Cybersecurity Data

Both machine-learning algorithms and previous cyber-crime data are crucial for predicting and detecting cyber-attacks. Machine-learning methods are sufficiently successful; support vector machines (SVMs) accomplish a prediction success rate near 60%. Special consideration must be accorded to malware and social engineering attacks (Bilen & Bedri Özer, 2021). Sources for cybersecurity data include cyber defense and situational awareness research, network intrusion detection and countermeasure selection, cyber-attack modeling and impact assessment, pre-emptive intrusion detection approaches, real-time episode correlation algorithms for multi-step attack detection, network attack forecasting, intrusion response management, security-enhanced recommender systems, and Bayesian network-based cyber-attack prediction. Real-time alert correlation and prediction with Bayesian networks, anomaly detection combined with Bayesian networks, physical impact assessment of attacks on industrial systems, and intrusion prediction based on optimised alerts and Hidden Markov models also provide valuable data (Martin et al., 2019).

5.2. Data Cleaning Techniques

The raw dataset constructed from diverse online resources, including professional articles and government reports, typically contains irrelevant and non-informative records. To make the dataset suitable for training and testing, the first-stage procedure performs the initial data cleaning process to glean information from the dataset and discard irrelevant records. The data cleaning pipeline involves four consecutive data cleaning procedures implemented successively on the entire raw dataset through custom Weka filters.

To remove records containing irrelevant samples, the deletion of stored data procedure evaluates every record according to independent criteria. When the records are found to contain no stored information about a cyber-attack, the procedure deletes the record. It also checks if a record exists in the raw dataset, where several of its attributes are not filled, and deletes the record in such cases. The parameter selection procedure distinguishes those records containing an agent, service, or payload malicious activity and erases the records that do not meet these specific scenarios. The keyword selection procedure imposes another query on the dataset and excises the records without pertinent information. The record resize procedure addresses the discrepancies in the number of attributes among records. It investigates the dataset to identify those records with a smaller or greater number of attributes in comparison with the largest record in the dataset. Half of the records with fewer attributes are then removed, and the records containing a greater number of attributes are reduced to have a number of attributes consistent with the largest record. The cleaned dataset, after this initial filtering, contains cyber-crime-related information spanning 2004–2015 (Bilen & Bedri Özer, 2021).

6. Feature Selection and Engineering

Feature engineering can be defined as a process that uses domain knowledge to generate descriptors based on the model. The motivation behind feature engineering stems from the acknowledgement that different machine learning algorithms invoke different mechanisms for modelling, mapping, dependency and non-linearity. Accordingly, transformations are discouraged from overlapping with the learnt model and presence of redundant features is not favoured. The domain knowledge should point out features that can be enhanced or extracted with a suitable mapping function within the context of the model. A common method is to combine features that are more or less related into an environmentally oriented context by considering rules that the model identifies. Combinations, or non-redundant transformations, of these features should be used in addition to the original features. For example, neutron features should be avoided when the model tries to map bursts in activities at a certain timescale (Hajaj et al., 2020). By contrast, the combination between the number of antineutron particles and the burst size is a more suitable feature because the dependency between space and time has been encoded. Features indicate straightforward predictive tasks, such as the differentiation between flow types, the recognition of periodicity or the prediction of recurrence. The feature space can be informed by known patterns and behaviours to be found in social networks; however, the surveyed models reveal that information can only be inferred but not easily integrated to favour improved learning.

6.1. Importance of Feature Selection

Feature selection performs the task of selecting useful features from the dataset. It is vital to machine learning since it saves time and memory during data training (Bilen & Bedri

Özer, 2021). If the features are improperly selected, the time required for training may increase. This makes the interpretation of the model difficult and increases the error rate in the model. The selection of vital and informative features is crucial in domains where accurate classification is important (Hajaj et al., 2020). A robust feature selection mechanism was introduced to lessen vulnerability against evasion attacks targeting malicious-domain classifiers. This method provides robust and novel features for malicious domain detection. Two sets of features showed significant resistance to malicious perturbations and excellent effectiveness in classifying non-manipulated data. The feature sets offer a reduction in dimensions from nine to four while simultaneously increasing the combined F1-Score from 92.92 to 95.81.

6.2. Techniques for Feature Engineering

Feature Engineering in Cybersecurity. Planning machine learning (ML) models requires feature engineering — preparing the dataset for analysis and learning. Ideally, this preparation does more than feed data into the pipeline; the model should extract key information from the project and scenario. Feature engineering itself can benefit from natural language processing and other analysis tools.

Manual and Automated Approaches. Manual feature engineering leverages domain knowledge and intuition to generate two types of features: engineered features—statistical or operational aggregations reflecting expert insight—and emergent features, which aim to discover new information within data (Zhu, 2019). On the other hand, automated feature engineering uses algorithms to generate candidate features and subsequently models their importance as a random variable, often employing techniques like Gaussian mixture models or nonparametric neural representations for estimation, thereby reducing reliance on human input.

Analogies in Natural Language Processing. Datasets can be further refined by drawing analogies with natural-language-processing (NLP) frameworks. Here, theobjects within the dataset—such as network flows represented by a source, a destination, and specific connection details—correspond to text concepts. The objects encapsulate the information conveyed, while the features parallel documents in NLP. Relationships can then be established between individual datapoints and an overall analytic objective.

Illustrative Example. For instance, a flow indicating a transfer of data from a bank may become part of an overall goal to estimate civil unrest. Such examples been abstracted from entrants at the Cyber Threat Intelligence Challenge hosted at the Los Alamos National Laboratory (Martin et al., 2019).

7. Model Development

Preliminary investigations into candidate predictive variables were conducted using Spearman's rank correlation. The relationship between the quality of attacks and their

quantity is undisputed; given this inherent dependency, only quality-related variables were shortlisted (Martin et al., 2019). Both the targeted industry and the detected country possess predictive potential. Different industries navigate the malware street-price marketplace differently, resulting in a heterogeneous affordability landscape (Bilen & Bedri Özer, 2021). Similarly, various countries exhibit discernible pricing patterns that influence the relative cost of exploits.

The employed models are single-step-ahead predictors. At a given time t, variables of interest are historical features associated with time points $\tau < t$. The principal quantity to predict is K_t, the count of exploitation attacks at time t. A reduced variable set is utilized due to limited availability of historical variables. Specifically, the model ingests: the sought-after count K_{t−1} from the previous time step; the previously discussed domain counts for concurrent time t across N and H; and the relevant frequencies of active attacks observed during the prior week.

7.1. Supervised Learning Models

Machine-learning (ML) methods for cyber-attack classification and prediction encompass a wide range of techniques, both with and without human supervision. (Bilen & Bedri Özer, 2021) propose a method that predicts and detects cyber-attacks using ML algorithms and data from previous criminal cases. On average, all ML methods considered achieve a 50% success rate in attack prediction. These algorithms classify cases according to various features; successful classification forecasts attack methods or criminals involved in cases with similar properties. The focus is on characteristics of potential victims and attack modalities. Among all approaches, support vector machines (SVMs) perform best in attacker prediction, with a 60% success rate. The analysis indicates that malware and social engineering warrant particular attention. Furthermore, higher victim education levels and income correlate with lower probabilities of cyber-attack. Based on these insights, law enforcement agencies can better identify cyber-crimes and perpetrators. New training and warning systems derive from victim profiles. Future work addresses deep learning algorithms for crime, victim, and attacker profiling, comparison of regional datasets, and development of intelligent criminal-victim detection systems to support law enforcement and mitigate crime rates. ML continues to gain popularity within the research community. Neural networks and SVMs feature prominently, although their diverse applications hinder cohesive categorization.

7.2. Unsupervised Learning Models

Unsupervised learning models find latent structures within high-dimensional and unlabelled data, allowing a system to perform advanced data analysis without supervision. These techniques are primarily used for failure and anomaly detection (Martin et al., 2019). K-means clusters data points by measuring dissimilarity between them, partitioning observations into K clusters to minimize variance within each cluster.

As one of the simplest and fastest algorithms, it requires only a moderate understanding of data and offers scalability for extensive feature spaces. The autoencoder takes samples as input and reconstructs them by creating a bottleneck for the underlying data to pass through. An anomaly is then detected by calculating the reconstruction error: points with high errors are identified as "out-of-distribution." Autoencoders might leverage feature-learning abilities to reduce the number of necessary dimensions and provide greater flexibility. Association rules identify frequently occurring patterns within a dataset, returning rules when one or more items appear together in a transaction such as a database or query log. This technique can reduce the dimension of data before analysis, as it can select key features with respect to specific criteria. Blind source separation separates a set of input signals into independent source components, which can be used to discover hidden subnetworks of an analyzed target network. N-grams extract sequences of tokens from input data. These tokens are converted into feature vectors for machine learning algorithms, making this a very popular technique for text and malware analysis.

7.3. Hybrid Models

Cyber incidents are increasing in prevalence and complexity. Systems designed to identify and counter the broad range of possible threats are necessary for pre-emptive mitigation. As a result, numerous specialized detection and prediction algorithms have been combined in hybrid models (Martin et al., 2019).

Seven hybrid approaches address cybercrime scenarios at different stages of attack that facilitate discovery and responsive mitigation: • Preemptive intrusion-detection systems monitor for suspicious activity and parameter shifts that indicate an attack before the attack can actually be mounted, allowing for preventative action. • Correlation systems continuously analyze data flow to identify the interrelations among suspicious events and acquire a holistic understanding of performance through multivariate data fusion. • Verification models employ arbitration mechanisms that elicit feedback and seek confirmation from alternate sources to minimize false-positive events that may result in unnecessary countermeasures. • Forecasting techniques estimate the probable time, location, and weaponry of an impending attack by mining knowledge from historical information. • Exposure assessment methods analyze network security and vulnerability data to identify points of concern and opportunities for exploitation. • Response mechanisms apply guidance and control so that countermeasures align with ongoing strategic and tactical objectives. • Repositories of events, information, and actions document activity to assist in the examination of past attack scenarios and identify past vulnerabilities to address in the future.

The performance of these versatile models can vary, but the collective combination of techniques offers an effective means of predicting and managing complex cyber threats.

8. Model Evaluation Metrics

Cybersecurity threat prediction models require thorough evaluation through specific measurement techniques in order to assess the progress and effectiveness of these methods. Popular metrics for metric-based methods encompass classification accuracy, false alarm rate, and precision. Time-series-based approaches, such as time series analysis, employ metrics including the confusion matrix, Area Under the Curve (AUC), hyper-volume, Modified Hausdorff Distance (MHD), and probability distribution as their primary evaluation tools. In the domain of attack method and perpetrator prediction, the success rate of correctly identifying the attacker attains approximately 60%, revealing an inverse relationship between the victim's education and income levels and the likelihood of cyber-attack (Bilen & Bedri Özer, 2021). Despite these seemingly promising outcomes, the applicability of current cyber security predictive methods in operational environments remains dubious. While accuracy rates exceeding 90% have been reported on virtual datasets, the same models exhibit a considerable decline to 60–70% when tested on real-life datasets. Utilities should also consider prediction speed and reaction time, which in some cases provides over 39 minutes advance warning, offering a reasonable window for precautionary measures. Equation-based methods, though less accurate than exhaustive algorithms, nevertheless yield reasonable results. The development of appropriate evaluation metrics for cyber attack prediction constitutes an ongoing challenge, and further assessments aimed at determining the real-time effectiveness of existing techniques are necessary (Martin et al., 2019).

8.1. Accuracy and Precision

Accuracy and precision measures are employed in cyber-security assessments, model evaluation, and intrusion detection. Accuracy metrics quantify match degree between a predicted trend or value and the actual timeline, while precision metrics quantify how distinct a prediction is from other outcomes. A system is accurate if most of its predictions match actual events, and precise if it minimizes false positives, avoiding excessive reporting of non-occurring events (Martin et al., 2019).

Machine-learning algorithms and previous cyber-crime data enable cyber-attack and perpetrator prediction. Success rates for attacker prediction are approximately 60%, with heightened attention required for malware and social-engineering attacks. Victims' higher education and income levels correlate with a lower probability of attack. These insights support law-enforcement efforts in crime detection and prevention (Bilen & Bedri Özer, 2021).

8.2. Recall and F1 Score

Recall is the quantity of positive events found by a model. In intrusion detection it represents the rate at which attacks are identified by the model. A high recall indicates

that an approach has found a large proportion of the attacks within the dataset, signalling an effective model. The Recall metric can be improved by the identification of anomalies in time series data because some attacks in ICS datasets present themselves as anomalous sequences through the system variables (Raghavendra Narayan et al., 2023).

The F1 is the harmonic mean of precision and recall, and indicates the percentage of class decisions that are accurate, in the context of machine learning models. The F1 score depends on precise, correct classifications so an approach which maintains the accuracy of the DT classifier whilst improving model recall will also demonstrate improvements in F1. The highly accurate nature of time series classification means that DTs are better able to classify samples anomalous to a particular class. This ability allows the F1 score to be increased on ICS datasets with minimal topological disruption.

8.3. ROC Curves and AUC

The Receiver Operating Characteristics curve (ROC curve) is a central tool for diagnostic test evaluation. Given a predictor variable, such as the result of a medical test, it plots the estimated false positive rate against the estimated true positive rate as a function of the classification threshold. The ROC space, that is, a 2-D plot of sensitivity (or true positive rate) versus 1-specificity (false positive rate), is considered the most appropriate for visualizing and evaluating classifiers outputting class membership probabilities . Area Under the Curve (AUC) is most often used to compare the performance of different classification methods.

9. Challenges in Threat Prediction

Cyber-attacks are fast-growing at an exponential pace; the frequency and severity of intrusions, malware, and instances of hacking have significantly increased in the past few years, resulting in huge financial losses. Cyber criminals use a broad array of attack techniques to exploit weaknesses. Predicting these attacks at an early stage is necessary to reduce the violence caused by cyber threats and to take proper security measures such as detecting the upcoming attack, forecasting the region to be targeted, and identifying the attacker. A predictive method is proposed for detecting cyber-attacks by utilizing machine-learning algorithms and data from multiple historical cyber-crime cases.

9.1. Data Imbalance Issues

The selection of data used to train and develop threat prediction models has a substantial impact on their performance, particularly when carried out through manual acquisition or direct querying of online repositories and honeypots. Depending on the resulting sources, threat data may not be representative of the target ecosystem because a system's characteristics evolve during its lifetime and may differ from those observed during data preparation. Additional features, such as resource availability, usage patterns, and the number of viable attack points often remain undetected, resulting in limited

transferability of models. Existing big data repositories used in the training of models commonly encompass real-world threat and interaction data, yet produce a significant number of false positives and atypical examples.

Imbalance issues (Fig. 9.1) arise when the available data contains a largely disproportionate share of some classes, causing models to become biased towards the most frequent ones. In cybersecurity applications, where data is frequently derived from the observed behaviour of legitimate system operation, models typically continue to adapt to the same benign patterns and consequently neglect many anomalous conditions; as a result, the detection of unexpected but unfrequent conditions is underrepresented (Pawlicki et al., 2020). Unbalanced datasets therefore lead to a high number of false negatives and anomalous data being misclassified as legitimate, consequently preventing response to silently propagating, persistent threats.

9.2. Adversarial Attacks on Models

Intelligent systems widely exploit machine learning to detect cyberattacks in both research and operational domains (Pauling et al., 2022). Adversaries adapt to detection mechanisms by probing models with inputs to circumvent defenses and generate incorrect outcomes. Attack scenarios targeting these systems are examined across different application taxonomies (Ibitoye et al., 2019). Notably, sophisticated attacks during the inference phase aim to produce erroneous outputs by exploiting vulnerabilities without corrupting the underlying model. These can be categorized as white-box or black-box attacks, depending on whether the adversary has access to the model's architecture. The attacker's objectives, framed within the confidentiality, integrity, and availability (CIA) triad, encompass: extracting sensitive information about the model or training data (confidentiality); inducing faulty model behavior such as misclassifications or suppressed output confidence (integrity); and obstructing access to model outputs or impairing performance through denial-of-service or slowdown tactics (availability). Within network security applications, machine learning models remain vulnerable to poisoning attacks during training and to evasion techniques or false-positive inducements during inference.

10. Case Studies of Successful Implementations

In a recent study, a cyber-attack method and perpetrator prediction approach was developed by leveraging machine learning algorithms. The approach analyzes data from prior cyber-crime cases in Turkey to anticipate the types of attacks, potential victims, and possible perpetrators. The system also predicts broader attributes of illegal activities and likely offenders. Machine learning techniques demonstrate the most effective performance compared to alternative methods. Support vector machines (SVMs), which stand out among machine learning algorithms, achieve a prediction accuracy of around 60%. The analysis reveals that higher education and income levels of potential victims

reduce the probability of falling prey to cyber-attacks. The proposed framework aims to enhance the capabilities of law enforcement agencies in detecting cyber-crimes and identifying responsible individuals. Future directions include the application of deep learning algorithms to improve estimations of the types of crimes, as well as profiling of offenders and victims. Additionally, acquiring cyber-crime data from multiple provinces will enable comparative assessments based on geographic parameters. The development of advanced criminal-victim detection systems is expected to further support law enforcement efforts and contribute towards lowering crime rates (Bilen & Bedri Özer, 2021).

10.1. Case Study 1: Financial Sector

The ever-evolving landscape of cyber threats necessitates agile and robust predictive models that can bolster preemptive defense mechanisms. Confronted with unpredictable challenges and a multitude of possible attack vectors, cybersecurity practitioners require tools that can identify threats before they manifest. Drawing insights from historical attack patterns thus emerges as a crucial strategy for forecasting future incidents. Machine learning (ML) contributes significantly to this endeavor by enabling the analysis of extensive historical datasets, facilitating the evaluation of numerous potential threats, and generating probabilistic forecasts of impending attacks. Consequently, ML-generated predictions can support proactive defensive measures, contributing to the timely safeguarding of information and assets (Bilen & Bedri Özer, 2021). In the financial sector, where the rapid development of digital infrastructure has increased vulnerability to cyberattacks, ML-based models have been proposed to anticipate potential threats more effectively.

10.2. Case Study 2: Healthcare Sector

Threat modeling is a fundamental activity to understand the threats that the healthcare organization has to deal with. Important threats to healthcare systems include ransomware, data breaches, DDoS (Distributed Denial of Service), and insider attacks, specific threats to hospital services and medical devices. Measures such as patch and incident management are key elements of the control environments. Recent works on regulatory compliance often focus on threat and vulnerability detection adopting machine learning (ML) and deep learning (DL) methods as complementary approaches to the analysis of vulnerabilities of healthcare or medical systems. While ML applications to healthcare generally cover patient diagnostics, health monitoring, and disease or compliance prediction, ML approaches to security of healthcare systems still represent an underexplored domain. Different complementary approaches utilize ML and DL techniques to reveal, understand and predict threats and vulnerabilities of the healthcare ecosystem. Initially, software metrics can be predicted using ML classifiers to identify potentially vulnerable code. Anomaly-driven frameworks enable the

detection of malicious activities and sophisticated attacks through monitoring and interpreting network and host information. For embedded medical systems, supervised and unsupervised ML models analyze data from power consumption, execution time, temperature, and network traffic to identify abnormal behaviors. To enhance Android app security, vulnerable code patterns are recognized through source code analysis combined with NLP and word embedding techniques. Furthermore, ML facilitates assistance in compliance evaluation by analyzing regulatory documents, highlighting and classifying key clauses and definitions according to regulatory domains or specific standards (Silvestri et al., 2023).

11. Future Trends in Cybersecurity Threat Prediction

Cybersecurity threat prediction models employ mathematics and physics to analyze alphanumerical data, identify patterns, and build predictive models. Future trends in this domain can be grouped into four primary categories: (i) randomness optimization, (ii) hybrid systems, (iii) content-based analysis, and (iv) graph-based methods.

Randomness optimization aims to optimize randomness measures such as linear and non-linear complexity, 2-adic complexity, and entropy. These metrics illuminate the inherent unpredictability of data, which is essential for analytical models. By optimizing randomness, prediction models can enhance the accuracy of their inferences regarding potential cyber-threats.

Hybrid systems combine various machine learning and deep learning techniques to improve overall prediction capabilities. These hybrid approaches maximize the strengths of their constituent methods and mitigate individual weaknesses. An example is the development of cyber-attack prediction models that draw upon multiple algorithms to foresee the characteristics and methods of potential attacks. Such models can aid law enforcement in detecting cyber-crime and formulating targeted training and warning systems (Bilen & Bedri Özer, 2021).

Content-based analysis models extend to packet contents rather than focusing solely on network topology. This category is highly relevant to Intrusion Detection Systems (IDS) and enables more granular inspections of network traffic to identify malicious patterns. Interpretable content-based models facilitate critical decision-making by providing transparent justifications for predicted threats (Schmitt, 2023).

Graph-based methods apply predictive analytics to communicate the chronological progression of attacks following an initial breach. These techniques harness graph theory to model potential propagation paths and evaluate the impact of attacks within specific network segments. Graph-based prediction can be augmented with concepts from chemistry and quantum physics to provide formulations at different levels of abstraction (Martin et al., 2019).

11.1. Evolution of Machine Learning Techniques

Machine learning (ML) has seen increasing adoption across research domains, including cybersecurity, and encompasses diverse approaches such as neural networks and support vector machines (Martin et al., 2019). Neural-network methods have been applied to attack detection, with back-propagation models reporting an accuracy of 42%. Wavelet neural networks combined with genetic algorithms achieve slight improvements over back-propagation, whereas cascaded neural network ensembles outperform simpler models. Support vector machines have been used for real-time detection of malware and specific attacks, including SQL injection, though some implementations restrict the range of detectable attack types. Data-mining techniques—such as frequent pattern mining and sequence mining—analyse network data and reveal insights into attack patterns. Additional learning algorithms such as decision-tree classifiers and random forests facilitate the prediction of malicious websites and data breaches, with true positive rates approaching 90%.

Intelligent systems that utilize machine learning constitute a leading paradigm for applying data science to cyber operations. These systems detect malicious activity by evaluating data features, thereby strengthening security monitoring. Classification methods trained on historical data predict labels with high accuracy, underpinning a popular approach to malware identification (M. Devine & D. Bastian, 2019). However, the same mechanisms render systems vulnerable to data-poisoning attacks, which can degrade performance or conceal malware. Enhanced robustness is achievable by exposing candidate models to perturbed inputs and combining them through linear stacking to mitigate adversarial effects. Machine learning forms a critical dimension of intelligent systems and represents a principal attack vector for adversaries.

11.2. Integration with AI Technologies

AI technologies have become popular tools for system protection. Integrating machine learning and deep learning models with existing security architectures enables network intrusion detection and malware detection in smart infrastructures and digital industries. Ensemble mechanisms and multi-dimensional feature fusion further increase detection accuracy. For high-stakes decisions, interpretable models are preferred. Call data record and other cybersecurity datasets support malicious-activity verification and intelligence. The Edge-IIoTset 10-terabyte heterogeneous IIoT datasets provide broader opportunities. GPU-based and cloud security tools increase detection capabilities. Additional topics covered include IoT cybersecurity management, malware attack techniques, and adaptive systems supported by AI for predictive cyber-risk analytics (Schmitt, 2023).

Investigations support integrating artificial intelligence with network security. Manickam, for example, proposed a Grey Verhulst prediction model to address limited

data on security situation prediction. Liu et al. forecasted cybersecurity incidents using a cloud-based model. Zheng and colleagues provided strategies for autonomous security-awareness. Chen et al. developed a small-world echo state network for prediction. Zhang et al. applied BP and RBF neural networks to security-situation prediction. Xing-zhu created an intrusion-prediction model based on RBFFeatures Classification. Zhang et al. also used wavelet neural networks with optimized parameters. He et al. proposed a mixed wavelet-based neural network, employing MODWT and Hurst Exponent Analysis. Prediction and dynamics of network-security situation were analyzed, and attackers' behaviors estimated in social networks. Other approaches combine computational intelligence, machine learning, and pattern-driven analytics (Martin et al., 2019).

12. Ethical Considerations in Cybersecurity

The deployment of machine-learning and mathematical computational models in the prediction of cybersecurity threats is of growing significance. Statistical analyses reveal an upward trend in cyber-attacks, underscoring the necessity of accurate predictive models (Martin et al., 2019). High prediction accuracy is fundamental to practical application. Models frequently achieve over 90% accuracy on selected datasets, yet this figure decreases to approximately 60–70% when applied to live network data. The time interval between prediction and attack onset remains critical; certain frameworks reportedly offer up to 39 minutes of advance notice, affording sufficient opportunity for manual scrutiny and response. An approach employing machine learning trained on datasets comprising 609 cyber-attack instances succeeded in forecasting the perpetrator of various cyber-crimes with predictive probabilities ranging from 44% to 71%, contingent on the specific crime and individual (Bilen & Bedri Özer, 2021). These predictive capabilities not only enable preemptive countermeasures but also guide law-enforcement investigations towards the most probable crime types and culprits.

12.1. Privacy Concerns

Machine learning (ML) is widely adopted in various domains, including crime, education, finance, healthcare, and law enforcement. ML models trained on sensitive personal data pose substantial privacy risks through model predictions and parameters (Strobel & Shokri, 2022). The lagging development of privacy-enhancing techniques creates an impediment to trustworthy ML adoption. Assessing ML privacy leakage and mitigating privacy threats to training data are necessary to adopt ML models in real-world applications while respecting data protection regulations (Kumar Murakonda & Shokri, 2020).

12.2. Bias in Machine Learning Models

Bias is an impediment to fair decisions in domains such as human resources, public administration, and healthcare. Despite hopes that machine-learning methods could

reduce such bias, models may also be biased. These forms of bias depend on the data on which the model was trained (Gu & Oelke, 2019).

Algorithmic unfairness is the phenomenon by which model predictions benefit or harm certain groups of people in society. Notably, unfairness in fraud detection may limit access to financial services for particular subpopulations. The field of Fair ML studies, measures, and mitigates unfairness, typically with respect to a protected group such as race or gender.

A formal understanding recognizes that algorithmic unfairness emerges through the interaction between models and data bias. Data bias follows a taxonomy that characterizes the type and magnitude of unwanted correlations in the data. An accounting of such biases helps to understand the trade-off between fairness and accuracy. Certain bias configurations entail particular trade-offs, affecting fairness in both expected value and variance, while models perform differently depending on the biases present in the data. Simple pre-processing interventions sometimes balance group-wise error rates under certain biases but often fail in more complex scenarios (Pombal et al., 2022).

13. Conclusion

Cybersecurity threats, which prevail across various computer or network environments, involve intrusions, malware propagation, attacks, and exploits. These threats target not only private or public enterprises but also governments or military organizations. As a consequence, a significant amount of data or assets can be lost, unless appropriate countermeasures are enforced. Therefore, an automatic detection-based taxonomy of attack methods and perpetrators is used to forecast threats and secure networks. This approach is supported by data from previous cyber-crimes and machine learning techniques. Assigning high priority to network or host security is critical for determining more efficient responses and defending against cyber-crime. More accurate information on threats would also reduce the efforts and costs related to insurance claims or investigations by private enterprises or governments.

A model that forecasts device specifications, cyber-crime types, information on cyber-crime victims, and perpetrators is presented. The detected cyber-attack methods, predicted or labeled with this model, are also used to forecast perpetrators. An automatic detection-based cybersecurity crime pair forecasting framework is proposed using a dataset of past cyber-crimes (Bilen & Bedri Özer, 2021). Future work includes exploration of hardware or software system specifications and use of deep learning algorithms to forecast damaging cyber rackets. When an event involving a victim is detected, the forecasting model identifies the cyber-crime type, proposes the perpetrator, and facilitates an intelligent investigation (Martin et al., 2019).

References

Bilen, A. & Bedri Özer, A. (2021). Cyber-attack method and perpetrator prediction using machine learning algorithms. ncbi.nlm.nih.gov
Martin, H., Jana, K., Elias, B. H., & Pavel, Čeleda (2019). Survey of Attack Projection, Prediction, and Forecasting in Cyber Security.
Ibitoye, O., Abou-Khamis, R., el Shehaby, M., Matrawy, A., & Omair Shafiq, M. (2019). The Threat of Adversarial Attacks on Machine Learning in Network Security - A Survey.
Schmitt, M. (2023). Securing the Digital World: Protecting smart infrastructures and digital industries with Artificial Intelligence (AI)-enabled malware and intrusion detection.
M. Devine, S. & D. Bastian, N. (2019). Intelligent Systems Design for Malware Classification Under Adversarial Conditions.
Hajaj, C., Hason, N., Harel, N., & Dvir, A. (2020). Less is More: Robust and Novel Features for Malicious Domain Detection.
Zhu, Z. (2019). AUTOMATIC FEATURE ENGINEERING FOR DISCOVERING AND EXPLAINING MALICIOUS BEHAVIORS.
Raghavendra Narayan, K. G., Mookherji, S., Odelu, V., Prasath, R., Chand Turlapaty, A., & Kumar Das, A. (2023). IIDS: Design of Intelligent Intrusion Detection System for Internet-of-Things Applications.
Pawlicki, M., Choraś, M., Kozik, R., & Hołubowicz, W. (2020). On the Impact of Network Data Balancing in Cybersecurity Applications. ncbi.nlm.nih.gov
Pauling, C., Gimson, M., Qaid, M., Kida, A., & Halak, B. (2022). A Tutorial on Adversarial Learning Attacks and Countermeasures.
Silvestri, S., Islam, S., Papastergiou, S., Tzagkarakis, C., & Ciampi, M. (2023). A Machine Learning Approach for the NLP-Based Analysis of Cyber Threats and Vulnerabilities of the Healthcare Ecosystem †. ncbi.nlm.nih.gov
Strobel, M. & Shokri, R. (2022). Data Privacy and Trustworthy Machine Learning.
Kumar Murakonda, S. & Shokri, R. (2020). ML Privacy Meter: Aiding Regulatory Compliance by Quantifying the Privacy Risks of Machine Learning.
Gu, J. & Oelke, D. (2019). Understanding Bias in Machine Learning.
Pombal, J., F. Cruz, A., Bravo, J., Saleiro, P., A. T. Figueiredo, M., & Bizarro, P. (2022). Understanding Unfairness in Fraud Detection through Model and Data Bias Interactions.

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Chapter 8: Optimization in Resource Allocation for Smart Grid Systems

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Abstract: The evolution of smart grid systems has introduced a transformative approach to modern energy distribution and management, aiming to achieve higher efficiency, reliability, and sustainability. One of the key challenges in this domain is the optimal allocation of resources—such as electricity generation, storage, and consumption—across diverse, interconnected grid components. This paper explores various optimization strategies employed in resource allocation within smart grids, focusing on both centralized and decentralized models. Advanced computational techniques such as linear programming, dynamic programming, genetic algorithms, and machine learning are utilized to solve multi-objective optimization problems under constraints of time, cost, and energy balance. The integration of renewable energy sources, electric vehicles, and distributed energy storage further complicates the allocation problem, demanding adaptive and real-time decision-making frameworks. Simulation results discussed in the paper highlight the efficiency gains from employing such optimized solutions, demonstrating significant improvements in load balancing, peak shaving, demand-side management, and operational cost reduction. Additionally, the paper emphasizes the role of predictive analytics and artificial intelligence in enhancing grid responsiveness and resilience. Security, data privacy, and interoperability are addressed as vital concerns in implementing optimization solutions. The study also examines recent trends in cloud-based and edge computing platforms that support scalable optimization models for smart grids. Overall, the work underlines the importance of robust optimization techniques for achieving sustainable and intelligent energy systems. It provides a foundation for future research into scalable, secure, and adaptive optimization methodologies tailored for dynamic smart grid environments.

Keywords: Smart Grid, Resource Allocation, Optimization Techniques, Renewable Energy Integration, Load Management.

1 Introduction

Smart grid systems optimize energy allocation by employing techniques such as approximate dynamic programming (ADP) and fast optimal power flow (OPF) algorithms. Optimal control policies for grid-connected battery energy storage systems (BESS) require consideration of time dependence and a finite horizon, while enhanced OPF algorithms accelerate computations through reduced system modeling and distributed solution retrieval. ADP approaches have been shown to outperform classical dynamic programming in this context (Das, 2017). The proliferation of renewable energy and demand-response assets introduces significant uncertainty. Clustering and network-reduction techniques combined with cumulant-based methods and Gram-Charlier expansions enable efficient probabilistic analysis of OPF (Liang, 2019). In a 100-resident system, average comfortableness and total financial rewards for various demand-response rates and durations demonstrate the effectiveness of the energy-optimization approach. Smart grid technologies that establish two-way communication of electricity and information thereby improve the efficiency and reliability of power-grid systems. The rapid development of advanced computing platforms offers unprecedented opportunities for large-scale smart grid analysis and optimization. Clustered and reduced systems allow rapid calculation of system-state statistics, facilitating efficient management of smart grid operations.

2. Overview of Smart Grid Systems

Smart Grids are electrical grids enhanced using digital commination to provide intelligent remote control, monitoring, and improved governance of the system. The key components of Smart Grid systems include smart metering infrastructure, smart appliances, micro-generation (distributed energy resources), energy storage systems, and the energy management system. Micro-grids emerged as a promising concept to help modernize the power grid and aim to provide fast and accurate responses to the ongoing demand and supply balance. Optimization is the foundation for considering resource allocation. Optimization methods include Spanning tree, Linear Programming, Genetic Algorithms, and Mixed Integer Linear Programming. (Das, 2017) (Yuan Xu, 1970).

3. Importance of Resource Allocation

Resource allocation is pivotal in the execution of services across every sector. In energy systems, optimal allocation crucially ensures the efficient operation of battery energy storage systems (BESS) and microgrids. Determining the ideal state of charge (SOC) for a battery, aligned with its lifetime characteristics, supports the achievement of a maximum feasible cycle life. The intermittent and variable nature of renewable energy sources (RESs) complicates the optimization of distributed systems, threatening power quality, reliability, and operational expenses. Interest continues to grow in renewable energy and distributed generation; alongside this, the widespread deployment of electric vehicles (EVs) introduces additional challenges in managing energy flow effectively.

4. Challenges in Resource Allocation

The scarcity of energy resources has led to the extensive application of Distributed Generation (DG) in power systems, predominantly integrating solar and wind energy (Das, 2017). The allocation of optimal resources entails determining the best placement, sizing, and resource type within a network. Inherent characteristics of renewable energy sources (RESs) introduce uncertainty and intermittency, complicating power system optimization and making the balance between power generation and load demand critical. Imbalances can cause significant deviations in power system operation and jeopardize stability, resulting in confiscation costs or penalties (Sindi, 2018). Battery Energy Storage Systems (BESS) present an efficient strategy to counteract these issues. The allocation process stipulates specific requirements and optimizations guided by operational conditions during allocation. Multipliers of the day-ahead electricity price suggest utilizing battery energy storage to exploit price differentials between peak and off-peak periods. The daily peak reduction must consider the system's maximum reserve capacity, a constraint that prevails over the incentive to reduce peak demands at end-user locations. Residual load considerations emphasize prioritizing the most desirable location for BESS placement to maximize impact during these periods. The operation of BESS significantly influences the battery's life cycle. As such, an Optimal Battery Energy Storage System Sizing and Operation technique (OBESSO) integrates battery lifetime characteristics into both the sizing and operational management of BESS within the simulation framework.

5. Optimization Techniques

To improve efficiency and reduce cost, various optimization techniques have been developed to schedule residential appliances while fulfilling consumer and grid constrains. One approach employs an approximate dynamic programming (ADP) method with automatic value function approximation that outperforms classical methods as data size grows. Another strategy uses demand-side management, enabling residential energy systems to act as agents that allocate demand reduction requests efficiently without compromising user comfort and provide strategic rewards; this approach has been validated through simulations involving multiple households. Additionally, a multi-phase optimal power flow (OPF) technique for distributed generation capacity planning addresses issues such as unbalanced loadings, voltage regulation, and reactive power compensation in unbalanced networks. This method, implemented via a co-simulation framework with constriction factor particle swarm optimization (CF-PSO), has been tested on an IEEE 8500-node distribution system and offers a new tool for planning problems where existing OPF solutions cater primarily to balanced networks (Das, 2017) (Anwar & N. Mahmood, 2014).

5.1. Linear Programming

The simplest method is linear programming (LP), which has been extensively used for distributed generation planning. In some approaches of this category actual power trade-off between participants is not considered; planning can be based on system load level, energy loss, voltage deviation, optimal source capacity, or DG unit size. Sensitive indexes are considered in . An LP-based model was proposed in for DG allocation with relaxed voltage constraints for non-firm generation; AC power flow is used in when problems with an optimal solution exist. AC optimal power flow (OPF) is also frequently applied for economic dispatching. For this reason a DG allocation technique was proposed in that is based on traditional nonlinear programming-based OPF to satisfy the required constraints and achieve the desired objectives. A variation COPF approach was proposed in that minimizes power losses. Increasing DG hosting capacity is also investigated in . In all cases these techniques rely on passive representation of DGs with peak-load modeling, insufficient for smart grid applications that require more system-aware models. Optimal sizing and placement approaches for smart loads that result in larger benefits is discussed in . The procedure considers not only maximizing DG capacity but also security, voltage stability, and protection coordination. Traditional nonlinear programming (NLP)-based AC power flow or OPF cannot incorporate integer

programming; a mixed-integer NLP framework is developed in but its complexity increases with the system size and number of periods. Aggregated temporal and spatial units are employed in to reduce simulation time, at the expense of accuracy resulting in a less reliable approach. Stochastic planning techniques—Monte Carlo, analytical, and hybrid—are also used for DG allocation, taking into account financial, network, and supply reliability requirements. These methods rely on large amounts of data that increase dramatically with the system size.

5.2. Dynamic Programming

In smart grid systems, energy management can be crucially optimized by employing dynamic programming. (Huang et al., 2023) proposed an energy scheduling scheme by integrating a revised dynamic programming algorithm and a long short-term memory (LSTM) network. The derived power purchasing and discharging schedules of plug-in electric vehicles (PEVs) can smooth out the overall system load profile with incremental costs substantially reduced. This suggests that the proposed scheme can be a powerful tool for smart grids to maintain system stability and improve economic benefits. In a broader context, recent technological developments have transformed the traditional power grid into a more intelligent future grid with the tremendous progress of information and communications technology. The electrical power network is also gradually developing to a large-scale, highly complex, and smart grid, which is based on power electronics and information technology. It integrates power generation, power transmission, power distribution, and loads.

Looking beyond power grids, dynamic programming already finds diversified applications in contemporary engineering and sciences. A practical dynamic programming based methodology was developed for aircraft maintenance check scheduling optimization. The derived policy allows flexible rescheduling of checks according to limitations on maintenance crews, facilities, and budget availability. A survey was conducted on smart grid technologies and applications to better tap the full potential of smart grids. The dynamic programming technique was used to optimize the performance of fuel cell hybrid vehicles operated in different drive cycles. A uniform dynamic programming (UDP) algorithm was employed for dimensionality reduction of hydropower systems in the optimization of hydropower system operation. More broadly, smart grids can dramatically reduce the emissions of the conventional power sector. The integration of big data, machine learning, and smart grids was therefore reviewed, together with the security concerns and solutions. In electrical power systems, the fast

Newton–Raphson (FNR) economic dispatch and reactive power/voltage dispatch (RPVD) by sensitivity factors was applied to optimal power flow, aiming at the minimization of the total production cost and system active power loss. Additional examples of relevant advances include machine learning and deep learning in smart grids, artificial intelligence techniques, adaptive dynamic programming for control, improved ant colony algorithms for path planning, deep-convolution-based LSTM networks for life prediction, grey wolf optimization applied to economic load dispatch, enhanced particle swarm optimization for non-convex economic load dispatch, random forests, particle swarm optimization, and improved dynamic programming algorithms for sequential decision processes. Optimal scheduling of electric bus fleets also benefited from dynamic programming by simultaneously considering battery capacity fade.

5.3. Genetic Algorithms

Genetic Algorithms (GAs) cover an optimization method modeled broadly on natural selection processes at the population level. Underlying the GA is the notion that natural selection can be formulated to solve global and combinatorial optimization problems. GA techniques involve iterative manipulation of chromosomal structures, or strings. Each string represents one potential solution to the problem, and a population of these enables parallel exploration. Each string is first evaluated to determine its fitness to the problem. The fittest strings then combine during a mating process that involves crossover, mutation, and selection. Conventional GAs, however, suffer from slow convergence, premature marginalization, and reduced final solution quality, challenges unresolved through improved information sharing or probabilistic selection. An Adapted Genetic Algorithm (AGA) aligned with the multicellular organism mechanism—the GAMOM algorithm—addresses these issues. The approach modifies GA operations based on human meiosis, integrating mitosis concepts to accommodate asexual chromosome behaviors. Control parameters guide the algorithm's dynamics post population initialization. A test case on the IEEE 33-bus system, incorporating four distributed generators, two wind sources, and a breaker for emergency grid disconnection, demonstrates effective operational cost minimization despite constraints such as load balancing, utility purchase limits, generator capacities, ramp rates, and minimum up/down times (Jamaledini et al., 2018).

Energy cost reduction objectives persist in microgrids containing multiple distributed generators. Availability of conventional units subject to scheduled or forced outages and alternative energy sources susceptible to weather-dependent power fluctuations

complicate operations. Multi-step methods offer expedited unit outage calculations that preserve solution quality, facilitating large-scale urban energy system modeling. Improved mixed-integer linear programming (MILP) formulations also yield substantial performance enhancements for extensive grids. Comparative microgrid evaluations suggest that GAs outperform MILP approaches in scheduling efficiency. Decomposing scheduling into integer programming for unit commitment and nonlinear programming for economic dispatch captures start-up and shut-down costs more tractably, enabling Enhanced Genetic Algorithms to jointly optimize commitment and dispatch. Memory-Based Genetic Algorithms tailored for energy cost minimization further surpass Particle Swarm Optimization variants. Fuzzy multi-objective optimization supports analyses of storage and renewable sizing under operational considerations (Alvarado Barrios et al., 2019).

5.4. Heuristic Methods

Power system planning is often addressed as a combinatorial optimization task. Meta-heuristics such as mixing switching, line reinforcement, and new line measures serve as optimization strategies to find solutions to this problem. A comparison of iterated local search and genetic algorithms reveals that performance depends on factors including the initial grid state, grid size, and the specific measures applied. Iterated local search often demonstrates robust performance, while more exploratory heuristics can identify solutions in shorter run times on larger grids (Schäfer et al., 2020). Smart grid technology enables consumers and utility companies to reduce electricity costs and regulate generation capacity by permitting optimization of appliance operation over a range of demand scenarios. Scheduling algorithms rely on accurate information exchange between the main grid and smart meters. Consumers must schedule loads, respond to demand signals, participate in energy bidding, and monitor price fluctuations. Enhanced communication infrastructure supports these capabilities and improves consumer satisfaction. A heuristic demand side management model facilitates dynamic scheduling of smart home appliances to maximize satisfaction. Simulations demonstrate a reduction in the peak-to-average energy demand ratio and lower total energy costs without compromising user comfort (Ullah Khan et al., 2019).

6. Data Analytics in Smart Grids

Data analytics technology constitutes a fundamental element of a high-performance smart grid (ZHANG et al., 2018). Whereas traditional power systems were designed with a one-way flow, modernization has introduced a two-way electricity and information flow. At the same time, monitoring, control, communication, management, and security technologies have been widely deployed throughout power grids, thus enabling the generation and collection of a large volume and variety of sensing data. The development of intelligent equipment and data sensors such as smart meters, phasor measurement units (PMUs), and micro-synchrophasors has paved the way for data-driven smart grids. Data analytics serves as a bridge between the abundant data, information, and knowledge present in grid operations. The broad integration of data analytics in power systems has attracted considerable attention, and artificial intelligence (AI)-based data analytics has risen to prominence as a cutting-edge research topic.

6.1. Big Data Applications

The extensive deployment of smart meters and household sensors in Smart Grid Systems generates a considerable volume of intricate data characterized by diversity, velocity, and privacy concerns. For example, smart metering data underpins advanced pricing schemes and load control utilities. Data acquisition stages include conventional sampling, compression, and transmission processes. Considering the computation and communication capabilities in the field and control centers are comparable in different scenarios, exchanging large data volumes among Smart Grid players becomes a plausible and beneficial alternative. Smart Grid data can also inform the tactical placement of measurement devices. For instance, various factors like location importance, observability, spacing requirements, and data quality must be considered (ZHANG et al., 2018).

6.2. Machine Learning Approaches

The complex nature of power systems often requires the transformation of unfeasible points into feasible solutions to sustain reliable operation. Starting from an arbitrary point, iterative techniques are typically employed to approach a feasible one; however, such methods may be computationally demanding and potentially divergent. Recent

efforts have concentrated on developing generalized mappings capable of ensuring feasibility without resorting to iterative steps. A learning-based approach to power dispatch leverages a generalized gauge map, which efficiently transforms any infeasible solution into a feasible point within a linearly constrained domain. This technique exhibits reduced sensitivity to input variations and significantly accelerates the search process. Consequently, the framework guarantees near-optimal and strictly feasible solutions without dependency on computationally intensive post-processing procedures (Li & Mohammadi, 2023). Machine-learning-assisted optimal power flows (OPF) rely on off-line training to mitigate the complexity of non-linear, non-convex constrained optimization problems. Systematic comparisons among fully-connected, convolutional, and graph neural networks reveal that locality properties between features and targets are generally limited; when the grid topology is fixed, the advantage of convolutional and graph architectures over fully-connected models remains marginal. Nevertheless, graph-based networks effectively incorporate topological variations and surpass other configurations when the network structure changes (Falconer & Mones, 2021). The development of intelligent wireless systems demands the balancing of utilities and constraints within extensive device networks. Optimal resource allocation aims to maximize expected capacity under system restrictions, yet non-convexity and infinite dimensionality complicate the challenge. As an alternative to model-dependent, high-complexity methods, machine learning and regression techniques have been employed to approximate strategies. Neural networks trained via supervised learning adapt to available solutions but hinge on their accuracy. Reinforcement learning, conversely, optimizes performance measures without requiring a preexisting solution set. These adaptable approaches offer the potential to outperform conventional heuristics. Formal methodologies draw connections between resource allocation and constrained statistical learning; however, training these models entails solving highly dimensional optimization problems, thereby introducing additional difficulties (Randall Eisen, 2019).

7. Modeling and Simulation

The design of an optimal system for the allocation of resources requires a detailed model. This model is used to explore the design space via simulation. The model must accurately represent the most important components of the system and support experiments that evaluate different configurations. Input data and results must be traceable to confirm that observed behaviors correspond to real phenomena rather than anomalies in the modeling process. Statements regarding model validity therefore require transparency of data and methods. Modeling and simulation can support a wide variety of investigations. When the relevant objective functions are known, a validated model can be used for design

space exploration and optimization, providing decision-makers with an understanding of the trade-offs among alternatives. When the goals of the system are unclear, modeling and simulation can facilitate the formulation of policies, the definition of requirements, and the identification of good strategies (Das, 2017). Simulation models have been used to investigate time-dependent factors such as planning horizons, storage capacity, and demand profiles. Resource management strategies for individual computing units and corresponding policies have been studied. The challenges of predictive and run-time power management and partitioning of resources have also been addressed.

7.1. Simulation Tools

Simulation constitutes an indispensable component in smart grid development, offering a means to analyze, design, model, and investigate various scenarios. The choice of simulation tools similarly influences results and their reproducibility. Two widely adopted open-source simulators are GridLAB-D and RAPSim, which provide support for distributed generation integration and offer a broad spectrum of modules for modelling distribution systems cooperative to smart grid concepts. A comparative case-study approach highlights the diverse modelling capabilities that result in divergent power-flow and renewable-energy-integration outcomes. Key features, including weather-profiling algorithms and load-model accuracy, substantially impact performance and output reproducibility, underscoring the importance of appropriate tool selection for specific applications (Jdeed et al., 2018).

7.2. Case Studies

The integration of renewable energy sources into the smart grid allows distributed generators (DG) of different natures—such as wind, photovoltaic (PV), biomass, and fuel cells—to supply clean energy. Optimal planning and operation of distributed energy resources (DER) are essential to preventing end-user interruptions and reducing costs to acceptable levels. Stochastic models capture the intermittent and random output powers of wind, PV, and bio-DG units, enabling their integration within an existing load flow (LF) model. A penalty cost models excessive reversed power relative to limits, improving the accuracy of the solution process (Sindi, 2018).

The IEEE standard 33-bus system exemplifies the impact of depletion rates of all utilized DGs on planning horizons ranging from a single day to a whole year. Allocations to minimize total real power losses at various buses demonstrate that numerous parameters significantly influence the planning results. Optimal DG location requires a WDGS model that balances load and generation. Plug-in electric vehicles (PEVs) at selected load buses extend the ADL framework to distributed generation scheduling (DGS), with total load reduction and scheduling validated via a cost benefit analysis (Parsa Sirat, 2018).

Energy management with the smart community (SC) moves toward a new era where the optimal energy management system (EMS) aims to achieve minimum operating cost while accounting for the power consumption model of a battery energy storage system (BESS). An approximate dynamic programming (ADP) approach solves the control policy for a time-dependent and finite-horizon BESS problem, with performance compared to classical dynamic programming (Das, 2017).

8. Economic Impact of Optimization

Electricity is the basic infrastructure of modern human society and, because it is a product that cannot be stored in large quantities easily, production and consumption must be kept in balance at every moment at an extremely high level of reliability and quality. The electricity industry was restructured in the 1990s in many countries, and for the newly liberalized industry the production/demand balance had to be managed by means of auctions. On the supply side, the application of a smart grid widens the area of available resources through the large-scale introduction of distributed energy resources and, on the demand side, a smart grid provides more ways to control consumption using flexible demand in the form of demand response, demand-side management, load control, and the like. Managing the supply and demand of electricity is an economically important problem (Das, 2017).

A generic problem is addressed that captures a wide range of practical pricing forms currently being considered for use within smart grid markets. This generic problem becomes a pure convex geometric programming problem when decisions at different times are interconnected by convex constraints. In this case, a variety of algorithms for convex optimization could be immediately applied (Parsa Sirat, 2018). Several specific classes of problems are identified for which the generic formulation is appropriate. Since

the problem is relatively new, a number of model extensions to accommodate additional features in smart grid applications are also described; in particular, stochastic programming and multi-utility formulations (Michael Flath, 2013).

8.1. Cost-Benefit Analysis

A smart grid is expected to converge and expand its functions as the power system, communications among power-system users (namely consumers) and providers, and various control systems. Operations of the smart grid have been provided with advanced mechanisms in the areas of reliability, resilience, stability, as well as energy and cost efficiency. Cost emission analysis is a very useful framework for quantitatively assessing the energy saving and emission reduction of the smart grid, but only a limited number of studies have been conducted (Das, 2017) , (Li & C. Qiu, 2010). The dynamics of power price are modeled as a Markov chain by modeling the random process of load as a Brownian motion-like process and employing the LMP-load mapping curve. Then, the decision of power inquiry is considered as an MDP problem, and dynamic programming is employed to compute the optimal strategy. To avoid the high computational cost, a simple and suboptimal myopic strategy is also studied. A PJM five-bus system is used for numerical simulation, which shows significant performance gain of the optimal strategy of price inquiry, as well as the near-optimality of the myopic approach.

8.2. Impact on Energy Prices

Electric power transmission and distribution systems constitute the fundamental infrastructure that facilitates the transfer of electrical energy from power plants to end consumers. Modernizing the transmission and distribution grids leads to improved grid efficiency, enhanced communication, greater reliability, and increased resiliency while simultaneously reducing electricity expenses and greenhouse gas emissions. Integrating renewable energy resources further contributes to energy independence and security (Ahmadzadeh-Ghahnaviehei, 2017).

Demand response represents a strategy to mitigate power system stress by influencing user energy consumption patterns. Real-time pricing schemes, as a demand response approach, incentivize customers to adjust their consumption in response to price signals. Wireless sensor networks enable cost-efficient residential energy management, wherein

residential customers can design their energy consumption schedules based on recommendations from an energy management system. By leveraging utility information and advanced models, it becomes possible to calibrate models that delineate customer time-varying demand behavior, energy service level requirements, and sustainable energy consumption patterns.

9. Environmental Considerations

Smart grid systems provide a cleaner alternative to traditional power systems with significantly improved environmental performance. In smart grids, distributed generation units such as wind turbines, solar panels and biomass generators should be optimally allocated to minimize losses. Cost reductions can be dramatic, as demonstrated in a case study on the IEEE 33 bus system. Nonetheless, the penetration of renewable-energy resources creates balancing challenges owing to their stochastic nature and to the added complexity introduced by electric vehicles. Power electronic interfaces facilitate renewable-energy integration. The deployment of distributed energy resources, advanced metering, control, communication technologies and smart-energy management further enhances system reliability. Smart grids also enable a shift from load following to energy positioning, helping to reduce the need for backup generation. Core features include distribution automation, electric transportation, demand response, and energy storage. Self-healing capabilities help to prevent failures and restore loads rapidly; they therefore constitute an important feature of modern power systems (Parsa Sirat, 2018).

9.1. Sustainability Metrics

Metrics serve as indicators for dynamic sustainability problems and are derived from the various optimization challenges and multiple objectives that result from the expansion objectives for different system parts (Das, 2017). Efficiency is a key aspect of sustainability, and metrics can be categorized into expenditure efficiency, resource efficiency, and emission efficiency. Expenditure efficiency relates to the level of effort or capital required to achieve additional performance. Indicators such as the ratio of marginal to average expenditure ascertain this efficiency. Resource efficiency reflects how well the system utilizes resources within its limits, and it is measured by the ratio of energy supplied to the maximum possible energy supply over a period. Emission efficiency pertains to environmental impact and is derived from the ratio of the

difference between feasible and expected emissions to the maximum expected emission reduction. These metrics facilitate the adoption of management and control approaches aimed at improving system sustainability.

9.2. Carbon Footprint Reduction

Smart grids significantly enhance technical, economic, and environmental aspects of conventional power systems. The strategic allocation of Distributed Generation (DG) units—including wind turbines, solar panels, and biomass generators—optimally reduces transmission losses and operational costs while respecting technical constraints (Parsa Sirat, 2018). Consequently, the careful placement of DGs is crucial for achieving substantial cost savings. One of the pressing challenges in modern power systems involves balancing supply and demand amid increasing renewable energy integration and the stochastic behaviors of electric vehicles and their drivers. Power electronics facilitate the seamless incorporation of renewables and strengthen system reliability through advanced metering, control, communication, and energy management functionalities. Key smart grid features such as demand response, distributed generation, energy storage, distribution automation, and self-healing capabilities collectively prevent failures or ensure rapid restoration. An improved carbon emission flow framework enables each load to trace its carbon flow rate, thereby assisting consumers in submitting accurate carbon quotas for trading markets (Yang et al., 2015). Based on this framework, an optimal dispatch strategy that accounts for large consumers and transmission losses seeks to minimize operational and power utilization costs. Simulations conducted on the IEEE 30-bus system confirm the strategy's effectiveness and reveal the influences of carbon pricing and generator types on dispatch outcomes. The implementation leverages Matlab R2010b and genetic algorithms, with a recommendation for more advanced computational techniques when addressing large-scale systems to maintain efficiency and accuracy.

Although the increasing adoption of clean energy sources mitigates emissions, a significant portion of grid demand remains reliant on carbon-intensive generation. To address this, emission-aware scheduling of distributed energy storage is formulated as an optimization problem. Employing a robust optimization approach caters to uncertainties in load forecasts, particularly under the intermittency of solar and wind resources (Jha et al., 2020). The resultant strategy achieves a reduction exceeding 0.5 million kilograms in annual carbon emissions, corresponding to a 23.3% decrease in electric grid emissions.

10. Policy and Regulation

Most power grids currently operate under monolithic utility ownership and increasing integration of distributed energy resources requires consideration of alternative market models and the development of new methods for integrating both generation and storage devices in the smart grid (Sindi, 2018). Progress presents many challenges for governments and regulators. Transitioning from traditional operating frameworks to a fully flexible and high-DER penetration environment necessitates significant systemic changes in current market and regulatory structures. Adapting to a changing resource mix entails reviewing existing regulatory and tariff structures and providing consistent price signals throughout the supply chain (Das, 2017). Philosophy suggests adoption of regulatory principles that adapt to uncertainty and highlight the need for greater consultation between regulators and system operators.

10.1. Government Incentives

Government incentives have played a significant role in developing the penetration, efficiency, sustainability, cost, and reliability of the smart grid (A. Brown & Zhou, 2012). Energy prices and net power injection constraints regulate the operational behavior of distribution grids and typically ensure that grid constraints are satisfied. During contingencies, customers can effectively contribute to preventing network outages by offering services to the network operator. An incentive mechanism can promote active user participation in providing distribution grid services by modifying the energy pricing scheme. These incentives can be described through a linear function whose parameters may be determined by the system operator by solving an engineering optimization problem. Feedback-based optimization algorithms enable the determination of optimal incentive parameters from grid measurements, even in the absence of full grid and user data (Cavraro et al., 2024).

10.2. Regulatory Frameworks

Electricity reforms in various countries have promoted deregulation of the electricity industry, with many countries pursuing deregulation globally (Sindi, 2018). Although smart grid projects are underway worldwide, a set of well-defined regulations for future implementation is not yet available. These projects face unresolved technical challenges

and threats arising from the lack of a comprehensive regulatory framework. For example, the absence of standards for smart grid communication can lead to incompatibility between devices from different vendors. There is no unique policy approach to smart grid development; different regions use diverse policies and business models based on their specific environments. Although broad consensus exists on the need to modernize the electric grid, regulatory policies present challenges that impede the diffusion of smart grid technologies (A. Brown & Zhou, 2012) and limit their ability to satisfy consumers. The existing regulatory environment reflects the way stakeholder interests and competing political forces converge to form coalitions in favor of specific policies. The fragmented nature of the electricity market, coupled with a complex technical and regulatory environment, creates inconsistent services and hinders the development of innovative products and services. The proliferation of new technologies in electricity generation and consumption has transformed the nature of regulation, whereas the demand for ancillary services and a variety of tariffs has led to the unbundling of previously vertically integrated functions.

11. Future Trends in Smart Grids

Advancements in Information and Communication Technologies (ICTs) facilitate efficient and cost-effective smart electricity distribution and storage. Building automation incorporates technologies such as Supervisory Control and Data Acquisition (SCADA) and Building Energy Management Systems (BEMS). SCADA enables the central control of distributed equipment using programmable logic controllers and intelligent electronic devices. BEMS optimizes energy generation, consumption, and storage in buildings through interconnected computers, sensors, and remote-control systems. Smart grids employ multi-objective optimization techniques to coordinate individual agents and optimize overall system performance. Many energy management systems seek a global optimum without considering individual entities' attitudes toward proposed solutions. Some approaches solve single-objective problems by converting conflicting objectives into a single, weight-dependent objective.

11.1. Integration of Renewable Energy

Because of worldwide environmental concerns, renewable sources are increasingly employed for power generation. The main problem related to their utilization is the unstable and unpredictable nature of wind and solar energy sources. At the smart grid

level, the use of a single alternative energy solution is inadequate; instead, a hybrid power system with more than one energy source is envisioned. Consequently, the integration of renewable energy resources in the grid is examined by highlighting the main aspects, challenges, and existing models. Electric systems are experiencing a remarkable revolution, with the smart grid becoming a reality in many countries. It is a modernized electricity system situated between the power plant and the consumer, endowed with innovative assets, including automated control, distributed intelligence, enhanced monitoring, smart sensors, advanced metering infrastructures (AMIs), smart appliances, and intelligent assets. Three different layers can be identified, each with specific missions: the component layer, the communication layer, and the application layer. A systematic architecture is proposed where, at the component level, generation, transmission, distribution, and consumption are encompassed as major components of the smart grid.

Conventional generators, distributed generators (DGs), storage units, electric vehicles, and prosumers produce energy at the generation level. Transmission infrastructure allows the generated energy to be conveyed through derived paths to distribution infrastructures, which supply power to consumers. Electrical loads are also characterized as significant components of a smart grid system. Figure 11.1 illustrates a typical HVAC grid configuration, also applicable to HVDC architecture and to different voltage levels of AC (primary, secondary, MV, and LV). It comprises a set of components, including transformers, switches, loads, and lines, each modeled according to the environment to be investigated. Load modeling may range from simple representations (e.g., fixed power or current) to complex formulations (e.g., composition of appliances, protection, and behavior models). Prosumers install photovoltaic and battery units at the consumer level, becoming producers as well. Their behavior can be characterized in terms of a load component or specified through dedicated profiles. Modern inverter-based renewable energy systems provide smart grid applications with an alternative to conventional plants for supplying active power and are capable of compensating voltage, reactive current, and harmonic distortion of linear and nonlinear loads at their point of common coupling. When included in a microgrid scenario, they offer the possibility to regulate voltage and frequency in the absence of grid support, prompting an updated definition of grid-code or regulation depending on the specific applications.

Renewable energy at the component level comprises renewable generation of electrical energy only, covering procedures and control of power units for PV and wind generators connected to the smart grid. Similarly, storage components represent the physical asset for storing available energy after production. Physical modeling of renewable sources

and storage units is detailed, delineating the structure and connections to the smart grid (Filipe Soares Pogeira, 2018) (Ramamoorthy & Ramachandran, 2016) (Strasser et al., 2015).

11.2. Advancements in Technology

Power systems have been undergoing rapid evolutions. Technological advances continue to transform traditional power grid systems to Smart Grid systems that integrate the communications infrastructures, distribution infrastructure, sensors, and control techniques to realize flexible power distribution networks, accommodate renewable energy sources, enable advanced metering and pricing, and provide user-oriented services (Sindi, 2018).

12. Case Studies of Successful Implementations

The electric power industry has made notable progress by integrating renewable energy systems, which presents a pathway to address environmental concerns and balance power generation with load demand. For instance, the problem of optimal operation of distributed energy storage systems in grid-connected microgrids can be formulated and solved through ADP-based control policies that take into account battery lifetime characteristics (Das, 2017). Similar challenges in multi-period studies are addressed through reinforcement or expansion frameworks that determine optimal size and allocation of new or existing distribution system equipment, such as substations, feeders, and transformers, while meeting technical and economic objectives (Sindi, 2018). Planning tools that incorporate stochastic techniques, multi-objective planning, and operational details show that optimal DG operation can provide voltage support at peak load and reduce power curtailment at minimum load, thereby increasing hosting capacity. However, solving allocation and sizing problems over longer terms requires more intricate load and DG representations coupled with algorithms for mixed-integer analysis. The strategic integration of DG, storage, and capacitor technologies further enhances the economic viability of smart grid investments. Nevertheless, long-term planning frameworks must still incorporate power curtailment and technical-constraint considerations to ensure comprehensive decision support.

12.1. International Examples

Smart grids play a critical role in utilizing renewable energy, whose disruption puts the whole system at risk. To increase sustainability, minimize investment, and reduce cost, Hatem Sindi suggests adopting an optimal economy-driven framework, as stated in Planning and Operation Framework of Smart Distributed Energy Resources in Emerging Distribution Systems (Sindi, 2018).

Hatem Sindi proposes a steer-by-wire framework to connect the estimation of services with the distribution system operator, electricity markets, and consumers. Economic principles define the operation, encouraging participation and enabling wide-scale application. A mathematical planning model optimizes location and size and aids operators in cost- and emission-efficient determination of system components.

12.2. Local Initiatives

A decentralized control method for a local electricity grid (microgrid) coordinates generation and consumption decisions of individual Distributed Energy Resources (DERs) to reduce energy costs. The approach employs the Alternative Direction Method of Multipliers (ADMM). Various scenarios demonstrate the coordination scheme's superiority over independent decision-making. In one scenario, the strategy lowers total expenses under variable energy tariffs. Another scenario ensures individual benefits for each user, even if the total benefit diminishes (Vinot et al., 2016). Multi-period studies address planning and operation of Smart Distributed Energy Resources (DERs) in emerging distribution systems. Expansion studies optimally size and allocate new equipment (substations, feeders, transformers) while serving technical and economic objectives and constraints. Reinforcement studies provide upgrade decisions on existing assets within technical and economic criteria. Three planning tools are identified: stochastic techniques, multi-objective planning, and system operational details. Operational aspects of distributed resources significantly influence the sizing and placement of installed units. Optimal operation of existing Distributed Generation (DG) systems offers two main benefits: voltage support at peak loading and minimal power curtailment at low loading, thereby increasing hosting capacity. Prior work applied linear programming (LP)-based Optimal Power Flow (OPF) in a single-year period for validation. Allocation and sizing problems require a more complex representation of loads and DG, coupled with algorithms capable of solving the resulting mixed-integer

problem over a longer horizon. Integration of DG, storage, and capacitors enhances the economic feasibility of smart grid investments. Nonetheless, long-term planning calls for operational details related to distributed generation power curtailment while satisfying reverse power constraints, alongside other technical conditions.

13. Stakeholder Engagement

A feedback system is advantageous, particularly for groups with lower interest in an SDS. Direct engagement and monitoring of all customer types constitute the primary focus of a successful transition. Multiple ownership and multiple stakeholder systems constitute the emerging framework and one that necessitates the inclusion of these stakeholders' goals. Conflicting objectives require compromises, and cooperative efforts become essential in future SDS planning (Sindi, 2018).

13.1. Community Involvement

Community involvement is necessary for the integration of distributed local energy systems into the utility-scale system. Current deployment modes for community energy-sharing systems include the island model, the interconnected model, and the Energy Service Companies model, along with other promising alternatives. Mathematical models are developed for the island model, the interconnected model, and the Energy Service Companies model, formulated as mixed-integer linear programming problems. A dedicated decomposition approach is introduced to enhance computational efficiency in large-scale cases. These models help to tackle key challenges in energy-sharing systems and facilitate community participation in the energy transition by addressing ongoing optimization problems. The models can be adapted for use in managing existing community energy-sharing systems or in the design of new ones, assisting policymakers, utility companies, and Energy Service Companies in the study of renewable energy investment projects. They contribute more broadly to the promotion of distributed renewable energy generation and the advancement of self-consumption within community energy-sharing frameworks (Ghaddar et al., 2024).

13.2. Industry Collaboration

Efficient communication among diverse parties plays a significant role in grid planning and resource allocation within emerging distribution systems (Sindi, 2018). Industrial actors possess a substantial market share in the power sector, and numerous algorithms aim to minimize the total cost of electricity during real-time operations. Coordinated resource deployment by distribution system operators tends to increase the electricity market price, whereas uncoordinated deployment has the opposite effect. Industrial operators can exploit this by adjusting real-time consumption in response to expected price trends from the day-ahead market. For this strategy to remain viable, strong collaboration, possibly via industrial associations or powerful energy management systems, is essential. Sharing aggregated loads enables operators to collectively optimize resource allocation, thereby reducing overall costs. Despite the attractiveness of a market-clearing-price approach, clarity regarding the governing organization remains a challenge.

14. Risk Management in Resource Allocation

Grid operators are faced with balancing uncertain supply due to renewables against flexible demand, which presents a two-sided risk management challenge. Delivering a balanced market clearing solution involves matching random supply bids and load bids that are functions of the zonal clearing prices. This formulation becomes tractable when supply bids are step functions, and load bids are strictly decreasing functions, aligning with the monotone-convex compositional programming framework. The resulting stochastic market clearing problem can be solved with a decentralized solver based on the alternating direction method of multipliers. An accept/reject decision scheme can eliminate cases where independent producers incur losses from delivering the committed power, which may be infeasible given the zonal clearing prices. Delivery performance can be enhanced through intra-hour bidding, allowing suppliers more frequent adjustment opportunities with the system operator (Zhang & B. Giannakis, 2015).

Risk-related challenges come into play with high penetration of mixed renewable energy sources (RES), such as solar and wind farm. The integration of renewables may introduce significant supply-demand imbalances into the smart grid. Advanced and scalable risk management schemes are needed to effectively hedge the violation of day-ahead commitments, in the absence of non-renewable generators, while hedging network congestion. A judicious optimal resource allocation balance of mixed generation units leads to economic dispatch, addressing this double energy-scheduling challenge.

Tractable formulations harmonize economic dispatch with the Conditional Value-at-Risk (CVaR) measure (Stover et al., 2022).

14.1. Identifying Risks

The risk assessment scheme for smart grids is based on a quantitative method where costs and energy losses are considered simultaneously. In a reliability program related to production cost and electricity sale, the total investment amounts to $1,921,000 with fixed costs of $94,090. When an accident occurs, risk assessment calculates damages while considering investments in reliability. The scheme proves reliable if the critical value remains below 75–80 % of the normal level. The assessment procedure involves identifying weak circuit sections, modeling electrical modes, defining reliability indicators, estimating failure probabilities, assessing damages due to energy under-supply, categorizing outage severity, and comparing damage costs with reliability-related investments. The system sustains reliability even when one transmission line is out of service, albeit with a slight increase in the critical sale volume (Andrukhova et al., 2017).

14.2. Mitigation Strategies

High-performance computing (HPC) strategies have focused on mitigating impacts of electro-magnetic, seismo-magnetic, or other geo-magnetic disturbances through approaches such as clustering, network reduction, and probabilistic analysis. Optimal placement of blocking devices in large power networks can minimize adverse effects during unpredictable geo-magnetic disturbances. While branch and cut algorithms offer optimal solutions for blocking-device placement, large-scale problems have become intractable in recent years. Alternative algorithms such as simulated annealing have been proposed to achieve near-optimal placements efficiently. By achieving economically feasible solutions, these enhancement strategies help maintain the reliability of smart-grids and day-to-day operation of power systems, even with increasing loads and environmental demands on electricity generation (Liang, 2019).

15. Conclusion

A study examined average comfort levels and total financial rewards across various demand response requests for a 100-resident system, presenting results for stochastic test problems that included total revenue calculations under real-time pricing and assessments of optimality percentages. Yearly simulations evaluated the impact of varying state-of-charge thresholds, while analyses of load profiles, personal preferences, and appliance priorities were conducted for a subset of ten residents. The investigation addressed challenges associated with incorporating renewable energy sources into smart grids, emphasizing the optimal operation of battery energy storage systems within microgrids. An approximate dynamic programming approach optimized control policies by accounting for battery lifetime characteristics, with performance benchmarks established against classical dynamic programming techniques (Das, 2017)..

References

Das, A. (2017). Efficient Energy Optimization for Smart Grid and Smart Community.

Liang, Y. (2019). High-performance computing for smart grid analysis and optimization.

Yuan Xu, F. (1970). Smart grid framework analysis and artificial neutral network in load forecast.

Sindi, H. (2018). Planning and Operation Framework of Smart Distributed Energy Resources in Emerging Distribution Systems.

Anwar, A. & N. Mahmood, A. (2014). Swarm Intelligence Based Multi-phase OPF For Peak Power Loss Reduction In A Smart Grid.

Huang, X., Lin, Y., Ruan, X., Li, J., & Cheng, N. (2023). Smart grid energy scheduling based on improved dynamic programming algorithm and LSTM. ncbi.nlm.nih.gov

Jamaledini, A., Khazaei, E., & Toran, M. (2018). Modified Genetic Algorithm Framework for Optimal Scheduling of Single Microgrid Combination with Distribution System Operator.

Alvarado Barrios, L., Rodríguez del Nozal, Álvaro, Tapia Córdoba, A., Luis Martínez Ramos, J., & Gutiérrez Reina, D. (2019). An Evolutionary Computational Approach for the Problem of Unit Commitment and Economic Dispatch in Microgrids under Several Operation Modes.

Schäfer, F., Menke, J. H., & Braun, M. (2020). Comparison of Meta-Heuristics for the Planning of Meshed Power Systems.

Ullah Khan, I., Ma, X., James Taylor, C., Javaid, N., & Gamage, K. (2019). Heuristic algorithm based dynamic scheduling model of home appliances in smart grid.

ZHANG, Y. A. N. G., Huang, T., & Bompard, E. (2018). Big data analytics in smart grids: a review.

Li, M. & Mohammadi, J. (2023). Toward Rapid, Optimal, and Feasible Power Dispatch through Generalized Neural Mapping.
Falconer, T. & Mones, L. (2021). Leveraging power grid topology in machine learning assisted optimal power flow.
Randall Eisen, M. (2019). Learning Optimal Resource Allocations In Wireless Systems.
Jdeed, M., Sharma, E., & Elmenreich, W. (2018). Smart grid modeling and simulation - Comparing GridLAB-D and RAPSim via two Case studies.
Parsa Sirat, A. (2018). Loss Minimization through the Allocation of DGs Considering the Stochastic Nature of Units.
Michael Flath, C. (2013). Flexible Demand in Smart Grids - Modeling and Coordination.
Li, H. & C. Qiu, R. (2010). Need-based Communication for Smart Grid: When to Inquire Power Price?.
Ahmadzadeh-Ghahnaviehei, S. (2017). Real-time pricing algorithms with uncertainty consideration for smart grid.
Yang, J., Feng, X., Tang, Y., Yan, J., He, H., & Luo, C. (2015). A Power System Optimal Dispatch Strategy Considering the Flow of Carbon Emissions and Large Consumers.
Jha, R., Lee, S., Iyengar, S., H. Hajiesmaili, M., Irwin, D., & Shenoy, P. (2020). Emission-aware Energy Storage Scheduling for a Greener Grid.
A. Brown, M. & Zhou, S. (2012). Smart-Grid Policies: An International Review.
Cavraro, G., Comden, J., & Bernstein, A. (2024). Feedback Optimization of Incentives for Distribution Grid Services.
Filipe Soares Pogeira, J. (2018). Implementing Dynamic System Reconfiguration with Renewables Considering Future Grid Technologies: A Real Case Study.
Ramamoorthy, A. & Ramachandran, R. (2016). Optimal Siting and Sizing of Multiple DG Units for the Enhancement of Voltage Profile and Loss Minimization in Transmission Systems Using Nature Inspired Algorithms. ncbi.nlm.nih.gov
Strasser, T., Andrén, F., Kathan, J., Cecati, C., Buccella, C., Siano, P., Leitão, P., Zhabelova, G., Vyatkin, V., Vrba, P., & A. Mařík, V. (2015). A review of architectures and concepts for intelligence in future electric energy system.
Vinot, B., Cadoux, F., & Héliot, R. (2016). Decentralized optimization of energy exchanges in an electricity microgrid.
Ghaddar, B., Ljubic, I., & Qiu, Y. (2024). Three Network Design Problems for Community Energy Storage.
Zhang, Y. & B. Giannakis, G. (2015). Distributed Stochastic Market Clearing with High-Penetration Wind Power.
Stover, O., Karve, P., Mahadevan, S., Chen, W., Zhao, H., Tanneau, M., & Van Hentenryck, P. (2022). Just-In-Time Learning for Operational Risk Assessment in Power Grids.
Andrukhova, A., Lenmirovna Batseva, N., & Mikhailovna Evseeva, A. (2017). Analysis of risk assessment algorithm from power supply interruption due to transmission line fault.

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Chapter 9: Optimization Techniques for Sustainable Transportation Logistics Using Metaheuristic Algorithms

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Abstract: Sustainable transportation logistics has emerged as a crucial area in supply chain management, addressing the rising demand for environmentally responsible and cost-effective logistics solutions. This paper explores the application of metaheuristic algorithms to optimize complex transportation logistics systems, considering environmental and economic objectives. The study begins by highlighting the challenges posed by rapid urbanization, population growth, and the environmental impact of traditional logistics operations, including increased CO_2 emissions and fossil fuel consumption. It discusses how green logistics and intermodal transportation offer alternatives that integrate sustainability into operational practices. Metaheuristic algorithms—such as Genetic Algorithms, Ant Colony Optimization, Simulated Annealing, and Particle Swarm Optimization—are emphasized for their efficiency in solving NP-hard problems like vehicle routing, scheduling, and location-routing under multiple constraints. These algorithms outperform traditional methods by finding near-optimal solutions in large, dynamic, and uncertain search spaces. The paper also presents several case studies demonstrating successful implementation of metaheuristics in urban, rural, and intermodal transportation contexts, achieving substantial reductions in delivery costs and emissions.Moreover, the work evaluates algorithmic performance and highlights the significance of hybrid methods and decision-support systems in addressing real-world logistics complexity. Challenges in scalability, data availability, and integration with existing Transport Management Systems (TMS) are also

explored. Overall, the study contributes to the field by proposing optimized models for sustainable transportation logistics, fostering eco-efficiency and resilience in global supply chains..

Keywords: Sustainable Transportation Logistics, Metaheuristic Algorithms, Vehicle Routing Problem (VRP), Green Supply Chain, Optimization Techniques.

1 Introduction

Sustainable transportation logistics integrates economic, environmental, and social imperatives within a multi-stakeholder context to address the increasing complexity and growth of distribution activities (Validi et al., 2020). The distribution side of supply chains, encompassing the transport of finished goods to final customers, presents key challenges that have inspired research efforts aimed at optimizing distribution strategies. A prominent issue relates to the environmental impact of distribution, which is rising concurrently with commercial expansion and the strong growth of transportation demand. The development of cost effective and environmentally friendly routing strategies represents a critical lever to reduce CO2 emissions and other pollutant gases generated by vehicle fleets. In this context, route optimization extends beyond minimizing the distance covered, highlighting the need for robust methods capable of managing the large size of logistics systems and real-time requirements, while simultaneously ensuring superior performance.

Metaheuristics constitute a promising framework suitable for addressing this category of problems. The capacity of metaheuristics to explore particularly large and complex search spaces has progressed in alignment with the growing complexity of logistics systems; they have been widely utilized in transportation, distribution, and logistics issues. Furthermore, the inherent scalability of metaheuristics eases eventual adaptations in tune with the expansion of logistics systems and service area extents.

2. Sustainable Transportation Logistics

Sustainable transportation logistics aims to develop efficient and optimized transportation planning and routing capable of accommodating fluctuations in demands and mitigates issues related to increasing associated costs and emissions from transportation activities (Validi et al., 2020). Recent supply chain structures have

become increasingly complex and multi-faceted, involving a wide range of stakeholders, such as shippers, customers, delivery companies, and third-party logistics providers. Strategic decisions within such structures encompass selection of intermediate facilities, design of distribution networks, and determination of suitable transportation modes, while tactical decisions include allocation of customers to facilities, planning of shipment quantities, and scheduling of pick-ups and deliveries. Sustainable transportation logistics aims to develop efficient and optimized transportation planning and routing capable of accommodating fluctuations in demands and mitigates issues related to increasing associated costs and emissions from transportation activities. Recent supply chain structures have become increasingly complex and multi-faceted, involving a wide range of stakeholders, such as shippers, customers, delivery companies, and third-party logistics providers. Strategic decisions within such structures encompass selection of intermediate facilities, design of distribution networks, and determination of suitable transportation modes, while tactical decisions include allocation of customers to facilities, planning of shipment quantities, and scheduling of pick-ups and deliveries.

2.1. Definition and Importance

Transportation plays a crucial role in ecology and environmental problems as it is responsible for the largest share of total energy consumption (Mehdizadeh & Afrabandpei, 2012). Designing and planning transportation in multi-stage, multi-product supply chain networks that involve suppliers, distribution centers, and customers are vital topics for transportation managers. The goal is to find the optimal number of routes and vehicle types within a limited budget. The problem can be formulated as a mixed-integer nonlinear programming (MINLP) model aimed at minimizing both transportation and holding costs of products and vehicles. Due to its NP-hard nature, the problem requires alternative solution techniques such as metaheuristics; the literature contains many metaheuristic algorithms with various efficiencies.

2.2. Current Challenges

Rapid urbanization and population growth have significantly increased fossil-fuel emissions in the transportation sector. This expansion elevates the cost of fuel and maintenance, both of which are important considerations in the viability of supply chains and in the preferences of both suppliers and customers for green products. The depletion of resources and loss of biodiversity greatly impacts future generations and can

overwhelm the planet, threatening its capacity to sustain life. Transportation and distribution systems influence the environment through emissions of toxic gases, the release of suspended pollutants, and reliance on fossil fuels, which ultimately decrease the sustainability of the supply chain. Furthermore, the added challenge of potentially unconventional transportation vehicles or network components may increase the complexity of determining the optimal design for the system and lead to increased emissions and transportation costs (Validi et al., 2020).

2.3. Impact on Environment

Green logistics has become a major concern for logistics stakeholders throughout the supply chain and especially for transportation planners (Demir et al., 2019). Its objective is to observe, measure, and minimize the ecological impact; transportation planning can no longer ignore these requirements. Freight carriers have started to pay more attention to the negative externalities of their operations, such as CO2e emissions. The latter must therefore be quantified accurately. Reducing emissions also presents advantages for the logistics providers. Besides, transportation companies rely heavily on Transport Management System (TMS) software to plan, execute, and monitor their activities. Recent advances focus mainly on the management of logistics operations in highly dynamic and stochastic environments. The complexity and non-deterministic nature of shipments generate fundamental changes to the conception of planning approaches. To make each effort sustainable, logistics operations need to be optimized efficiently.

Since the determinants of the final freight transportation mode choice are usually changed, the intermodal transportation model is an innovative transportation mode that has become an attractive transport alternative, satisfying the limitations on freight transportation. The intermodal freight transportation has received considerable attention among challenges due to the rapid growth of the economy and environmental concerns. Intermodal transportation is also considered a green and sustainable transportation strategy, because greenhouse gas emissions from intermodal transportation are less than for other transportation modes, especially road transportation (Validi et al., 2020). This study proposes an intermodal freight transportation model between pairing locations, including fixed and flexible-feeder service modes for further addressing economic and environmental issues. In this regard, an innovative green approach based on bi-objective optimization is proposed by considering two conflicting objectives minimizing transportation cost and CO2-e emissions simultaneously.

Sustainable transportation concerns the development of services and infrastructure in an efficient way that does not harm the social and environmental aspects of a place while meeting users' needs. A sustainable transportation strategy promotes the benefit of economy, environment, and society. On the other hand, transportation activities are the most significant sources of air pollution and greenhouse gases. Due to the fact that logistics operations have a significant impact on a company's carbon footprint as well as a considerable impact on cost, designing an efficient outbound logistics plan is a critical element when it comes to the sustainable movement of products.

3. Optimization Techniques Overview

Optimization refers to a collection of mathematical methods designed to identify the most effective parameters or variables that optimize a particular objective function subject to certain constraints. The primary goal of optimization is to determine the best system configuration that maximizes or minimizes the objective function according to specific criteria (Validi et al., 2020). Transportation logistics optimization model, therefore, incorporates a wide array of business and economic factors as decision variables, addressing various transportation problems such as route planning, load optimization, mode selection, inter-terminal distribution, fleet scheduling, and production planning. A sustainable three-echelon bi-objective integrated location-routing optimization model, for example, considers multiple interconnected decisions to design a logistics network that enhances sustainability. This model integrates demand-side supply chain considerations and utilizes the Analytic Hierarchy Process to align vehicle selection with decision-makers' priorities. Given the NP-hard nature of the problem, a two-phase approach is adopted: the first phase manages transportation from plants to distribution centers and retailers, while the second phase identifies non-dominated Pareto optimal routes. A meta-heuristic method combining a Multi-Objective Genetic Algorithm and TOPSIS facilitates the search for optimal, realistic solutions. The model aims to minimize CO2 emissions and transportation costs on the demand side, employing two distinct vehicle fleets for different transport stages. Routes are differentiated by road type and speed limits to accurately represent transport conditions.

3.1. Need for Optimization

The growing demand for transportation services has sparked a surge in energy consumption and pollutant emissions by the logistics sector. Optimizing transportation

contributes to sustainable development by reducing costs and environmental impacts and helps cut costs and travel times at container terminals (Gulić et al., 2018). Multi-objective models have been developed for optimizing intermodal freight transportation to reduce operational costs and environmental consequences such as greenhouse gas emissions. Green logistics minimizes ecological impact by integrating environmental, economic, and social considerations to support corporate, regional, and global sustainability. Incorporating environmental aspects into freight transportation planning requires a holistic approach, a view that transportation companies should adopt. The use of environmental feasibility studies will be increasingly considered by regulators before granting access to infrastructure and at various stages of a carrier's life cycle. Transport Management System (TMS) software now supports planning, execution, and monitoring, supplemented by methods and algorithms that address realistic, dynamic, and stochastic conditions (Demir et al., 2019). Urban freight distribution has gained prominence due to increasing freight transport demand. The logistics activities at ports and terminals underpin the global supply chain and passenger traffic, with navigation, fleet management, and logistics services depending more on public and private information systems that exploit static and real-time data.

Optimizing supply chain management has become the cornerstone of many strategic decisions, as multinational firms face stiff competition. The design phase is crucial to define the supply chain before operation, along with decisions on sourcing, dynamic requirements, and manufacturing processes. Modelling and measuring work-in-progress inventory through different SCM systems maintain synchronization with customer demand and manage production. The increased complexity of supply chains aggravates synchronization problems when a robust plan is not devised, while real-time monitoring helps analyze deviations in scheduled and actual activities (Hfeda, 2018). Comprehensive freight optimization models integrate cost and environmental dimensions to identify green transportation plans. Shipping companies prioritizing sustainability seek methods or business models to optimize operational performance, decrease air pollution, and enhance energy efficiency. Parameters such as distance, payload, and shipping technique influence the calculation of emissions, and higher customer service levels are tied to increased energy consumption.

Designing optimal collection logistics routing plans mitigates economic and environmental impacts by reducing fleet size and optimizing vehicle routes. Improving transport vehicle productivity through optimized work schedules minimizes transfer times and empty distances. Minimizing crane waiting times and synchronizing vertical with horizontal transport at a terminal's container yard are pivotal to quality logistics.

3.2. Traditional Methods vs. Metaheuristic Algorithms

Transportation companies use Transport Management System (TMS) software for planning, execution and monitoring and seek new methods to handle the dynamic and stochastic nature of real-world transportation. Traditional planning becomes complex, with larger shipments leading to non-deterministic problems that are difficult to solve rapidly (Demir et al., 2019). Metaheuristics-based optimisation reduces transport costs and environmental impacts of intermodal solutions and uncovers new, more sustainable solutions for large problems. Vehicle Routing Problem (VRP) optimisation can achieve significant fuel savings, useful for last-mile and same-day deliveries. VRP encapsulates a NP-hard problem: allocating resources to customers at lowest cost. Exact methods are computationally infeasible, so heuristic and metaheuristic methods seek near-optimal solutions. Heuristics explore promising search space areas and divide into constructive, two-phase and improvement methods. Constructive heuristics rapidly build solutions; improvement methods refine existing solutions, with higher compute times. Enhanced computing power boosts metaheuristics' accuracy (Peric et al., 2024).

Optimising container loading from the stacking area to rail trains requires maximising transport productivity through work schedules that minimise transfer times, vehicle travel distances and crane waiting times at both stacking and railhead areas. Horizontal and vertical transport synchronisation guides logistics. Genetic algorithms addressed specific issues. Because container-transfer optimisation is NP-hard, metaheuristics produce good solutions. Established variants include genetic algorithms, ant colony and particle swarm optimisation, but nature-inspired methods such as artificial bee colony, firefly and bat algorithms emerge as promising alternatives and often outperform traditional approaches (Gulić et al., 2018).

4. Metaheuristic Algorithms

The Vehicle Routing Problem (VRP) is highly applicable for motor carriers and is considered computationally difficult because the number of potential solutions typically grows exponentially with problem size, often requiring excessive time for exact methods to find optimal solutions. Consequently, exact-exponential methods are limited to small problems, and more efficient approaches are needed.

Heuristic methods deliver high-quality solutions in reasonable time without guaranteeing optimality and are often classified as constructive methods, two-phase methods, or improvement methods (Peric et al., 2024). Constructive methods produce a solution by successively adding new elements, while two-phase methods generally first determine the assignment of customers to vehicles and subsequently find a minimum cost sequence for the customers assigned to each route. Improvement methods take an existing feasible solution and attempt to improve it using local-search procedures. Improvement methods tend to yield solutions with smaller average suboptimality but require longer execution time.

Many meta-heuristics, which are generally more computationally expensive than heuristic methods, have received considerable attention. Examples include simulated annealing, tabu search, genetic algorithms, Ant Colony Optimization (ACO), and Variable Neighborhood Search (VNS). Metaheuristic algorithms have been proposed to solve routing problems such as multi-objective vehicle routing (Validi et al., 2020). Both tabu search and variable neighborhood search methods have been successfully applied to real-world vehicle routing problems. Metaheuristic methods can be applied to instances of realistic size and frequently outperform classical heuristics.

4.1. Genetic Algorithms

Genetic algorithms (GAs) are nature-inspired metaheuristics guided by Darwin's principle of natural selection, that is, "survival of the fittest." Since the introduction of genetic algorithms in 1975, these solution methods have found applications in a wide range of fields and, in particular, many application-driven variants. Genetic algorithms maintain a population of candidate solutions (encoding each solution to the problem at hand as an artificial chromosome) and manipulate them through genetic operators—such as crossover, mutation, and reproduction—to generate alternative solutions. Efforts to overcome some of the shortcomings of the basic model have resulted in a plethora of genetic algorithm variants, such as the introduction of new selection strategies, the development of alternative encoding techniques, the use of multiple and hierarchical populations, the integration of local search procedures, and the hybridization with other optimization methods and solution strategies.

An instance of reverse logistics for waste (RLW) determines the flow of a waste (e.g., plastic household waste) from a group of waste generation nodes (GNs) through a

hierarchical system of waste recycling facilities (WRFs) to be finally disposed at one (or more) final disposal plants (FDPs). Metaheuristic methods were used to solve a rock and mineral business supply chain problem in Chile, to address the waste collection–transfer–disposal problem for hazardous waste in Bulgaria, and to analyze the cost and location problems in reverse logistics of waste (Serrano Elena, 2016). Several crossover operators (e.g., single-point, multiple-points, linear order crossover, uniform crossover, and position-based operators) were tested and compared for solving the vehicle routing problem with soft time windows (VRPSTW) (Josef Geiger, 2008). The results revealed that problem structure, especially customer distribution, strongly influences algorithm behavior. Genetic algorithms outperform local search approaches in complex problems with dense and small time windows and random customer distribution. Mutation operators were found to have a stronger impact than anticipated, highlighting the significance of simple mutation methods. In contrast, the studied crossover operators proved relatively weak for the multi-objective problem as they failed to effectively recombine desirable structures. The study concluded that the development of specific multi-objective operators remains necessary and that combining genetic operators with local search heuristics represents a logical progression based on the findings.

4.2. Ant Colony Optimization

The ant colony optimization (ACO) is another metaheuristic technique inspired by the foraging behavior of ants. In nature, ants search for food by laying down a pheromone trail. Other ants follow this trail but also explore randomly for other food sources. Eventually, the trail to the nearest food source receives the highest concentration of pheromone, since food can be fetched fastest in large quantities, and thus attracts more ants travelling from and returning to the colony. In ACO, a set of artificial "ants" is deployed each iteration in parallel. The state transitions of ants build a solution in a probabilistic way generating new solutions from previous ones. These constructed solutions are evaluated and pheromone information is updated accordingly. The pheromone update guides the search in the proceeding iteration by biasing the transition probabilities towards decisions that have yielded better solutions. The search process terminates when the pheromone information is sufficiently converged or when some terminate criterion—such as a time- or iteration-bound—is reached.

4.3. Simulated Annealing

Simulated annealing (SA) originated from the annealing procedure in metallurgy where, by slowly cooling, a material's internal structure achieves a minimum energy configuration at each temperature. This concept was adapted for optimization by Kirkpatrick, Gelatt, and Vecchi (1983), who treat the objective function to minimize as the energy of the system at a given configuration. The algorithm initializes at some reference temperature and an initial configuration. New configurations are sampled from the neighborhood of the current configuration. If the new configuration yields an improvement in the objective function, it is always accepted. Otherwise, it is accepted with a probability that depends on how much worse it is and on the current temperature. This mechanism allows the algorithm to escape local minima by moving to worse solutions early on, with this possibility gradually diminishing as the temperature decreases according to an annealing schedule. Solutions can be continuous or discrete, with the latter common in combinatorial optimization. In transportation logistics, SA has been applied to problems such as railway timetabling and vehicle routing. For the vehicle routing problem with time windows (VRPTW), SA explores the solution space by randomly performing moves like 2-opt and 3-opt, where feasible positions for relocating customers are sampled uniformly but only moves that maintain feasibility with respect to capacities and time windows are considered ((Titi) Iswari, 2017). Further work has combined SA with variable neighborhood search (HRSA-VNS) to enhance solution quality and diversification capabilities for the VRPTW (Iswari, 2017). In all applications, the solution quality improves monotonically with execution time, making SA a graceful degradation algorithm well-suited to real-time decision-making scenarios.

SA's domain of application also extends beyond transportation logistics. For example, it is used in the calibration of climate system parameters and the design of speckle-reducing laser modulation signals, both requiring the exploration of complex, rugged search spaces. Given its efficacy in these diverse fields and the extensive existing literature, SA is frequently employed as a reference or baseline for benchmarking newly proposed metaheuristics.

4.4. Particle Swarm Optimization

Particle swarm optimisation (PSO) is a metaheuristic developed in 1995 that is inspired by the social behaviour of a flock of birds. It is one of the most widely researched metaheuristics since its introduction, attracting more attention than any other swarm-intelligence technique. PSO has been combined and hybridised with other metaheuristics; for example, with genetic algorithm, particle swarm with levy-flight and

A-star, external-memory-based chaotic PSO, and multi-objective QPSO. It has application across diverse domains such as engineering, routing, scheduling, anomaly detection, job-shop scheduling, pattern recognition, health, decision-making, modelling, robot path planning, variable selection, neural network training, protein-folding, assembly optimisation, mining, target operation allocation, crop yield optimisation, economy and marketing among many others.

Solving optimisation problems with a metaheuristic involves a search for an optimal or near-optimal solution among a large combination of solutions in a solution space. In this process, all the possible solutions to the problem are represented as points in the space, and each of these points has associated coordinates also referred to as position. Based on a specific criterion, the points are evaluated for their fitness and each point has an associated value referred to as the fitness value. In metaheuristic terminology, solution points in the solution space are referred to as particles and each particle represents a potential solution to the optimisation problem. Similar to particles in the physical world, the particles in PSO scientific discipline move through the solution space by a series of fitness-driven leaps (Ab Wahab, 1970).

Table-01 Comparative Study

Authors	**Year**	**Objective**	**Findings**	**Limitations**
Laura Antón, Marina Leal, José Luis Sainz-Pardo	2021	To optimize trip planning for electric vehicles using wireless support.	Developed methods that improve energy efficiency and reduce travel time for electric vehicles.	Limited to specific types of electric vehicle networks.
Hanwen Liu, Xiaobing Liu, Sardar M. N. Islam, et al.	2021	To design a strategy for low-carbon vehicles and optimize route planning.	Proposed a combined strategy that enhances sustainability while meeting	Assumes accurate demand forecasting, which may not always be possible.

			customer demand.	
Angel Alejandro Juan, Carlos Alberto Mendez, et al.	2016	To survey the operational challenges of electric vehicles in logistics and transportation.	Identified challenges like infrastructure, cost, and operational inefficiency in EV deployment.	Lacks quantitative data and focuses mainly on qualitative insights.
Marko Gulić, Livia Maglić, SanjinValčić	2018	To explore nature-inspired metaheuristics for container terminal optimization.	Showed that metaheuristics significantly improve logistic operations at container terminals.	Applicability may vary based on terminal size and type.
Antonio Serrano Elena	2016	To analyze metaheuristic approaches in reverse logistics for waste management.	Metaheuristics effectively optimize waste collection routes, reducing costs.	Focuses primarily on local scenarios, limiting broader applicability.
Bartosz Sawik, Javier Faulin Fajardo, et al.	2017	To perform a multicriteria analysis for green vehicle routing problems (VRP).	Developed a model integrating environmental criteria, resulting in lower emissions.	Model complexity increases with the number of criteria considered.
Sahar Validi, Arijit Bhattacharya, P.J. Byrne	2020	To design a sustainable distribution system using a	Balanced cost, service level, and sustainability through	Requires extensive computational

		metaheuristic approach.	systematic design.	resources for large datasets.
Romanov Petr, Romanova Irina	2019	To model logistics processes in urban environments.	Optimized urban logistics, improving delivery efficiency and reducing congestion.	Urban models may not translate well to rural logistics.
Hanwen Liu, Xiaobing Liu, Sardar M. N. Islam, et al.	2021	To optimize strategies for low-carbon vehicle routes.	Developed a model for reduced emissions and increased efficiency in logistics.	Relies on the assumption of stable vehicle performance metrics.
Camelia-M. Pintea, Petrica C. Pop, Mara Hajdu-Macelaru	2012	To address transportation problems with gas emission constraints.	Proposed hybrid methods that minimize gas emissions while maintaining efficiency.	Results may not apply to all transport contexts due to varying operational rules.

5. Application of Metaheuristic Algorithms in Logistics

Metaheuristic algorithms find extensive applications in addressing location routing, vehicle routing, and supply chain optimization problems within the logistics sector. For instance, ant colony algorithms, Tabu Search, and hybrid heuristics have been tailored to solve green location-routing problems that emphasize sustainable supply chain management. Such algorithms facilitate the minimization of carbon emissions during product transportation and distribution, as demonstrated in complex location-routing studies featuring bi-objective frameworks that integrate the Analytic Hierarchy Process

(AHP). Beyond green logistics, metaheuristic approaches have also been employed to develop eco-friendly distribution systems, optimize recycling logistics in multi-echelon networks, and balance profitability with environmental considerations in green supply chains (Validi et al., 2020). Complementing algorithmic developments, modelling and analysis techniques for intermodal freight transportation incorporate environmental criteria to support the design of transportation practices that advance ecological performance. Bi-objective models applied to real-world scenarios underscore the feasibility of integrating operational efficiency with sustainability goals. Transportation companies leverage Transport Management System (TMS) software equipped with advanced algorithms to plan, control, execute, and track activities, a necessity driven by increased market demands, operational complexity, and the dynamic, stochastic nature of transportation networks (Demir et al., 2019).

5.1. Routing Problems

Routing problems represent a large family of vehicle path design issues (Validi et al., 2020). These problems describe additional constraints or extensions to the original vehicle routing problem. In typical cases, a given fleet of vehicles is available at a designated depot, and the objective is to select and visit customers by satisfying a number of constraints. Various heuristic algorithms are investigated to find optimal routes for freight transport vehicles. The main goal is to identify routes that enable distances to be covered in the shortest possible time, thereby reducing traffic and considering transport costs, social impact, clearance times, and delays (Zadobrischi & Negru, 2022). Classic routing methods, heuristic algorithms, and standard algorithms such as bee swarm, ant colony, and parallel heuristic searches are used in the analysis.

5.2. Scheduling Issues

The scheduling issue has attracted much attention in the literature owing to the crucial role of scheduling in transportation. Efficient scheduling can minimize the transport time and cost while increasing mobility and customer service. Vehicle scheduling is a particularly crucial task since improper vehicle schedules may lead to imbalanced demand and supply, wasted labour and resources, as well as insufficient or delayed services and late shipments. Indeed, the problems experienced by the transportation system can be accentuated even by a good vehicle-designing solution, when an inappropriate schedule is used (Ionut Andreica et al., 2009).

Optimizing delivery schedules is a primary concern for last-mile logistics (E Dunbar et al., 2018). The vehicle routing problem with time windows is a widely studied model for scheduling and routing under bounded delivery delay. The problem involves assigning a set of customers to a finite set of vehicles from a depot and designing routes and schedules for the vehicles so that all customers are served within their time windows and the total cost of the routes is minimized. The solution is a collection of vehicle routes and an associated service schedule such that the overall routing cost is minimized and the time window of each customer is respected; each vehicle starts (and ends) at the depot and each customer is served by a single vehicle, within its time-window constraints.

5.3. Inventory Management

Inventory management involves optimizing the quantity and storage of stock on hand, as well as its replenishment, to meet demand efficiently. Effective inventory management reduces costs and the risk of stockouts while improving overall supply chain performance. Available techniques include demand forecasting, safety stock calculation, and replenishment policies designed to accommodate fluctuations in demand (Validi et al., 2020). Integration with logistics and transportation strategies is critical when developing sustainable, responsive supply chains.

In the automobile industry, each vehicle requires between 2,000 and 4,000 components (Hfeda, 2018). A manufacturing plant studied in Germany produced 850 vehicles daily, of which only 15 shared identical component combinations. Complex supplier arrangements ensure that multiple suppliers deliver components to various assembly plants, while supply methods depend heavily on picking frequency and transport volume. Direct deliveries enable larger lot sizes and reduced storage but incur higher transport costs for each supplier visited. Centralized deliveries to a dock center allow easier consolidation but increase handling costs and trailer utilization rates. Primarily two types of delivery arrangements are in use: direct shipping, characterized by simplicity but large lot sizes and high inventories, and centralized shipping with cross-docking operations, which lowers transportation costs and inventory levels but involves greater coordination complexity. SC flow in automobile manufacturing is evolving from a push-centered model relying on forecasts and stable production schedules to a pull-based approach driven by actual customer demand. However, the transition presents challenges since order lead times generally exceed the desired delivery window, motivating the adoption of lean SC strategies.

6. Case Studies

The implementation of metaheuristic algorithms in the optimization of sustainable transportation logistics is exemplified by three case studies. Each applies a different metaheuristic approach to a problem characterized by attributes that include environmental constraints, multimodal transport options, and stochastic demand.In the first, a hybrid approach combines simulated annealing and genetic algorithms to determine optimal locations for distribution centres, assign customer demand across multiple products, and design vehicle routes to minimize distribution system costs (Validi et al., 2020). The resulting optimisation model respects capacity and time-window constraints, effects a two-phase design of experiments (DoE) screening of solution parameters, and employs an analytic hierarchy process (AHP). A large-scale, three-echelon supply network is used as a case study.

The second studies green intermodal freight transportation with a simultaneous focus on cost and emissions minimization (Demir et al., 2019). The integrated green transportation network combines road and rail as the problem is formulated as a bi-objective pick-up and delivery value-routing problem. After a comparison of solution methods, the Pareto front is explored using the ε-constraint approach. An instance-transfer based local search, which is shown to advance the efficacy of each method, is introduced and the solution strategy is applied to the Danish railway system. The third employs an adaptive memory procedure (AMP) to solve a real-world vehicle routing problem that honours requirements for capacities, time windows, heterogeneous vehicles, time-dependent routes, multi-trip delivery, crew skills, split delivery and dynamic fuel consumption (Peric et al., 2024). Stochastic distribution attributes are accommodated through a dropout factor in a Clarke-Wright (CW) initialisation routine. The local-iterated AMP procedure discretely navigates the solution space with an escape facility that enable reductions in both delivery times and transportation costs.

6.1. Case Study 1: Urban Logistics

In large metropolitan areas, it is imperative to seek management solutions that simultaneously increase the efficiency of goods transportation and reduce its environmental impacts. Modern traffic management systems strive to curb congestion by controlling traffic flows either within the network or in the vicinity of critical intersections. Logistics flows are consequently optimized with the help of routing and

scheduling techniques. A case study based on the supply of retail outlets is proposed to illustrate the field of application.

Commercial activities in urban areas have become sensitive to the current economic and environmental context. Older retail outlets and franchised outlets with an important logistics component have both a high frequency of goods transportation and a large consumption of private vehicles, respectively. Various types of goods are often delivered from warehouses located in a large urban area to commercial outlets that specialize in such products. These goods are often transported by a dedicated fleet of vehicles using motorways at the inner city entrance or traversing the city whom length and travel time distributions are uncertain due to incessant traffic congestion. Planning vehicles' routes to supply these outlets is consequently challenging. This problem, which is not addressed by usual modelling and optimisation tools, is a relevant issue for service inefficiencies and environmental impact (Petr & Irina, 2019). The strategy to reduce transportation time is twofold. From a macro model standpoint, one objective is to forecast the origin of congestion and its possible spread. The other objective is, given the complex turn assignment at each network node, to reduce the traveling time of an individual vehicle using route choice. Offering alternative systems for goods delivery at urban scale would also contribute to this challenge. Various systems have emerged since the 1970s and are implemented in several cities. These systems could reduce the number of vehicles by consolidating freight flow, differentiate the origin of these flows, and reduce the distance traveled by goods.

In the case of supply to stores, most companies invest their resources in large outlets; therefore, large vehicles are the only ones authorized to reach each retail outlet with the product. The homogenous fleet model corresponds to this type of working such that all vehicles are of the same size and volume. While goods may be carried by smaller vehicles, the selection of transport capacity and production levels is not the focus, as the fleet size, vehicle size, and discrete production levels are fixed to simplify the model (Jiang et al., 2019).

6.2. Case Study 2: Rural Transportation

Innovating approaches in transportation logistics remains central to economic and sustainable development. Rural transportation presents particular challenges for effective distribution. A logistical network supporting villages remote from regional

centres offers a further case study. A bi-objective location-routing model aims to minimize CO2 emissions and transportation costs in a three-echelon supply chain. Two vehicle fleets serve extensive networks from processing plants to distribution centres and from centres to retailers. Distance and time criteria feature prominently. A design of experiments methodology supports a meta-heuristic optimization procedure. The location-routing model divides decisional complexity into inter-connected phases. Phase-I specifies transportation from plants to multiple distribution centres and from centres to retailers. Phase-II applies Phase-I outcomes to determine non-dominated, Pareto-optimal routes among retailers. The model allocates centres to plants and retailers to centres, routing vehicles accordingly. Adaptive memory metaheuristics and local search improve routing for real-world vehicle problems that include capacities, time windows, heterogeneous vehicles, dynamic fuel consumption, multi-trip delivery, skills, split delivery, and time-dependent routes. An extended Clarke-Wright algorithm incorporates a stochastic dropout factor in initial planning. Benchmarks and real cases report average savings of 2.03% in delivery time and 20.98% in total delivery costs. (Peric et al., 2024) (Validi et al., 2020)

6.3. Case Study 3: Intermodal Transport

Transportation is a significant source of environmental pollution, and about 80% of goods movement is by road alone. Efficient planning of freight transportation requires a comprehensive look at a wide range of factors to ensure safe, fast, and environmentally suitable movement of goods while offering flexibility and the right type of transport model to meet requirements (Demir et al., 2019). Combining transportation modes for a reliable network offers flexible and environmentally friendly alternatives to move high volumes of goods over long distances. To reflect the advantages of each mode, models and algorithms are developed and implemented in Transport Management System software.

7. Performance Evaluation of Algorithms

Metaheuristic tools inspired by natural phenomena provide effective strategies for solving complex combinational optimization problems. In this work, five metaheuristic algorithms—Artificial Bee Colony (ABC), Particle Swarm Optimization (PSO), Firefly Algorithm (FA), Genetic Algorithm (GA), and Differential Evolution (DE)—were implemented to address a transportation system featuring multiple production plants and

customer locations. All algorithms incorporated an identical encoding scheme to ensure uniformity in solution representation. Comparative results revealed that ABC (Peric et al., 2024) delivered superior solutions by a considerable margin and exhibited the quickest convergence rate. In contrast, PSO (Serrano Elena, 2016) , despite its fast convergence, produced solutions of noticeably inferior quality. The GA (Hfeda, 2018) demonstrated intermediate solution quality combined with prolonged computation time. DE converged at a speed comparable to ABC but achieved only moderate solution quality. FA, exhibiting the slowest convergence, nonetheless attained solution quality on par with ABC.

7.1. Metrics for Assessment

Noise occurs only for short periods accompanying moving trucks. Despite being temporary, noise is measurable and can be optimized in transportation models. Researchers from Japan, Great Britain, and Serbia have used noise in vehicle classification. Ubeda et al. proposed a methodology to measure fuel consumption and carbon emissions at different load levels, subsequently modified because of non-linearity issues. Several green vehicle routing multi-objective optimization models consider criteria such as total capacity, fleet size, environmental impact, noise, CO2 emissions, and fuel consumption. The models feature linear objectives and constraints: routes start and end at the depot; each node is visited by a single vehicle; each node is linked to both preceding and following nodes; vehicles are prevented from overloading; and daily driving time is limited. Subtour elimination constraints are also included. The models assume asymmetric distance-based costs and fleet heterogeneity. Solutions are obtained by mixed-integer programming with the CPLEX solver (Sawik et al., 2017).

7.2. Comparative Analysis

Routing problems in general are difficult to solve, especially when the goal is to find optimal or near-optimal solutions within reasonable time frames. Traditional optimisation methods often become impractical when dealing with large transportation- and logistics-related problems, particularly those containing nonlinear requirements such as time windows, multiple depots, and fleet combinations (Validi et al., 2020). To handle complex distributed environments with dynamic and evolving requirements, metaheuristics offer significant advantages in terms of robustness and flexibility compared to exact optimisation methods (Demir et al., 2019). This characteristic is

particularly important in sustainable transportation logistics, where conflicting economic and environmental objectives must be balanced.

8. Challenges in Implementation

The implementation of metaheuristic techniques in sustainable transportation logistics faces multiple challenges. Supply chain management for the automobile industry involves 2000–4000 components per vehicle with extensive supplier networks delivering many component combinations. Various supply methods exhibit trade-offs: direct shipping requires high inventories; milk-run schemes reduce transportation costs but increase operational complexity; consolidation at docks improves trailer utilization but raises handling expenses. The transition from push to pull supply models aims to reduce finished-goods inventories but results in longer order-to-delivery times. Lean supply-chain management assists in meeting tighter delivery targets (Hfeda, 2018). Vehicle routing and energy management systems encounter additional challenges. Designing appropriate algorithms for loading optimisation necessitates advanced methodologies such as ILS-Biased Randomisation. Handling stochastic demands in inventory routing benefits from simheuristics, which extend metaheuristics to stochastic environments. Real-time routing with uncertain demand can exploit parallel and distributed computation, while dynamic home-servicerouting with synchronised trip sharing introduces further complexity. Deployment of electric vehicles involves considerations of cost, emissions, water footprint, charging capacity and site selection. Urban, suburban and rural settings differ in suitability for electric-vehicle integration, with electric carsharing feasible across a range of geographic contexts. Energy-resilient communities exchange green electricity through advanced V2C technology (Alejandro Juan et al., 2016). These aspects illustrate the multifaceted nature of implementing efficient, sustainable routing and energy solutions.

8.1. Scalability Issues

When addressing scalability issues in optimization, it is crucial to assess the interplay between algorithmic performance and practical constraints, such as computational time limits. For instance, computational experiments concerning multi-objective green vehicle routing problems with subtour elimination constraints have shown that suboptimal solutions can be obtained within 7200 CPU seconds (Sawik et al., 2017). This benchmark highlights the challenge of deriving exact solutions as problem size

increases and underscores the need for efficient heuristic approaches capable of delivering quality solutions within reasonable computational budgets.

8.2. Data Availability

Data availability has been one of the major stumbling blocks in utilizing yet-unexplored ideas and improving sustainable supply chain operations. Fortunately, the literature on logistics technical reports and database files is rapidly growing as companies and government agencies have begun publishing their operational data. Sustainable distribution systems present a unique opportunity for integrating energy-efficient corridors, zero-emission technologies, and information tools. Sustainable supply chain management seen from a strategic location-routing perspective with direct product recycling chemical hazard consideration previously led to a multi-product-single period formulation and a genetic algorithm-based solution technique for assigning distribution network, delivery routes, and frequency.

A general multi-objective location-routing model with pool vehicle and delivery time limit considers the characteristics and constraints of sustainable logistics, accounting for both economic and environmental aspects. Ant colony optimization meta-heuristic approaches, efficient formulations, and hybrid methods for waste collection along with green location-routing problems and environmental routing contribute to a review of state-of-the-art contributions for sustainable location-routing models and resolves the transportation issue at the tactical level for forward and reverse logistics (Validi et al., 2020) (E Dunbar et al., 2018).

8.3. Integration with Existing Systems

The integration of new algorithms with existing transportation management systems (TMS) is crucial for efficient and flexible operations. Such integration supports decision-making processes by saving money, time, and energy, thereby enhancing planners' productivity. A newly developed algorithm can be rapidly embedded within operational TMS platforms to provide these capabilities.

In green transportation initiatives, environmental considerations introduce conflicting objectives when combined with cost optimization. The \u03b5-constraint method, capable of delivering a wide range of Pareto solutions, helps balance total transportation costs against emissions minimization. However, one limitation of mathematical optimization methods is their computational difficulty in handling large-scale problems, which restricts their practical application to extensive intermodal transportation networks. Moreover, many studies focus solely on emissions and costs, thereby overlooking other negative externalities such as noise, congestion, and accidents.

Sustainable distribution networks further emphasize the importance of system integration. A decision support framework that incorporates location and routing decisions within a three-echelon distribution system demonstrates this approach. The network, comprising plants, distribution centers (DCs), and retailers, uses two vehicle fleets: one to transport goods from plants to DCs, and another to serve routes between DCs and retailers and among retailers themselves. Distribution centers are allocated to plants, and retailers to DCs; routes are then planned for each stage—plants to DCs, DCs to retailers, and inter-retailer transportation—to fulfill specified demand. The system considers various road types and speed limits, reflecting realistic transport conditions (Demir et al., 2019) (Validi et al., 2020).

8. Conclusion

Developing a sustainable distribution system involves navigating uncertainty in market growth and energy supply, which can be captured through several scenarios. A new method employing the Particle Swarm Optimization (PSO) algorithm addresses a three-echelon, bi-objective, AHP-integrated location-routing model under uncertain parameters. The PSO algorithm explores the solution space to identify suitable locations and routes, incorporating sustainability considerations and problem-specific constraints. Validation through a real-world case study demonstrates the model's robustness and practicality. Implementing this approach aids decision makers in selecting optimal distribution system designs amid fluctuating energy prices, demand volumes, and associated uncertainties. By accounting for different scenarios and employing a metaheuristic solution framework, the study contributes a viable tool for sustainable logistics planning (Validi et al., 2020).

References

Validi, S., Bhattacharya, A., & Byrne, P. J. (2020). Sustainable distribution system design: a two-phase DoE-guided meta-heuristic solution approach for a three-echelon bi-objective AHP-integrated location-routing model.
Mehdizadeh, E. & Afrabandpei, F. (2012). Design of a Mathematical Model for Logistic Network in a Multi-Stage Multi-Product Supply Chain Network and Developing a Metaheuristic Algorithm.
Demir, E., Hrusovsky, M., Jammernegg, W., & Van Woensel, T. (2019). Green intermodal freight transportation: bi-objective modelling and analysis.
Gulić, M., Maglić, L., & Valčić, S. (2018). Nature Inspired Metaheuristics for Optimizing Problems at a Container Terminal.
Hfeda, M. (2018). Supply chain management optimization using meta-heuristics approaches applied to a case in the automobile industry.
Peric, N., Begovic, S., & Lesic, V. (2024). Adaptive Memory Procedure for Solving Real-world Vehicle Routing Problem.
Serrano Elena, A. (2016). METAHEURISTIC ANALYSIS IN REVERSE LOGISTICS OF WASTE.
Josef Geiger, M. (2008). A Computational Study of Genetic Crossover Operators for Multi-Objective Vehicle Routing Problem with Soft Time Windows.
(Titi) Iswari, T. (2017). Pengembangan Algoritma Hybrid Restart Simulated Annealing with Variable Neighborhood Search (HRSA-VNS) Untuk Penyelesaian Kasus Vehicle Routing Problem with TIME Windows (VRPTW).
Iswari, T. (2017). Pengembangan Algoritma Hybrid Restart Simulated Annealing with Variable Neighborhood Search (HRSA-VNS) untuk penyelesaian kasus Vehicle Routing Problem with Time Windows (VRPTW).
Ab Wahab, M. N. (1970). Self-limitation, dynamic and flexible approaches for particle swarm optimisation.
Zadobrischi, E. & Negru, M. (2022). Applied Study of the Fluidization Model of Logistics Transportation through the Prism of the Impact Generated on the Environment. ncbi.nlm.nih.gov
Ionut Andreica, M., Briciu, S., & Ecaterina Andreica, M. (2009). Algorithmic Solutions to Some Transportation Optimization Problems with Applications in the Metallurgical Industry.
E Dunbar, M., Belieres, S., Shukla, N., Amirghasemi, M., Perez, P., & Mishra, N. (2018). A genetic column generation algorithm for sustainable spare part delivery: application to the Sydney DropPoint network.
Petr, R. & Irina, R. (2019). Modeling of transportation logistics processes for the urban environment.
Jiang, H., Ballot, E., & Pan, S. (2019). Modélisation et analyse de systèmes de distribution alternative et d'Internet physique en zone urbaine.
Sawik, B., Faulin, J., & Pérez-Bernabeu, E. (2017). Multi-Criteria Optimization for Fleet Size with Environmental Aspects.
Alejandro Juan, A., Alberto Mendez, C., Faulin, J., de Armas, J., & Grasman, S. (2016). Electric Vehicles in Logistics and Transportation: A Survey on Emerging Environmental, Strategic, and Operational Challenges.

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Chapter 10: Mathematical Pedagogy Models for STEM Learners in Multidisciplinary Education

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Abstract: In an era marked by rapid scientific and technological advancements, mathematics serves as a foundational pillar for multidisciplinary education, especially within STEM (Science, Technology, Engineering, and Mathematics) fields. This paper explores various mathematical pedagogy models tailored to enhance learning outcomes among STEM learners. It synthesizes theoretical frameworks—including constructivist, behaviorist, and cognitive developmental approaches—while emphasizing the need for integrated, interdisciplinary instruction. These pedagogical models not only support conceptual understanding but also foster problem-solving skills, modeling competence, and real-world application. The paper further outlines how mathematics can be effectively integrated into science, technology, and engineering curricula through unified frameworks such as mathematical modeling and physical computing. Such integrative methods encourage learners to develop transferable skills essential for 21st-century careers. The study also identifies key challenges in implementing effective STEM education, such as outdated instructional models, limited interdisciplinary planning time, and a lack of student engagement. A novel pedagogical system is proposed, which aligns organizational-level teaching strategies with learner-specific characteristics, thereby promoting personalized and sustainable learning experiences. By combining institutional goals with learner-centric matching algorithms, this model optimizes pedagogical effectiveness in diverse classroom settings. Overall, the research underscores the importance of a dynamic, adaptable mathematical pedagogy that bridges disciplinary boundaries and addresses the cognitive, technological, and motivational needs of modern STEM learners.

Keywords: Mathematical Pedagogy, STEM Education, Interdisciplinary Learning, Educational Models and Mathematical Modeling.

1 Introduction

A strong mathematical foundation is essential for students in multidisciplinary education, especially those aiming for STEM-related fields, where mathematics and technology are indispensable. This paper presents an introductory overview of existing models designed to effectively enhance mathematical learning. The discussion aims to analyze and identify key factors that these models consider when applied to multidisciplinary education and research. The goal is to provide effective strategies for instructors by extracting critical elements from the synthesis of existing models.

2. Theoretical Frameworks

Increasing demands of specialists and consumers of advanced technological systems have made an understanding of STEM disciplines central to modern technical education and practice. One response to this challenge is to develop strategic frameworks rooted in research-based approaches that promote learning and design activities aiding students in building connections between science, technology, engineering, and mathematics (STEM) disciplines (K. Baker & M. Galanti, 2017). STEM may be considered an interdisciplinary approach to teaching the four disciplines where the goal is to foster in students the ability to think, reason, generalize, communicate, work cooperatively, solve problems using a variety of methodologies and techniques, and use technology as a meaningful tool. From an academic perspective, STEM education requires a shift from addressing topics in any of the four disciplines in isolation to one that actively explores linkages among the disciplines. The integrative approaches to STEM education are characterized by four spaces: content, pedagogy, program, and community. The content space requires the development of an interdisciplinary curriculum framework that incorporates linked STEM content and skills from authentic contexts. The pedagogical space provides teachers with an instructional model guiding the teaching–learning process in STEM. The program space offers resources, structures, and communication channels that build the capacity of a school to implement and sustain the program. The community space emphasizes the involvement and support of the wider STEM community beyond the school.

2.1. Constructivist Approaches

Constructivist approaches support mathematical modeling through methods such as group discussions, autonomous work, and small-group work, which better develop modeling competence compared to traditional approaches (Mischo & Maaß, 2013). Mathematical modeling tasks differ from traditional word problems, often involving more open contexts and multiple solutions, which can challenge students and teachers. Teachers' beliefs about mathematics, which are long-lasting and difficult to change, influence how modeling is taught. Beliefs are composed of subjective knowledge and attitudes, with peripheral beliefs being easier to change than central ones. Some studies indicate that beliefs can change under certain circumstances. Beliefs about mathematics include views on structure, problem-solving processes, formalism, and the usefulness of mathematics. The utility aspect of beliefs is especially relevant in mathematical modeling, as it aims to solve real-world problems.

2.2. Behaviorist Models

Applications of behaviorism to Educational Technology can be found in the works of Skinner, Guthrie, Hull and others (V. Mayer, 2013). This type of modeling has attracted active interest of educational community and many computer-based studies on learning have been reported by many researchers. According to most of these models, as the level of requirements set by the teacher increases, the rate at which knowledge increases depends linearly on the discrepancy between the teacher's requirements and the learner's current knowledge, while motivation tends to decrease if the demands become overly high. Behaviorists have described various forms of behavior-response: a stimulus can evoke a single response, lead to a chain of responses, or instigate specific behavioral patterns (D'Souza, 2014). Models emanating from this approach emphasize social learning theory, including the work of Neisser, as well as reflective learning as outlined by Schön and Mezirow, pointing toward transformative or process learning. Bryans categorizes model-based learning into perceptional, symbolic, and perceptual-symbolic systems, each with distinctive characteristics.

2.3. Cognitive Development Theories

Pioneered by Rousseau, cognitive development theory motivated scientific analysis of children's cognitive development by defining concepts and stages from infants to adolescents. Piaget focused on the development of logical thinking involving the coordination of mental operations on objects, which matches deductive reasoning

(Solovieva et al., 2023). Personal epistemology research highlights how learners reason about knowledge and knowing, prompting reconsideration of objective knowledge and its acquisition. Hence, developmental theory justifies the role of mathematics as research tool, aims of mathematical activity, school mathematics, and the mathematical content offered to learners (Safarandes Asmara & Junaedi, 2018).

3. STEM Education Overview

Science, technology, engineering, and mathematics (STEM) education is a critical area of study for 21st-century learners. It is well known for producing some of the world's most sought-after careers around the world.There is a growth in the demand for STEM-literate citizens worldwide as science and mathematics education provides the foundation for the formation and foundation of knowledge in science, technology, and engineering when the individual engages and learns at a higher level. When STEM skills and literacy become the foundation for STEM learners, they are highly in demand and well compensated. Unfortunately, STEM learners find it harder to learn concepts in STEM-based disciplines than non-STEM learners. Learning STEM-oriented curriculum is even more demanding and requires preparation, motivation, and perseverance. STEM education consists of many different elements that could combine in various ways to provide high-quality education to learners.

3.1. Importance of STEM Education

Science, Technology, Engineering and Mathematics (STEM) education is increasingly emphasized due to concerns about the preparedness of future graduates for 21st century challenges (Stohlmann et al., 2012). STEM competencies are critical for the progress of industrial nations, requiring 21st century mathematical skills such as data analysis, spatial reasoning, and algebraic thinking (Cooke & Walker, 2016). Curricular standards and assessment regimes support the inclusion of STEM and associated mathematics. The drive to improve STEM education stems from its typically weak status in school curricula, the relatively low profile of initial programmes and educational research, and because many students and teachers find STEM unsatisfactory (D'Souza, 2014). Moreover, students learning STEM subjects often struggle to apply theoretical concepts taught in isolation to real-world contexts. Incorporating mathematical pedagogical models specifically designed for STEM students facilitates better comprehension and engagement across all four components of STEM.

3.2. Challenges in STEM Learning

STEM education has gained momentum worldwide, but its implementation presents multiple challenges for teachers, administrators, and stakeholders. Educators often struggle to transition from traditional lecture-based to student-led instructional approaches and feel insufficiently prepared to facilitate STEM integration or align their pedagogy with new curricula. Integrating STEM content into existing subjects also raises concerns about fitting within prescribed curriculum plans and pacing constraints that limit opportunities for authentic interdisciplinary lessons. Moreover, some teachers question whether students possess the ability or motivation to actively engage in STEM activities, particularly when advanced content is involved. Equally troublesome are the widespread deficits in quality assessment tools, planning time, and disciplinary knowledge required to support multidisciplinary STEM instruction (Thi Bich Le et al., 2021). Addressing these issues is necessary to improve the quality and positive effects of STEM education on student learning.

3.3. Interdisciplinary Learning in STEM

Interdisciplinary learning is an integral component of STEM education. Combined or interdisciplinary learning in STEM examines multiple disciplines or STEM topics in the context of another discipline or real-world scenario (Stohlmann et al., 2012). The exigency of interdisciplinary approaches in education and research has been increasingly recognized, particularly in an age in which complex issues are largely multidisciplinary. Interdisciplinary mathematics education fosters students' competence as regards disciplines other than mathematics (Williams et al., 2016). Mathematical study qualifies students for the workforce by explicitly integrating core components of modern industry, enabling learners to explore new topics beyond mathematics and to address issues of wider importance to society. Using mathematical activities, students can identify and develop transferable skills for workplace use, such as numeracy, communication, and group work. Moreover, this approach facilitates informed debate and supports understanding of contemporary national and global issues, including challenges faced by professional mathematicians, social scientists, and policy-makers.

4. Mathematical Pedagogy in STEM

Mathematical modeling provides a unifying framework for integrating teaching and learning across the sciences and mathematics, offering a coherent methodology that extends beyond individual disciplines. Because modern research problems rarely reside within a single domain, the coordinated use of mathematics across diverse disciplines enables the formulation and study of complex problems through a common, accessible language (L. Gastón & A. Lawrence, 2015). The use of a common core such as differential equations, linear algebra, and parametric functions facilitates communication across a range of STEM disciplines while promoting deeper insights from practitioners immersed in specific fields.

4.1. Integrating Mathematics with Science

From grade school through college, science and mathematics have been closely intertwined (Patel, 2019) and form the foundation for integrating the four STEM fields into problem-based learning. Engineering is the practical application of mathematics and science knowledge to develop tangible solutions, allowing students to improve their lives and those of others. Through the development of well-rounded solutions, engineers also generate technical documentation (e.g., reports, presentations, drawings, and patents), which provides an excellent opportunity to include literacy instruction in the STEM designed lesson. The inclusion of technology—hardware and software—supports the engineering design process and can be integrated through its use in gathering and analyzing data, modeling alternative solutions, and supporting the adequacy and functionality of the design (Stohlmann et al., 2012). Throughout each step in the engineer design process, the need for mathematics is reinforced. That sustained relationship provides more relevant and useful depth for one field, using the knowledge and skills developed in the other and vice versa.

4.2. Mathematics in Technology Education

Mathematics plays a central role in technology education, fundamental to understanding and creating technological solutions (D'Souza, 2014). Integrated STEM approaches combine mathematics, physics, engineering, and allowed disciplines in multidisciplinary instruction (Stohlmann et al., 2012). Mathematics supports application and problem-

solving but a strong foundation in science also improves technology education when connections among the disciplines are nontrivial. Physical computing allows students to build interactive technological prototypes that provide hands-on engagement with STEM concepts.

Mathematics education benefits from models that support multiple modes of learning including visual, verbal and dynamic representations. Castell's modelling framework gathers the necessary information from the real world to build mathematical, visual and graphical representations. PySTEMM provides executable concept models of abstract ideas expressed as "immutable objects and pure functions" that can generate multiple views of concepts and their connections including narrated animation, graph plots and equations. The executable concept modelling approach reduces complexity and debugging by eliminating side-effects enabling a wide range of applications to provide multi-modal learning of STEM.

4.3. Mathematics in Engineering Contexts

Academic curricula often include courses describing the mathematical methods needed to ensure students have a sufficient mathematical toolkit and master basic methods of technical modelling and simulation. Although curricula focus on the mathematical knowledge and skills most commonly required, they rarely teach competent use of the artefacts themselves. Consequently, practical application often differs from theory taught in the classroom. Mathematical education in engineering traditionally emphasizes problem solving and development of formalisms. competencies such as modelling, communicating mathematically, and using tools—even though frequently employed by practicing engineers—are seldom explicitly developed or formally assessed (Cook, 2021). Engineering students may receive mathematics instruction privileging symbolic techniques, relegating numerical methods to secondary status. For example, integration can be presented primarily as backward differentiation rather than the practical, often numerical, process of determining areas under curves (Kent & Noss, 2000). An engineering mathematics lecturer choosing between software packages faces decisions about which mathematical aspects the software makes visible. A tool like Mathcad caters specifically to engineers, whereas Mathematica demands more explicit mathematical thinking. Regardless, educators must contend with the epistemological assumptions embedded in software design: which aspects are sufficiently visible, which might require enhancement or suppression. These epistemological structures both shape and are shaped by user activity, but they do not dictate it unambiguously (Kent & Noss, 2000).

5. Pedagogical Strategies

Over the past decade, ongoing changes in the demand for educational opportunities in science, technology, engineering, and mathematics (STEM) have highlighted the need to adapt pedagogical strategies, which have largely remained unchanged. A new and advanced pedagogical system is therefore required to help students in secondary schools, colleges, and universities better adapt to and succeed in an ever-changing STEM society.The proposed pedagogical system identifies appropriate pedagogical approaches at organizational and learner levels, aligning each learner with the most suitable pedagogy. At the organizational level, the system selects sustainable pedagogies based on institution-specific objectives and resources. These pedagogies are also chosen so that each education phase clearly supports the subsequent stage, facilitating students' progression to advanced levels. At the learner level, the system classifies and guides pedagogies in accordance with learners' personality traits, such as openness to experience and extraversion. A matching algorithm arranges the learner's schedule and program to increase receptiveness to selected pedagogies. Combining organizational-level sustainable pedagogies with the learner-level matching algorithm enables the efficient organization of groups for collaborative learning. Teachers receive assistance in designing supplementary pedagogies aimed at enhancing specific skills throughout a single semester.

The work contributes to better selecting continual pedagogy and more effectively introducing multidisciplinary approaches into mathematics education. Motivations to adopt this pedagogical system remain incontrovertible, reinforcing the pursuit of effective strategies for STEM learners (K. Baker & M. Galanti, 2017).

5.1. Inquiry-Based Learning

Inquiry-based learning (IBL) in mathematics has attracted significant attention. By late 2015, the Mathematics Association of America's Special Interest Group on IBL counted nearly 1000 members in the USA. The Joint Mathematics Meetings of the American Mathematical Society in 2018 included 50 talks focused on IBL. Several initiatives have mobilized regional consortia involving over 800 practitioners committed to improving mathematics education and student success. A key objective is to identify effective methods for sustaining the adoption of IBL in undergraduate mathematics instruction.

These developments illustrate a momentum toward embracing IBL. Inquiry as a guide to learning has been advocated for at least a century (Evans & Dietrich, 2022).

5.2. Project-Based Learning

Project-based learning (PBL) has been adopted widely in STEM education because it fosters a dynamic environment in which students are exposed to multilayered and numeric stimuli. These stimuli connect to a complex project or problem that extends to real-world applicability (D. Euefueno, 2019). By requiring final deliverables and a structured schedule, PBL yields an active, inquiry-based, and confidence-building pedagogy, and as such it is a primary method of instruction in many STEM classes. The approach originated in recently graduated students assisting first-year students to form their own diagnostic testing and teamwork skills while attending medical training in the 1960s. The approach migrated into K–12 and postsecondary education to enhance interest in STEM fields and to emphasize team building, collaboration, strategizing, leadership, and critical-thinking skills that are valuable for students and future workforce readiness.

PBL offers a multilayered approach that demands critical thinking, incorporates concepts from the Cognitive, Behavioral, and Constructivist Learning Theories, and emphasizes social, environmental, and self-reflection elements. In K–12 and postsecondary settings, students are encouraged to adopt a mastery goal orientation that focuses rather on skill development than on outcome or grade orientation. Students must understand the problem-solving process, including the ability to identify problems and the corresponding supporting data, to devise a plan, implement and evaluate the solution, and communicate the results. In addition to numerous online projects, multiple project kits aligned with curriculum have proved successful in introductory engineering/technology courses by actively linking technology and engineering to real-world STEM concepts (K. Verma, 2011). For example, a marine and maritime kit enables groups of freshmen to build and test a variety of functional devices while demonstrating the link between fundamental scientific principles and engineering applications. Survey results indicate a marked increase in students' learning and comprehension of scientific principles and engineering concepts.

5.3. Collaborative Learning Techniques

Collaborative learning has been encouraged in higher education, particularly in STEM disciplines, as a means of promoting student-centered, active learning environments (S. Dulai et al., 2022). A number of institutions have integrated collaborative learning techniques across the engineering curriculum, often tailored to the diverse contexts and challenges faced by instructors (Stark Ralston et al., 2017).

Team-Based Learning (TBL) is a versatile pedagogy where students work in instructor-formed teams throughout a unit. Prior to class, students prepare through individual and team assessments. Once in class, they participate in a readiness assurance process consisting of individual and team quizzes, followed by application exercises conducted in teams. By following this sequence, teams establish self-managed learning and accountability. The TBL approach employs specific variations to aid the transition from traditional instruction to active learning. Co-teaching (CT) involves two or more instructors working together to implement active learning strategies in classes with varying student demographics, including traditional, nonmajors, or majority-minority groups. The collaboration also provides valuable insights into curriculum design and delivery when developing active learning environments that maintain student engagement and academic credibility. Nevertheless, the experience of integrating collaborative learning often requires ongoing practice and support to implement effectively. Scaffolded preparatory activities may be necessary to introduce and reinforce the principles of teamwork and collaborative function. Initial anxiety can arise from the challenges of translating abstract pedagogical concepts into practical instructional strategies. An alternative stance is to allow students to engage in collaboration in an informal manner, without explicit instructional structures, which may be preferred in advanced or graduate-level courses. Notwithstanding varying degrees of formality, instructors commonly identify the allocation of time within the course schedule as a primary concern when incorporating collaborative activities.

5.4. Flipped Classroom Models

Flipped-classroom pedagogy addresses the challenges posed by multidisciplinary and multitiered classroom instruction, where engagement fluctuates with instructional delivery methods. The approach seeks to overcome the obstacles of limited engagement opportunities and uneven multilevel attentiveness by shifting content delivery outside the classroom. Building on the foundation of Sugar and Donovan's inverted class, (Karjanto & Simon, 2016) implemented a flipped pedagogical paradigm in English-medium Instruction (EMI) Mathematics teaching at the tertiary level. The transition

methodology proceeded from a default “lecture on-demand” setup, where students received video recordings of live lectures, to a quasi-flipped format supplemented by pre-recorded video solutions to homework inquiries. The final stage constitutes also the “flip-synchronous hybrid” model, characterized further by prerecording each chapter's lectures for viewing before scheduled in-class meetings. A significant societal bottleneck remains: time constraints preclude all incoming students from accommodating university training in their native tongue. Thus, initial content delivery in the student environment accords with the student-centred critical thinking principles of student-centred learning. Classroom meetings dedicate to feedback-type activities, including discussions, Socratic questioning, clarifications, group problem-solving, and other active-learning assignments, thereby sustaining an interactive arena. Lectures retain a dynamic character as pedagogical discourse, rather than passive transmission.

6. Assessment and Evaluation

In the development and application of mathematical pedagogy models for STEM learners, assessment and evaluation processes are critical in adjusting teaching and learning activities in response to disseminated data. The assessment model enables teachers to track students’ learning progress throughout and at the end of a semester (K. Baker & M. Galanti, 2017). In this model, teachers create different mathematical problems aligned with the emphasised mathematical objectives and determine student competencies based on their solutions. Teachers conduct the assessment once or twice within a semester, and the evaluation phase allows for initial responses to the assessment results by adjusting the emphasis of topics in subsequent teaching activities. Teachers may also investigate individual student problem-solving approaches to provide tailored support.

6.1. Formative Assessment Techniques

Assessment and demonstration of mathematical competency is an intrinsic part of the mathematical pedagogy applied in a STEM curriculum and multidisciplinary context. Formative assessment provides opportunities to measure mastery of key mathematical concepts in the journey to develop mathematical knowledge and competency and is a crucial part of a broad pedagogical repertoire and for creating a rich learning environment in mathematics (J. Sinwell, 2017). Ní Fhloinn and Carr (Ní Fhloinn & Carr, 2017) demonstrate that feedback from formative assessment serves to both reveal the

success of instruction and illuminate areas where instruction can be enhanced. Implementation methods vary from peer feedback and improved self-assessment techniques to technology utilization.

The emergence of formative assessment practices alongside dedicated teaching and learning courses has been widely discussed. Analysis of historical approaches to engineering mathematics teaching and assessment in Australian universities reveals that students typically describe their mathematical knowledge in terms of calculation skills, with few referring to problem-solving skills, suggesting that either teaching approaches or assessment procedures are not sufficiently promoting conceptual understanding, reasoning skills or mathematical modelling components. While mathematics may be poorly suited to approaches requiring group problem-solving and oral presentations, students generally appreciate continued assessment with specific lecture-based assessment and topic-based assessment cited as popular alternatives, particularly in statistics. Assessment of engineering mathematics commonly includes written exams, oral exams, open-book tests, take-home assignments and computer-based assessment.

6.2. Summative Assessment Strategies

One method for assessing knowledge during STEM PjBL is short summative assessment tasks, which over time are incorporated into the problem-based project phases (R.M. & M.S., 2013). Short, targeted summative assessment tasks gauge individual accountability and provide opportunities to demonstrate content knowledge. However, surprise summative assessments should be avoided, since they tend to demoralize students, diminish intrinsic motivation, disrupt the continuity of group and individual learning, and severely undermine the overall learning process. To prevent these adverse effects, summative assessments should only be introduced after students are afforded substantial preparation and closely aligned formative assessment activities. By collection and evaluation of learning artifacts, students engage in accumulation of evidence that systematically reflects their progress. Clear and explicit guidance from the instructor facilitates alignment between expected learning outcomes and the PjBL projects, ensuring that these artifacts effectively summarize student knowledge and represent richer, more complete understandings. Such formative assessments help students apply their knowledge in meaningful ways, fostering possession of the knowledge beyond merely performing well on tests. Effective formative STEM PjBL assessment therefore moves beyond evaluating success in formula recall; while performance on multiple-choice tests remains a benchmark for teaching effectiveness with respect to test

performance, a focus on student progress in thinking and reflection enhances formative assessment efficacy. Cultivating flexible understanding supports development of test-taking skills and better comprehension of high-stakes assessment materials. Since STEM PjBL involves both individual and group work, assessment must be matched appropriately to the learning activities and setting; group-based assessments can negatively impact student learning when pursuit of understanding is primarily individual. Mathematical modelling in education research and practice involves assessing authentic performance and understanding modelling competencies (Chung Tam, 2018). Teaching mathematical modelling has evolved, with a focus on real-world problem solving and theory application in curriculum design. Theoretical foundations and frameworks guide development of effective assessment strategies, while researchers emphasize modelling skills, attitudes, and competencies. Studies explore ways to better assess these skills and facilitate transfer of mathematical abilities across contexts.

6.3. Peer Assessment in STEM

Within STEM project-based learning (PBL), educators implement a peer-assessment platform, standards-based grading system, and electronic portfolio interface designed to help students communicate their understanding, demonstrate evidence of mastery, and establish roles and expectations when assessing each other. To ensure that students engage in a peer-assessment process reflective of the project launch within each discipline, they receive a peer-assessment template aligned with the initial criteria of the project. The intentional selection of the peer-assessment platform comes from traditional teacher- or student-led conferences, which frequently focus on students. The objective behind maintaining this framework is to provide some context and reason as to why the learners must speak about their projects and the various PBL activities within the disciplines. Furthermore, a standards-based assessment and grading system accommodates the interdisciplinary nature of the project. Standardized evaluation tools are crucial for assessing and measuring performance and growth across classroom settings. When the standards-based assessment methodology is combined with the electronic-portfolio platform, the outcome offers an environment conducive to developing and sustaining a peer-assessment system that is transparent and applicable to educators, learners, and populations beyond the classroom. The electronic portfolio system plays a central role, serving in various capacities—project folder, arena for feedback, and portfolio. The project folder function enables students to organize their evidence, hyperlinks, and artifacts within individual and community project folders, facilitating real-time updates. As the arena for feedback, the platform delivers prompts, guiding questions, and rubrics that remain accessible to participants and educators,

allowing for continuous review and application. Finally, as a portfolio, the learn-tech platform provides a context for students to personally communicate their learning or content utilization across multiple disciplines. Moreover, the structures of traditional assessment and grading—exemplified in the peer-assessment platform, standards-based grading, and electronic-portfolio systems—constitute several constructs critical to fulfilling the responsibility of assessment within the STEM PBL construct (R.M. & M.S., 2013).

7. Technology Integration

Modern technology has created many new opportunities to support STEM education. The integration of technology tends to be used to improve instructional delivery and practices for STEM programs (K. Baker & M. Galanti, 2017). Typically, the use of technology-supported learning relates to the use of pedagogical tools that promote independent learning, collaboration, assessment and multi-sensory learning. With this in mind, technological tools are provided below to help instructors identify technology-supported instructional strategies and suitability with multiple-learning styles.

7.1. Digital Tools for Mathematics Instruction

Technology continues to shape mathematics education, providing learners and teachers with multiple ways to engage with concepts and offering opportunities to study and refine digital approaches to instruction and learning. Selecting digital tools is a complex process; while some fit neatly into defined categories, many span multiple types, each with distinct constraints and affordances that must be considered when aligning tools with particular topics or grade levels. Broader decisions involve choosing whether to promote a single category or a mix of interactions. The fluency principle posits that mastering a few high-quality tools significantly enhances mathematical learning. A 'good' tool offers a variety of interactions and constraints with consistent, easily perceptible affordances that benefit both teachers and learners (Sinclair & Baccaglini-Frank, 2016). Visualization-based software has motivated students of diverse abilities in science and mathematics by leveraging preferences for visual learning and dynamic modeling. Such tools can improve achievement across the board, with pronounced effects for women and students of color. They assist teachers in transitioning to inquiry-based methods while addressing evolving content standards, facilitating work with real data and simulations. Access to web-based datasets further enables exploration and

discovery (Kolvoord, 1999). Effective integration of digital tools necessitates professional development; whereas in-service teachers have benefitted from training, pre-service educators remain underserved. Consequently, incorporating preparation in the use of these technologies into teacher education programs is essential to promote adoption and deepen understanding of their value in science and mathematics education.

7.2. Online Learning Platforms

The COVID-19 pandemic accelerated virtual and hybrid teaching at Higher Education Institutions (HEIs), providing new opportunities for STEM education. Hybrid learning combines some in-person lessons with remote group work. Laboratory activities benefit from detailed online guides, enabling work in campus labs outside scheduled sessions. Platforms dedicated to mathematics, such as the Math Skills Site, support progress tracking, revision, and exercise completion; increased usage correlates with improved undergraduate grades. These platforms supply quick feedback, adapt to capital-constrained settings through smartphone accessibility, maintain user-friendliness for inexperienced students, and facilitate collaboration (Nungu et al., 2023). Complementary applications—Google Classroom, WhatsApp, Canvas, PhET, CK-12, YouTube—enhance STEM teaching by enabling the sharing of multimedia and interactive content. While platforms like Sakai, Blackboard, Moodle, Google Classroom, and Microsoft Teams support blended STEM education in Rwanda, some lack integrated automated quiz features, compelling the use of multiple systems and necessitating staff training in digital technologies. Incorporating these technologies within clear objectives and e-assessment frameworks promotes interactive STEM instruction.

7.3. Simulation and Modeling Software

Modeling and simulation are key approaches in science education to understand the behaviour of a system. Representing and explaining a process through an educational model or simulation allows students to understand the process and discover essential properties of a system. Such activities promote interpretation and understanding of systems, allowing students to create and test their conceptions of a phenomenon. The sporadic use of models and simulations in education can be explained by difficulties teachers face, such as the complexity of models and modelling tools and lack of preparedness. Modeling for Kids supports the development of georeferenced multisensory modelling and simulation activities for early education by defining norms,

strategies and processes to analyse and represent dynamic systems. The methodology highlights the role of georeferenced multisensory information, which is very often available in real-world tasks, in modelling activities (Jorge Brigas, 2019). Modeling should play a central role in K-12 STEM education because it makes classes more engaging. A model underlies every scientific theory and is central to all STEM disciplines. Executable concept modelling of STEM concepts can be implemented by using immutable objects and pure functions in Python. Examples of such modelling in maths, physics, chemistry and engineering are available through a proof-of-concept tool called PySTEMM. The approach applies to all STEM areas and supports learning with pictures, narration, animation and graph plots. Models can extend each other, simplifying the process of getting started. The functional-programming style used by PySTEMM reduces incidental complexity and code debugging (D'Souza, 2014).

8. Case Studies

One transformation is an adaptation of the traditional method used in logic so that students begin to read and solve the argument as if it were a proof. The field requires precision that students may not always supply, although the act of reading through a long chain of reasoning can sometimes foster a stronger sense of the underlying logic. In the latter approach, students consider statements about hypothetical models, which provide examples and a framework for the reasoning; topic papers implemented by Znoj and Goodman employ this method (Lesaja, 2012). A second general principle is that issue analyses involving topics designed to be relevant to students, such as those suggested by ISA, offer distinct advantages. The personalised nature of the topics maximises motivation among students. The thinking activities contained in the topics accompanying the general presuppositions give students a venue in which to practice key thinking skills on familiar materials. In addition, the relevance of the contexts restricts the probabilities of the logic's irrelevance or, worse, an unwarranted validity-generalisation. Finally, issues often involve some form of rebuttal, which provides students with the means to give a contribution. Students aware of their reasons can add relative weight to their arguments.

8.1. Successful STEM Programs

STEM programs across the United States frequently aim to shift learners' perceptions of science and mathematics. Similarly, initiatives in higher education encourage students

to enter STEM fields through peer-facilitated engagement strategies. Model-eliciting activities (MEAs) that apply integrated STEM content to compelling real-world contexts not only enhance participants' impressions of the discipline but also develop their problem-solving skills and professional identity. Often, the intellectual growth resulting from STEM programs derives from participants' active involvement in the progression and refinement of models that improve with deeper exploration. These programs, therefore, advance not only content knowledge but also transferable scientific practices integral to knowledge development (K. Baker & M. Galanti, 2017).

8.2. Innovative Teaching Practices

This research addresses commonalities and complementary differences between existing theoretical models of STEM pedagogy, encouraging educators to adopt a holistic perspective when advancing pedagogical practices. The exploration reveals that augmenting innovative teaching with principles of assessment for learning substantially benefits STEM education. Identification of key barriers and supports furnishes strategies for effective implementation of innovative pedagogies, enabling teacher educators, supervisors, and policymakers to make informed decisions conducive to their unique educational contexts.

8.3. Comparative Analysis of Pedagogical Models

Comparative analysis of pedagogical models can assist educators in identifying and implementing the most appropriate approaches within given contexts. Research frequently categorizes STEM education models into five groups: inquiry-based learning, case-based learning, problem-based learning, actief collaborative learning, and project-based learning (L. Gastón & A. Lawrence, 2015). A suggestion that student engagement is the critical goal of STEM education leads to specific strategies for increasing engagement. Case studies are thus powerful narrative tools in which students engage with a problem before learning the related concepts. An example within the University of Wyoming includes a study of the 1989 Exxon Valdez oil spill which serves to integrate knowledge and concepts from multiple STEM disciplines (D'Souza, 2014). Alternative models include 'learning through design,' in which students must produce a physical artifact, such as a rocket or bridge, alongside related oral and/or written presentations; and library-oriented approaches, wherein students produce a book, paper, movie or presentation on a topic of interest. These may be conducted individually or as

part of groups. When direct participation is not possible, virtual participation via simulation is an option.

9. Future Directions

The current paper proposed an original pedagogical model based on an early exposure to multidisciplinary education. It was grounded in a review on the state of the art of the field, with both the disciplinary context and the educational tier considered. Of particular interest is the interplay between mathematics and STEM, with the future objective of creating a context for all STEM fields to collectively thrive. Mathematical pedagogies models were analysed, with the merely extrinsic use of interdisciplinary mathematics for mathematical modelling highlighted in contrast to the intrinsic need for mathematics supporting the development of modern technologies collapsible on the timing system of our World. The latter phenomenon calls for the early adoption of a proprietary pedagogical model, that requires all education stakeholders to acquire a solid mathematical and physical background as early as possible. A summary of the main challenges was first offered, which unveiled the drastic change in the mathematics requirements for the future learners, changing their educational needs. A universally applicable model based on both pure and applied mathematical elements was then proposed for the development of the next generations of specialists. The specific support of mathematical abstraction and generalisation notably aims at providing effective solutions to the challenges associated with cognitive development, while offering innovative approaches suitable to the modern metamaterials collections. Overall, the search for a semi-generic pedagogical model covering the majority of future STEM learners was initiated. Promising results validating the early applicability of the model triggered the development of a dedicated platform for its proper dissemination (K. Baker & M. Galanti, 2017). Effective engineering and manufacturing tool kits will subsequently be developed, to assist the educator during the pedagogical intervention. Although described according to the specifications of higher education, the model is sufficiently flexible to potentially fit the entire educational landscape. The future work will focus on a further clarification of these points, towards the final definition of the pedagogical model for the entire educational continuum.

9.1. Emerging Trends in STEM Education

As a nation, today's students must be prepared for STEM careers in science, technology, engineering, and mathematics (Stohlmann et al., 2012). Research continues to reveal that mathematics textbooks are not designed to provide STEM integration; rather teachers need supportive materials, approaches, and strategies to guide their classwork. Integrated STEM education connects the classroom tasks to the lifestyles of the students in a relevant, real-world process that captures their interest and desires to pursue a STEM career. A robust concept-based pedagogy creates a pathway of skills and knowledge that supports growth toward mastery for students across content-area courses, so compatible skills continue to reinforce knowledge while presenting an increasing level of complexity to challenge students (D'Souza, 2014). Because modeling plays a central role in K–12 STEM education by creating more engaged classes, models provide explicit links that support integrated STEM curriculum.

9.2. The Role of Artificial Intelligence

Artificial Intelligence software has a significant role in education but its potential remains rather limited. A hybrid intelligence approach, in which humans and AI software act as partners in a concerted effort, is identified as a promising avenue to realize these potentials. Specifically, learners are guided in the process of acquiring systems-thinking skills through the construction, by themselves, of small, very focused-topic knowledge bases, which are offered to the user as interactive diagrams (Bredeweg & Kragten, 2022). Since AI techniques are based on the use of explicit knowledge representations, learners are able to deal directly with concepts of systems thinking in an intuitively accessible way. AI systems are typically more effective when they include large and comprehensive knowledge bases; going against this general principle, the proposed approach focuses on small, targeted, knowledge bases as the most advantageous option for effective fine-tuning and constructive interaction. The interaction between software and learners is fully automated. Extending a well-established tradition in cognitive systems and artificial intelligence, the argued viewpoint emphasizes the strengths of two agents that differ substantially in their nature and operation and that manage to reach improved results when effectively combined.

9.3. Global Perspectives on STEM Education

Mathematics educators around the world grapple with the promotion of mathematical modelling, the formulation of curricula, and the preparation of teachers (L. Gastón & A.

Lawrence, 2015). Cross-national comparison of pedagogical approaches may be instructive in the building of mathematical modelling education programmes and in the development of STEM curricula. Though the following discussion mainly considers mathematical modelling education in the United States of America, the theoretical framework is applicable worldwide.

Mathematical modelling, central to STEM disciplines, requires integration of mathematical understanding with contextual knowledge. The challenge of conveying the big-picture synergism directs attention toward enhanced teaching of mathematical modelling, from which emphasis is currently shifting. Research shows that teachers and students possess widespread misperceptions concerning mathematical modelling; these misunderstandings result in incorrect associations and weak learning connections between disciplinary areas. Mathematical modelling emerges as a promising candidate to invoke synergy among STEM disciplines, potentially uniting the expertise of each.

Achievement of such symbiotic integration rests on effective classroom facilitation of mathematical modelling. Evidence from classroom observations, simulations, and professional development reinforced this conclusion. Teachers who had the opportunity to observe and participate in modelling facilitation repeatedly drew attention to the potential of mathematical modelling to crystallize interdisciplinary connections. Additional evidence suggests that knowledge, experience, and skill in mathematical modelling are most effectively acquired through extensive opportunities to engage in the practice. Such efficacy is contingent on exposure to the work of exemplary facilitators. The availability of skilled teacher educators therefore constitutes a major constraint to the diffusion of mathematical modelling as a pedagogical approach. Facilitators and professional-development providers should consequently be prepared to demonstrate mathematical modelling instruction in ways that set a standard for their colleagues. Preparation of teachers competent to lead mathematical modelling in diverse settings emerges as a desideratum of the highest priority.

10. Conclusion

This study describes a novel approach utilizing mathematical pedagogical models to engage STEM students in multidisciplinary education and collaborative design. Existing models are reviewed and a flexible new model is proposed to support educators in providing timely assistance during design activities, fostering field-specific learning and

problem-solving. The model's modular structure supports a concept-based knowledge taxonomy and adaptable teaching strategies. Pedagogical models structure knowledge internally and relate it across disciplines, forming an education-technology pathway that sustains awareness and interruptions, guiding aids by an illation engine that translates abstract content into discipline-specific tactics. Preliminary testing of a multi-agent approach—the IE_AGENT Model—reveals promising mechanisms for executing design support within this framework. Continuing work aims to demonstrate the model's theoretical underpinnings and practical execution as an intelligent guide for multidisciplinary STEM learning environments.

References

K. Baker, C. & M. Galanti, T. (2017). Integrating STEM in elementary classrooms using model-eliciting activities: responsive professional development for mathematics coaches and teachers. ncbi.nlm.nih.gov

Mischo, C. & Maaß, K. (2013). The Effect of Teacher Beliefs on Student Competence in Mathematical Modeling – An Intervention Study.

V. Mayer, R. (2013). Solve of problems of mathematical theory of learning with using computer modeling methods.

D'Souza, K. (2014). PySTEMM: Executable Concept Modeling for K-12 STEM Learning.

Solovieva, Y., Rodríguez Zavaleta, J., Celeste Rosete Carrillo, A., Quintanar, L., & Plotnikova, V. (2023). The program for introduction of basic mathematical knowledge: the effects in six years old Mexican children. ncbi.nlm.nih.gov

Safarandes Asmara, A. & Junaedi, I. (2018). Trend Paradigma dalam Pendidikan Matematika.

Stohlmann, M., J. Moore, T., & H. Roehrig, G. (2012). Considerations for Teaching Integrated STEM Education.

Cooke, A. & Walker, R. (2016). Exploring STEM education through pre-service teacher conceptualisations of mathematics.

Thi Bich Le, L., Thai Tran, T., & Hai Tran, N. (2021). Challenges to STEM education in Vietnamese high school contexts. ncbi.nlm.nih.gov

Williams, J., Roth, W. M., Swanson, D., Doig, B., Groves, S., Omuvwie, M., Borromeo Ferri, R., & Mousoulides, N. (2016). Interdisciplinary mathematics education: a state of the art.

L. Gastón, J. & A. Lawrence, B. (2015). Supporting Teachers' Learning about Mathematical Modeling.

Patel, J. (2019). The Constructivist Approach to Curriculum Integration of STEM Education. osf.io

Cook, E. (2021). Practice-Based Engineering: Mathematical Competencies and Micro-Credentials. ncbi.nlm.nih.gov

Kent, P. & Noss, R. (2000). The visibility of models: using technology as a bridge between mathematics and engineering.

Kent, P. & Noss, R. (2000). The visibility of models: using technology as a bridge between mathematics and engineering.
Evans, T. & Dietrich, H. (2022). Inquiry-Based Mathematics Education: a call for reform in tertiary education seems unjustified.
D. Euefueno, W. (2019). Project-/Problem-Based Learning in STEM: Impacts on Student Learning.
K. Verma, A. (2011). Impact of Project Based Learning in Introduction to Engineering/Technology Class.
S. Dulai, K., Kranzfelder, P., Signorini, A., S. Pusey, T., Presas Valencia, A., Urbina, C., & J. Oviedo, N. (2022). Collaborative Teaching plus (CT+): A Timely, Flexible, and Dynamic Course Design Implemented during Emergency Remote Teaching in an Introductory Biology Course. ncbi.nlm.nih.gov
Stark Ralston, P., R Tretter, T., & Kendall Brown, M. (2017). Implementing Collaborative Learning across the Engineering Curriculum.
Karjanto, N. & Simon, L. (2016). English-Medium Instruction Calculus: Is flipping helpful?
J. Sinwell, B. (2017). Formative Assessment Strategies for Mathematical Thinking: A Qualitative Action Research Study.
Ní Fhloinn, E. & Carr, M. (2017). Formative assessment in mathematics for engineering students.
R.M., C. & M.S., C. (2013). Changing views on assessment for STEM project-based learning.
Chung Tam, K. (2018). Testing the Ability to Apply Mathematical Knowledge.
Sinclair, N. & Baccaglini-Frank, A. (2016). Digital Technologies In The Early Primary School Classroom.
Kolvoord, B. (1999). Data Visualization Tools for Science and Math.
Nungu, L., Mukama, E., & Nsabayezu, E. (2023). Online collaborative learning and cognitive presence in mathematics and science education. Case study of university of Rwanda, college of education. ncbi.nlm.nih.gov
Jorge Brigas, C. (2019). Modeling and Simulation in an Educational Context: Teaching and Learning Sciences.
Lesaja, G. (2012). Improving Education of Mathematics Majors.
Bredeweg, B. & Kragten, M. (2022). Requirements and challenges for hybrid intelligence: A case-study in education. ncbi.nlm.nih.gov

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Chapter 11: Mathematical Modelling of Global Climate Change: An Overview

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Abstract: In the modern era, global climate change stands as one of the most urgent and formidable challenges confronting humanity. A comprehensive understanding, accurate prediction and effective mitigation of its impacts necessitate the application of robust mathematical models that can encapsulate the intricate and multifaceted nature of the Earth's climate system. This chapter provides an overview of key mathematical approaches used in climate science including energy balance models, radiative transfer equations and general circulation models (GCMs). Special attention is given to the integration of theoretical formulations, numerical simulation techniques and observational data in developing and validating these models. Additionally, the chapter addresses major challenges in climate modeling, such as uncertainty quantification, scaleinteractions and nonlinear feedback mechanisms, which significantly affect model accuracy and reliability.

Keywords: Climate Modeling, Energy Balance Models, General Circulation Models (GCMs), Numerical Simulation.

1 Introduction

Climate change is an outcome of intricate interactions among atmospheric, oceanic, terrestrial, and biological systems. These interactions operate across various spatial and temporal scales and involve numerous feedback loops, nonlinearities, and uncertainties. To understand and predict climate behavior, researchers employ mathematical models, a critical bridge between theory, simulation and observation. Early climate models began with energy balance models (EBMs), which simplified Earth’s radiation budget into

algebraic or differential equations. EBMs help estimate average global temperature changes based on greenhouse gas concentration scenarios (North et al., 1981). As computational power increased more complex models emerged, notably General Circulation Models (GCMs) which discretize the Earth's surface and atmosphere to solve fundamental equations of fluid dynamics, thermodynamics and radiative transfer (Washington & Parkinson, 2005; Trenberth, 1992).Modern models incorporate processes such as carbon cycling, cloud dynamics, aerosol forcing, and ice-albedo feedback, all governed by systems of partial differential equations (PDEs) and numerical algorithms (Trenberth, 1992). For instance, the Navier-Stokes equations are used to simulate atmospheric and oceanic flow, while radiative transfer equations calculate energy absorption and emission across spectral bands (Randall, 2000).Climate models are calibrated and validated using satellitedata, paleoclimate records, and in situmeasurements. Mathematical tools like data assimilation, machine learning, and Bayesianinference are employed to reduce model uncertainty and improve forecasting skill (Liou, 2002; Kalnay, E. 2003).As the Intergovernmental Panel on Climate Change (IPCC) emphasizes, reliable climate projections are indispensable for policymaking and global environmental governance (Reichstein et al., 2019).This chapter reviews key mathematical frameworks used in climate modeling and evaluates their capabilities, assumptions, and limitations in the context of global climate change.

2. Mathematical Foundations of Climate Modelling

Mathematical climate models are structured systems of equations that simulate energy flow, mass transport and chemical processes. These models range in complexity:

2.1 Energy Balance Models (EBMs)

Energy Balance Models (EBMs) are one of the foundational tools in climate science. They describe the balance between incoming solar radiation and outgoing longwave terrestrial radiation to estimate the Earth’s average surface temperature. The simplest form of a zero-dimensional EBM is represented by the following ordinary differential equation (Masson-Delmotte et al., 2021; Budyko, 1969)

$$C\,dT/dt = S(1-\alpha)-\epsilon\sigma T^4$$

Where:

C effective heat capacity of the Earth system ($J \cdot m^{-2} \cdot K^{-1}$)

T global mean surface temperature (K)

S solar constant (~1361 $W \cdot m^{-2}$)

α planetary albedo (typically ~0.3)

ϵ effective emissivity (~0.612 for Earth)

σ Stefan–Boltzmann constant (~5.67×10^{-8} $W \cdot m^{-2} \cdot K^{-4}$)

This equation models the net radiative energy gain or loss at the Earth's surface. The term S(1-α) denotes the absorbed solar radiation, while ϵσT^4represents the outgoing longwave radiation as per the Stefan–Boltzmann law (Peixoto & Oort, 1992) EBMs are useful for studying climate sensitivity, ice-albedo feedback, and radiative forcing scenarios under changing atmospheric compositions. By introducing temperature-dependentalbedo and emissivity, the model can be extended to analyze tipping points and bifurcation behavior, indicating transitions such as ice ages or runaway warming (Ghil, (1976; Fraedrich, 1979). Though simplistic compared to General Circulation Models (GCMs), EBMs remain valuable in conceptual climate studies and policy frameworks for evaluating the long-term effects of greenhouse gas emissions (Holton& Hakim, 2012).

2.2 Radiative Transfer Models

Radiative transfer models use integro-differential equations to describe the absorption,scattering, and emission of radiation as it passes through the Earth's atmosphere. These equations are fundamental to simulating energy exchanges between the Earth's surface, atmosphere, and space, and are crucial in both weather forecasting and climate modeling (Goody & Yung, 1989).

$\mu \, dI\nu/dz = -k_\nu I_\nu + j_\nu$

Where:

I_ν spectral radiance at frequency ν ($W \cdot m^{-2} \cdot sr^{-1} \cdot Hz^{-1}$),

$\mu = \cos\theta$ is the direction cosine of the radiation path relative to the vertical,

z is the vertical coordinate (height),

k_ν is the absorption coefficient (m^{-1}),

j_ν is the emission source function ($W \cdot m^{-3} \cdot sr^{-1} \cdot Hz^{-1}$).

This equation balances the loss of radiance due to absorption and the gain due to emission. In more realistic models, especially for climate and atmospheric remote sensing applications, scattering terms are also included, turning the equation into a full integro-differential form.

2.3 General Circulation Models (GCMs)

GCMs solve the primitive equations, a system of PDEs representing fluid flow on a rotating sphere:

Continuity equation

Momentum equation (Navier–Stokes)

Thermodynamic energy equation

Moisture equation

Radiative transfer equations

To numerically solve these equations over the globe, discretization techniques such as finite difference, spectral, or finite volume methods are applied over a three-dimensional grid of cells spanning latitude, longitude, and vertical layers (Washington & Parkinson (2005).

3. Components of a Climate Model

3.1 Atmospheric Module

This module simulates:

Wind velocity vectoru=(u,v,w)

TemperatureT

Pressurep

Humidityq

Governing Equations

The Navier-Stokes equations for incompressible flow in a rotating reference frame are essential to large-scale geophysical fluid dynamics and climate modelling. They offer a useful framework for simulating atmospheric and oceanic processes when combined with radiative transfer models, the continuity equation, and the thermodynamic energy equation (Vallis, 2017; Goody & Yung, 1989).

3.1(a) Momentum (Navier-Stokes) Equation (Rotating Frame):

$\partial u/\partial t+u\cdot\nabla u=(-1)/\rho\ \nabla p+g+\nu\nabla\hat{}2\ u-2\Omega\times u$

Where:

u: velocity vector

ρ: air density (~1.2 kg/m³ at sea level)

ν: kinematic viscosity (~1.5×10^{-5} m²/s)

Ω: Earth's angular velocity vector (Coriolis effect)

g: gravitational acceleration (~9.81 m/s² downward)

p: pressure

This formulation accounts for Earth's rotation $2\Omega \times u$, which plays an important role in the dynamics of atmospheric and oceanic flows (Vallis, 2017).

3.1(b) Continuity Equation (for incompressible flow):

$$\nabla \cdot u = 0$$

This ensures mass conservation for incompressible fluids (Vallis, 2017).

3.1(c) Thermodynamic Energy Equation:

$$dT/dt = Q/C_P$$

Here, T is the temperature, Q is the heating rate per unit mass, and C_P is the specific heat at constant pressure. This equation describes how temperature evolves due to radiative and convective heating processes (Goody & Yung, 1989).

3.1(d) Radiative Transfer: Beer's Law

$$I(z) = I_0 e^{(-kz)}$$

Beer's Law characterizes the reduction in solar radiation intensity during its transmission through the atmosphere. where I(z) is the intensity at depth z, I_0 is the incoming solar intensity at the top of the atmosphere, and κ is the absorption coefficient. This law is a cornerstone of radiative transfer in climate models (Pitman, 2003; Flanneret al., 2007).

3.2 Ocean Module

Simulates oceanic currents, stratification, and mixing layers.
Governing Equations:
Uses the Boussinesq approximation for incompressible flow with buoyancy effects:
$\partial u/\partial t+u\cdot\nabla u=(-1)/\rho_0\ \nabla p+g\ \Delta\rho/\rho_0+\nu\nabla^2 u$
Where:

$\Delta\rho=\rho(T,S)-\rho_0$
Temperature (T) and salinity (S) impact density via the equation of state.
Heat transport: modeled via advection-diffusion equations for T and S.

3.3Cryosphere and Land Surface Module

This module handles complex interactions involving snow, glaciers, permafrost, vegetation, andsoil, which are essential components for simulating land-atmosphere feedbacks in climate models (De Vries, 1952).

Processes Modeled:

Snow/ice albedo feedback: Highly reflective surfaces, such as fresh snow, can return up to 90% of incoming solar radiation to space, resulting in localized cooling. This cooling effect can promote additional snow accumulation, creating a positive feedback mechanism. The elevated albedo of snow is a key factor in controlling the surface energy balance and influencing climate sensitivity (Sitch et al., 2003). Soil heat and moisture transfer: These processes are typically governed by Richards'equationfor moisture dynamics and Fourier's law (heat conduction equation) for thermal transfer in the soil column. They control the coupling between land surface temperature and subsurface water availability, crucial for vegetation growth and energy fluxes (Trenberth, 1992).

Vegetation dynamics: These are simulated using either empirical growth rate models or more complex Dynamic Global Vegetation Models (DGVMs). These models incorporate biophysical and biogeochemical processes such as photosynthesis, respiration and competition among plant functional types (Randall, 2000).

4. Climate Model Techniques, Uncertainties, and Applications

Numerical climate models simulate Earth's systems using advanced mathematical schemes. Common methods include Runge–Kutta and Euler time-stepping, Arakawa grids, spectral methods, and semi-implicit/Crank–Nicolson schemes to ensure stability and accuracy (Murphy et al.,2004)Sub-grid processes like clouds and turbulence are statistically parameterized and high-performance computing is essential to run simulations over decades (Randall, 2000).

Models face multiple uncertainties:

Initial condition sensitivity due to chaotic dynamics (Lorenz, 1963).

Parametric uncertainty (e.g., albedo, emissivity)

Structural uncertainty from model design differences.

To manage this, methods like ensemble forecasting, Bayesian inference, and Monte Carlo simulations are widely applied (Murphy et al.,2004) Climate models inform global assessments (e.g., IPCC) and guide policy on carbon budgeting, sea-level projections, extreme weather, and adaptation planning(Masson-Delmotte et al., 2021).Future efforts aim to improve cloud and aerosol physics, increase resolution with less computation, and integrate AI and socio-economic models for more holistic projections.

5. Conclusion

Mathematical modeling is essential for understanding and addressing the complex dynamics of global climate change. By employing tools such as energy balance equations, general circulation models (GCMs) and numerical simulations, researchers can systematically quantify the intricate interactions between the atmosphere, oceans, land and cryosphere. These models are instrumental in informing climate policy by

offering scientific foundations for carbon budgeting, emissions forecasting and risk assessment. With advancements in computational power, adaptive grid algorithms and machine learning techniques, climate models are becoming increasingly precise and efficient. Moreover, the integration of climate models with economic, ecological and social systems allows for more comprehensive and sustainable decision-making frameworks. As the urgency of climate risks escalates, these mathematical tools remain indispensable for evidence-based policymaking, international climate negotiations, and the design of long-term adaptation and mitigation strategies. Ultimately, mathematical modeling extends beyond theoretical exploration serving as a cornerstone in the global effort to safeguard the Earth's future.

References

Arakawa, A., & Lamb, V. R. (1977). Computational design for atmospheric models. Methods in Computational Physics, 17, 173–265.

Budyko, M. I. (1969). The effect of solar radiation variations on the climate of the Earth. Tellus, 21(5), 611–619.

DeVries,D. A. (1952). The thermal conductivity of soil. Mededelingen van de Landbouwhogeschool te Wageningen, 52(1), 1–82.

Flanner, M. G., Zender, C. S., Randerson, J. T., & Rasch, P. J. (2007). Present-day climate forcing and response from black carbon in snow. Journal of Geophysical Research: Atmospheres, 112(D11).

Fraedrich, K. (1979). Catastrophes and resilience of a zero-dimensional climate system. Quarterly Journal of the Royal Meteorological Society, 105(446), 147–167.

Ghil, M. (1976). Climate stability for a Sellers-type model. Journal of Atmospheric Sciences, 33(1), 3–20.

Goody, R. M., & Yung, Y. L. (1989). Atmospheric radiation: Theoretical basis (2nd ed.). Oxford University Press.

Holton, J. R., & Hakim, G. J. (2012). An introduction to dynamic meteorology (5th ed.). Academic Press.

Intergovernmental Panel on Climate Change (IPCC). (2021). Climate change 2021: The physical science basis. Contribution of Working Group I to the Sixth Assessment Report of the Intergovernmental Panel on Climate Change (V. Masson-Delmotte et al., Eds.), Cambridge University Press.

Kalnay, E. (2003). Atmospheric modeling, data assimilation and predictability. Cambridge University Press.

Liou, K. N. (2002). An introduction to atmospheric radiation (2nd ed.). Academic Press.

Lorenz, E. N. (1963). Deterministic nonperiodic flow. Journal of Atmospheric Sciences, 20(2), 130–141.

Murphy, J. M., Sexton, D. M. H., Barnett, D. N., Jones, G. S., Webb, M. J., Collins, M., & Stainforth, D. A. (2004). Quantification of modelling uncertainties in a large ensemble of climate change simulations. Nature, 430 (7001), 768–772.

North, G. R., Cahalan, R. F., & Coakley, J. A. (1981). Energy balance climate models. Reviews of Geophysics, 19(1), 91–121.

Peixoto, J. P., & Oort, A. H. (1992). Physics of climate. American Institute of Physics.

Pitman, A. J. (2003). The evolution of, and revolution in, land surface schemes designed for climate models. International Journal of Climatology, 23(5), 479–510.

Randall, D. A. (2000). General circulation model development: Past, present, and future. Academic Press.

Reichstein, M., Camps-Valls, G., Stevens, B., Jung, M., Denzler, J., Carvalhais, N., & Prabhat. (2019). Deep learning and process understanding for data-driven Earth system science. Nature, 566(7743), 195–204.

Roe, G. H., & Baker, M. B. (2007). Why is climate sensitivity so unpredictable? Science, 318(5850), 629–632.

Sitch, S., Smith, B., Prentice, I. C., Arneth, A., Bondeau, A., Cramer, W., Venevsky, S. (2003). Evaluation of ecosystem dynamics, plant geography and terrestrial carbon cycling in the LPJ dynamic global vegetation model. Global Change Biology, 9(2), 161–185.

Trenberth, K. E. (1992). Climate system modeling. Cambridge University Press.

Vallis, G. K. (2017). Atmospheric and oceanic fluid dynamics (2nd ed.). Cambridge University Press.

Washington, W. M., & Parkinson, C. L. (2005). An introduction to three-dimensional climate modeling (2nd ed.). University Science Books.

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Chapter 12: Statistical Inference in Pandemic Forecasting: An Integrative Approach

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Abstract: The unprecedented global impact of pandemics, such as COVID-19, has underscored the need for accurate and timely forecasting to guide public health interventions and policy decisions. This paper presents an integrative approach to pandemic forecasting based on statistical inference methods that combine data-driven modeling, uncertainty quantification, and real-time prediction. The study explores key statistical tools such as Bayesian inference, maximum likelihood estimation, regression analysis, and time-series modeling to interpret and predict epidemic dynamics. These tools enable researchers to estimate crucial parameters including infection rates, reproduction numbers (R_0), and recovery times, even under conditions of limited or noisy data. By incorporating both deterministic and stochastic models, the paper highlights how statistical inference enhances the robustness and adaptability of predictive models. It further examines the integration of real-world datasets—such as case counts, testing rates, mobility data, and vaccination coverage—to refine model accuracy. Challenges such as parameter identifiability, sampling bias, and data incompleteness are addressed with strategies like hierarchical modeling, ensemble methods, and cross-validation.

The paper also presents case studies illustrating how inferential techniques have informed early warning systems and scenario planning during recent pandemics. The synergy between classical statistical methods and modern machine learning algorithms is emphasized as a pathway to improved forecasting capabilities. Ultimately, the work advocates for interdisciplinary collaboration and transparent modeling practices to build resilient systems for future epidemic preparedness and response.

Keywords: Statistical Inference, Pandemic Forecasting, Bayesian Modeling, Epidemiological Parameters, Time-Series Analysis

1 Introduction

Refined statistical inference is the cornerstone of pandemic forecasting. Forecasting the extent and timing of an outbreak provides a basis for decisions that lessen its impact on populations. For example, forecasts of infected individuals help inform the management of public health resources. This work develops a comprehensive framework for integrating statistical inference with epidemic models and demonstrates its use across different pandemic outbreaks. For each outbreak, diverse models are calibrated to competing data streams, and inferences from different models and datasets are combined to generate more robust forecasts. Embedding inference within modeling frameworks allows for tracking the evolution of a pandemic as new data arrives (W. Taylor & S. Taylor, 2021) (Petropoulos et al., 2020) (Mehta & Kasmanoff, 2022). Statistical inference provides a framework for translating data into knowledge-of-parameters and knowledge-of-models-anchored forecasts, which inform policy decisions and prevention strategies designed to save lives.

2. Background and Rationale

With annual worldwide deaths reaching 18 million, a detailed understanding of the processes behind common diseases such as heart disease, cancer, and diabetes would constitute a major breakthrough. Analyzing complex health data collected in clinical trials, cohort studies, or registries through sophisticated statistical methods has the potential to unveil new insights into these diseases. Evolving evidence and information from clinical trials guide the selection or design of candidate competing models, which are then further refined using observational data. Despite contributions from many researchers, Covid-19 forecasting models often fail to systematically report prediction accuracy, complicating evaluation. A useful forecasting approach provides both the mean estimate and multiple levels of uncertainty, as wide prediction intervals may overestimate uncertainty to prepare for extreme scenarios, while some models have underestimated it. A single time series model can achieve consistent accuracy in forecasting cases and deaths, and combining forecasts from diverse models can enhance accuracy (Petropoulos et al., 2020). Governments rely on predictions of cases, hospitalizations, and deaths for planning, but forecasting models are limited by data scarcity and assumptions regarding immunity, asymptomatic transmission, and public response. Policymakers must understand these uncertainties and limitations. Probabilistic forecasts, such as distributional and interval forecasts, offer valuable information for decision making and situational awareness; combining forecasts from multiple sources leverages collective insights (W. Taylor & S. Taylor, 2021). Replicating and forecasting the spread of SARS-CoV-2 is possible using probabilistic programming languages, facilitating study of modeling assumptions and policy interventions to limit infectious disease spread. Existing compartmental models enable posterior estimates of disease parameters, with improvements to account for under-

reporting of cases and to model real-world interventions. An SEI3RD model serves as a reusable, flexible template, and a greedy algorithm assists in selecting optimal policy interventions to control infection levels under constraints. The framework is simple, modular, and reproducible, providing access to state-of-the-art probabilistic inference focused on policy measures (Mehta & Kasmanoff, 2022).

3. Statistical Methods in Epidemiology

Statistical methods in epidemiology play a prominent role in shaping public-health responses during pandemics but require refinement if they are to provide optimal support for decision-making. During the COVID-19 epidemic, forecasting methods have been used widely to generate planning scenarios, and several major groups have built statistical models of infectious disease to underpin those predictions (E. Moore et al., 2021). The challenge is that the infectious disease forecasting paradigm remains in its infancy, and there exist enormous opportunities to strengthen the approach on multiple fronts (L. Juul et al., 2020). Although assessment of epidemiological models typically involves comparison of predicted to observed values, the practice of assessing full-distribution models in such a manner is yet to be adopted widely. For example, Maishman et al. (2021) analyse the effective reproduction number (R t) produced by several groups, describing differences in bias and variability in point estimates. Drawing on data from a bespoke transmission model, we introduce a statistical framework designed to incorporate multiple sources of COVID-19 surveillance data simultaneously.

3.1. Descriptive Statistics

The COVID-19 pandemic has created enormous planning and resource allocation challenges, and governments rely on predictions of cases, hospitalizations, and deaths to decide actions. Short-term forecasting of reported COVID-19 deaths is therefore essential. Epidemiological forecasting models have been applied to various infectious diseases, including SARS, Ebola, and MERS. These models are based on different assumptions and answer different questions. Limited data prompt assumptions about immunity, asymptomatic transmission, and public reactions. Forecasting infectious diseases is considered among the most challenging data sciences problems, and models have inherent uncertainties.

Probabilistic forecasts (or distributional forecasts) provide a more complete picture than single point forecasts. Interval forecasts predict a range containing the true outcome with a specified probability and assist real-time decision making and situational awareness. Combining forecasts from multiple models leverages the collective wisdom of experts (W. Taylor & S. Taylor, 2021). Descriptive statistics describe either populations or samples. Since sampling real-time epidemics is not feasible, model-generated data sets surrogate a hypothetical population. Rubin (1993) demonstrates equivalence between Bayesian posterior uncertainty relative to an observed sample and uncertainty regarding

a super-population from which the sample is hypothetically drawn. Thus, samples from scenario analyses inform measures of central tendency and uncertainty rather than raw data.

Using ensemble simulations, the death toll and hospitalization demand are forecasted. Curve-based descriptive statistics develop measures of central tendency and uncertainty regions. To facilitate inter-scenario comparisons, the underlying SIR-type model is encapsulated within a scenario specification (L. Juul et al., 2020). The SIR-type model is a compartmental ordinary differential equations (ODE) model capturing asymptomatic cases and hospitalizations. Modelling approaches that diverge substantially from standard compartmental models (e.g. agent-based simulations) can also be considered within this paradigm.

3.2. Inferential Statistics

Common practice applies systems theory and pairwise coupling between system components to model mode failure and propagation under system-wide stress. Failure modes are described by graphs linking components to the dominant mechanism behind failed components; however, time series data considerations are often missing. Frequency domain methods quantify pairwise coupling between oscillatory components and are widely applied in economics to quantify causal relationships among fluctuating economic parameters. For COVID-19, problems arise due to incomplete data, requiring multiple assumptions regarding immunity and public response. Mechanistic models with multiple parameters can fit data well but are non-identifiable, permitting arbitrarily large uncertainty in their forecasts. Hence, robust quantification of uncertainty is essential to provide decision makers with informative and quantitative forecasts under scenarios involving quarantine or mitigation policies. In economics and epidemiology alike, the ability to quantify parametric and structural uncertainty is paramount, especially for COVID-19 where comprehensive data are lacking. Decision makers require methods that integrate scarce data, quantify uncertainty robustly, and support risk planning amid potential long-range contagion scenarios. A novel methodology fully integrates stochastic compartmental models with error structures to systematically analyze non-stationary epidemic time series at a country scale. The approach decomposes observed time series into stochastic components, tracks their evolution, and maps growth rates to effective reproduction numbers (R_{eff}). Historical scenarios are generated by sampling the posterior distribution of growth rates; subsequent propagation of epidemic models yields probabilistic forecasts, which can be combined with multiple models to enhance reliability.

Models have been proposed to track epidemics and estimate transmission parameters; their predictive capabilities are enhanced by statistical inference from partial observations. Foster et al. demonstrated inference of transmission parameters and hidden

states through the line list despite early data incompleteness. Estimating transmission parameters from time series data and applying models for consistent forecasts of epidemic trajectories remains pivotal. Emphasizing inference and forecasting for rapidly evolving pandemics, a stochastic compartmental model facilitates (i) statistical inference of transmission parameters from multi-component partially observed time series; and (ii) probabilistic forecasting for mitigating epidemic consequences. Observations are modelled as stochastic processes with Gamma noise, Serra and Kruk quantified additive or multiplicative measurement noise under MaxCal, and past epidemic data have been treated as partially observed. This methodology extensively quantifies measurement, structural, and parametric uncertainty in transmission models, deriving both pointwise estimates and probabilistic forecasts. Crucially, the approach addresses multiple observed components, incorporates suitable noise models, and accounts for both structural and parametric uncertainty (W. Taylor & S. Taylor, 2021) (Petropoulos et al., 2020) (L. Juul et al., 2020).

3.3. Bayesian Methods

The unfolding COVID-19 pandemic necessitates dependable model-based projections to inform policy (L. Daza-Torres et al., 2022). The volume of available data complicates inference, rendering it impracticable to fit an entire epidemic history, particularly when parameters such as contact rates vary temporally. Information older than one month is unlikely to significantly enhance nowcasting and prediction, prompting the use of regular model recalibration.

Consequently, a Bayesian sequential data assimilation and forecasting approach is developed, tailored to a broad class of non-autonomous dynamical systems and applied to COVID-19. The methodology assumes pre-validated transmission, epidemic, and observation models, which are amalgamated into a comprehensive, epidemiologically grounded dynamical system. The susceptible population and initial conditions are modeled as random variables governed by elicited prior distributions, while the contact rate is treated as a time-dependent parameter. Employing Markov Chain Monte Carlo sampling, the framework facilitates inference on parameters of interest and projections of derived quantities such as hospital occupancy.

Inference commences at the onset of community transmission and proceeds in one-week increments, incorporating successive data sets via a sliding temporal window. At each update, novel prior models are constructed from the current posterior distributions, imposing temporal coherence on parameter trajectories through auto-regressive specifications. The resulting Bayesian filtering scheme constitutes a promising avenue for enhanced epidemic data assimilation and forecasting.

4. Data Sources for Pandemic Forecasting

Forecasting pandemics depends on data about both the disease and the populations affected. Data about the pandemic include estimates of transmissibility, spread, case indicated rates, deaths, frequency, and incubation period. Population data may include changes brought on by a specific pandemic, such as mortality age distribution and policy intervention. Data requirements change over time. For example, before the first 100 cases are detected, information about estimates such as transmissibility and incubation period is needed. Later data requirements might focus on hospitalizations, deaths, and the impacts of non-pharmaceutical interventions.

Data feeds into estimation and prediction models in the form of historical data (e.g., age, sex, cases, deaths, hospitalizations), metadata about the data (e.g., definition of inflation-adjusted constant cases, determinations about recording of assisted suicide as a disease death), and other contemporaneous data. These data come from different source regions—infected and uninfected—with different demographics. The list of pandemic forecasting data sources is now long and may be found in repositories such as the World Bank Data or Our World in Data.

4.1. Public Health Databases

Effective responses to pandemics require the integration of statistical models with datasets. The latter fall into three broad classes: routinely collected infection data, public health interventions, and behavioral data.

Routine, high-quality data are available from administrative sources at the global and local level. Preparing such data for inference requires care, corroboration by multiple data types and, where possible, modelling the underlying surveillance system generating the data (M. A. Bettencourt et al., 2007).

Newer technologies provide indirect proxies of infection: e.g. electronic health records, search and social media, participatory syndromic surveillance, and crowd-sourcing.

These datasets are large, varied, heterogeneous, and often sparse. They also encode behavioral changes, particularly in response to vast non-pharmaceutical intervention (NPI) programmes implemented globally, from within-country restrictions through to national lockdowns. With epidemiological parameters consistent across settings, statistically capturing the impact of interventions is crucial (W. Taylor & S. Taylor, 2021).

4.2. Social Media Data

The ongoing COVID-19 pandemic has placed enormous strain on healthcare systems worldwide and highlighted the importance of accurate pandemic forecasting models. Statistical models of various forms have always been central to the inference of

pandemic forecasts, from basic epidemic models to more complex agent-based models and data-driven neural network models. At the same time, data sources have grown and are now more abundant than ever, making it possible to build rich data models that incorporate important social, behavioral, and environmental factors.

People tend to share their thoughts and opinions on social media, making these platforms critical tools for assessing awareness and attitudes. Over half of the world's population uses social media, a percentage that continues to grow. Given that social media platforms reflect, forecast, and shape behaviour, they are an important channel through which to capture attitudes, beliefs, opinions, awareness, intentions, and reported behaviour towards infectious diseases and interventions (Sooknanan & Mays, 2021). Social media platforms interact with their users, enhancing understanding and social awareness about interventions and treatments. COVID19 social media content acts as a multivariate indicator of public sentiment and pandemic evolution (Tran et al., 2023). Incorporating up-to-date information sources, such as social media content, is therefore important for refining disease models and supporting forecasting models with additional indicators.

4.3. Mobile Health Applications

Mobile health (m-health) applications collect high-frequency data on individual-level characteristics while preserving privacy to support timely collection and analysis of real-world data during pandemics. Mobile-device time-series data were combined with a stochastic susceptible–exposed–infectious–recovered (SEIR) model to forecast hospital admissions in Massachusetts for 1148 individual hospitals during the second COVID-19 wave (Klein et al., 2023). M-health applications initially provided Mobile Positioning Data (MPD) and Call Detail Records (CDR) for interventions, such as social distancing and face coverings, to curb virus spread. An SEIR model calibrated on data from the first wave is used as a mediator between epidemiological indicators and real-time mobile-device data, informing both the transmission rate and hospitalization-forecasting model. During the second wave, the resulting forecasting models demonstrate superior accuracy compared to models relying solely on admissions and test positivity, offering a longer lead time for individual hospitals to allocate resources. Mobile-device data enable the construction of large, time-varying contact networks, instrumental for pandemic modeling. However, while generative ultra-scale SEIR-like models based on mobility leverage such networks, their inference from time-series data poses computational challenges due to high dimensionality. A novel system-identification approach based on the Ensemble-Kalman filter (AutoEKF) addresses these challenges, enabling the inference of SEIR-like models from fine-grained GPS data for both in-sample fitting and out-of-sample forecasting across millions of individuals (Barreras et al., 2021).

5. Modeling Techniques

Outbreak forecasting constitutes a primary application of epidemiological modeling. Accurate forecasts of disease burden and case counts are essential to guide public health decision-making. The COVID-19 pandemic has further elevated the practical relevance of modeling; compartmental models, for example, have been used to explore notions of disease risk and probable impact of social distancing and vaccination (R. Biegel & Lega, 2021). Metapopulation approaches, which explicitly describe population connectedness and human mobility, provide estimates of the probability of contagion travel between different regions (Chowell et al., 2022). Complementary methodologies include statistical analyses and agent-based modelling. Limited availability of parameter data forces a delicate balance between model parsimony and complexity. Very simple models neglect many aspects of COVID-19 dynamics, yielding forecasts unreliable beyond short time horizons. Conversely, excessive model detail, especially when parameters are not well identified, can produce unacceptably large uncertainties. Ensemble models blending different approaches generally constitute more reliable forecasting tools. A computationally efficient forecasting technique combines the interpretability of compartmental frameworks with flexible curvature patterns in phenomenological profiles. The incompletely specified compartmental model (ISCM) underpins this approach, a flexible mechanism that retains compartmental interpretability without explicit differential equations. Uncertainty quantification utilizes an adaptive Markov chain Monte Carlo scheme that naturally high-lights multimodality of the parameter posterior distribution.

5.1. Compartmental Models

Compartmental models were first introduced in 1906 by Ross for malaria and further developed in 1927 by Kermack and McKendrick; they remain one of the most widely used tool for studying the transmission dynamics of infectious diseases. The most basic structure is a network of compartments, each of which represents a specific condition with respect to the disease under study; individuals pass between compartments according to a flow rate that may depend on the interaction between compartments. Several popular variants exist, including SIR (Susceptible–Infectious–Recovered), SEIR (Susceptible–Exposed–Infectious–Recovered), and SEAIR (Susceptible–Exposed–Asymptomatic–Infectious–Recovered) (Zhang et al., 2022). While these models often provide accurate short-term forecasts on reallife multi-peak datasets when combined with performance-enhancement strategies, undertaking long-term forecasting or modeling special scenarios like vaccination and quarantine remains challenging. Nevertheless, the relatively low computational demands of compartmental models facilitate their deployment over large spatial scales and enable the efficient execution of numerous forecast iterations. Such flexibility permits the generation of critical epidemiological outputs, including forecasts of active infections and cases averted,

which are instrumental in shaping pandemic intervention policies, optimizing medical resource allocation, and mitigating drug shortages.

5.2. Agent-Based Models

Agent-based models (ABMs) are an additional mechanistic modelling framework, which describe disease transmission at the level of the individual (Herriott et al., 2023). ABMs allow population heterogeneity to be accounted for explicitly; every member of the population is represented, along with a set of traits that remain fixed or evolve according to user-defined rules. ABMs produce detailed, informative predictions when inter-individual variability in traits, behaviour and interactions is influential. Age structure, household structure and population-level mobility can be included natively, without adding additional compartments or differential equations. Stochastic effects become important when predicting transmission among small groups of individuals, which cannot be accounted for with continuous differential equation models, yet can be incorporated readily in an ABM. The impact of a range of interventions on disease spread can be assessed, providing evidence to inform government policy. Individual contacts can be simulated on an interaction-by-interaction basis, which is often straightforward to implement in ABMs, whereas the corresponding formulation would be considerably more involved in a compartmental model. The additional model complexity can, however, translate to considerably longer runtime than alternatives such as compartmental models; this can present challenges with Bayesian inference, which requires a large number of evaluations of the likelihood function (Li et al., 2018).

5.3. Machine Learning Approaches

Several recent deep-learning approaches have been proposed for epidemic prediction. EpiDeep co-training exploits seasonal and intra-seasonal data, while DEFSI encodes a deep latent space representation of disease trajectories to forecast multiple diseases at various spatial resolutions (Rodríguez et al., 2020). These deep methods can leverage data from additional cities to improve performance. Nonetheless, they typically require external data sources—such as mobility—and do not accommodate expert guidance, which is important for model calibration and real-world impact.

6. Parameter Estimation

An outbreak forecasting method combines data-driven parameter estimation with variational data assimilation to capture the fundamental components of nonlinear disease transmission (R. Biegel & Lega, 2021). Stochastic fluctuations are simplified as a process with independent increments, reducing the characterization to four core parameters. This minimalist scheme supports computational efficiency and enables applicability to other diseases or locations provided case counts and/or death data are available. Given limited knowledge in the early phase of a novel virus pandemic, key

parameters may be uncertain and measurements sparse or noisy (Swallow et al., 2022). Bayesian inference offers a framework for combining model and data with prior distributions that summarize available information. When knowledge from related viruses is unreliable, imposing a prior distribution on parameter ranges mitigates the risk of bias inherent in fixed unknowns. Systematic prior elicitation techniques support the construction of plausible distributions to guide early-stage simulations. Subsequent systematic sensitivity analyses reveal output variables that are particularly sensitive to parameter variation, which, in turn, informs targeted data collection and study design aimed at more accurate estimation.

6.1. Maximum Likelihood Estimation

Maximum likelihood estimation (MLE) endeavors to identify the parameterization, within a specified family, that maximizes the probability (or probability density) of the observed dataset (R. Biegel & Lega, 2021). In typical applications, the dataset comprises independent points, each governed by a distinct probability distribution. The likelihood function assumes a multiplicative form, derived from the individual density values evaluated at the data points. Statistical theory predicates that this choice possesses strong frequentist attributes, implying desirable properties in repeated-sampling scenarios, when the selected family is well-specified and sufficiently flexible (E. Moore et al., 2021). The same strong statements do not necessarily hold if the data points are not independent, underscoring the necessity for cautious interpretation in time-series contexts. When confronted with a time series, the discretion lies with the practitioner to decide between presuming independence or resorting to a parametric model. The first alternative, albeit not underpinned by robust theory, is readily applicable when the data-generating process remains elusive. Under this assumption, within the class of models that satisfy it, the inferences can be deemed the most reliable.

6.2. Markov Chain Monte Carlo

Mechanistic epidemic models are widely used for forecasting and estimating infectious-disease parameters from noisy case-report data. Despite their prevalence, little is known about the comparative performance of Bayesian Markov chain Monte Carlo (MCMC) approaches in this setting. We formulate a stochastic, discrete-time, discrete-state epidemic model with both process and observation error to assess the capabilities of different MCMC techniques. Models that accommodate discrete versus continuous latent states and varying levels of stochasticity are fitted using JAGS, NIMBLE, and Stan (Li et al., 2018). Parameter estimation in epidemic models poses particular challenges early in an epidemic, when data are necessarily limited. We compare the performance of simple MCMC methods on simulated epidemic data featuring transmission stochasticity, observation errors, and a flexible generation-interval distribution.

Stochastic epidemic models describe the dynamics of an outbreak as a disease spreads through a population. Often, only a subset of cases are observed at discrete times, which generates a complex latent-variable problem. For even moderately sized populations, the associated state space becomes prohibitively large, rendering integration over the missing data infeasible. A data-augmentation MCMC framework for Bayesian inference is proposed, wherein the measurements are supplemented with additional subject-level information. Each new subject-level path is proposed conditional on the augmented data by means of a time-inhomogeneous continuous-time Markov process with transition rates determined by the infection histories of other individuals (Fintzi et al., 2016). The methodology is both general and applicable to a broad class of stochastic epidemic models. An illustration with binomially sampled prevalence counts is presented alongside an application to an influenza outbreak at a British boarding school.

7. Forecasting Techniques

Forecasting techniques are typically classified into three general schools: statistical, mechanistic, and judgmental (Petropoulos et al., 2020). Statistical approaches predict behaviours of time series according to historical data; simple models are easier to interpret but typically lack the complexity of mechanistic approaches. Mechanistic models divide the population into epidemiological compartments to simulate the progression of disease; a prevalent class is SEIR-type models (Susceptible, Exposed, Infectious, Recovered or Removed). Judgmental, or expert, methods use collective human judgment to arrive at forecasts. Judgmental methods can be particularly valuable when historical data do not exist for the current phenomena and for the early development of new epidemics and novel pathogens Specialised approaches from each school have been proposed for epidemic forecasting of COVID-19, and combinations of different models into ensembles can further improve forecasting accuracy (Kandula et al., 2018).

7.1. Time Series Analysis

Methods from time series analysis are widely used to characterize the propagation of pandemics and to forecast the evolution of cases, hospitalizations, and fatalities (L. Daza-Torres et al., 2022). Given a time series of daily counts—number of new reported cases, number of new hospitalizations, or number of new fatalities—the goal is to predict the temporal evolution of any of these variables. The Bayesian sequential data assimilation framework developed by Daza-Torres et al. can be implemented with any dynamic epidemic model that produces forecasts compatible with the data. In this approach, L denotes the length in days of the period used to train the model, D the duration of the reporting delay, F the forecasting horizon, and n the frequency of forecast updates, typically weekly. The epidemic is mathematically formulated as an initial value problem for a nonlinear dynamic system of differential equations, $x˙(t)=f(x(t),\theta k)$, where

θk represent model parameters. Probabilistic prediction of state variables x(t) is carried out by integrating a predictive distribution p(x(t) | y1:k) over the joint space of initial conditions xk and parameters θk, with sequential updating: today's posterior informs tomorrow's prior.

Free-of-assumptions frameworks such as the n-sub-epidemic approach proposed by Chowell et al. (Chowell et al., 2022) also enable short-term forecasting of epidemic trajectories from time series data. The model phenomenologically represents complex epidemic trajectories as the sum of asynchronous and overlapping sub-epidemics, each described by a generalized logistic growth model. It naturally accounts for diverse epidemic dynamics, including plateaus, resurgences and multiple peaks.

7.2. Exponential Smoothing

Exponential smoothing represents a widely applied forecasting technique well-suited to pandemic data. It considers the phenomenon as a weighted moving average in which the more recent observations receive greater weights. The weights are determined as an exponentially decreasing function of time from the observation, resulting in a smaller number of parameters and less demand on historical data compared to autoregressive methods. The simplest variant, Simple Exponential Smoothing (SES), takes a weighted average between the most recent observation and the previous smoothed average. This technique is most appropriate for time series devoid of clear trend or seasonal patterns. In the SES model, given a time series \, {Q t} \, with an observed value at time \, t \, denoted by \, q t \, and a smoothed value \, s t \, based on all values preceding \, t \, including \, q t, the smoothed value is calculated by the formula \[s t = \alpha q t + (1 - \alpha) s t-1 \] where the smoothing parameter \, \alpha \, lies within the open interval (0, 1). The parameter set \, \boldsymbol\theta = \{\alpha, s_0\} \, comprises the smoothing coefficient and the initial smoothed value. The process initiates at \, t = 1 \, with the choice of \, s_0 \, often equal to \, q_1. The method iteratively computes the smoothed values for successive times and can generate point forecasts into the future by extrapolation from the latest smoothed value (E. Moore et al., 2021).

7.3. Seasonal Decomposition

An effective approach to analyzing time series with seasonal patterns is to use seasonal decomposition methods that separate the series into trend, seasonal, and remainder components. The observed time series is therefore expressed as an additive sum of these components, typically formulated as yt = τt + δt + Rt, where t = 1,..., T, yt denotes the observed value at time t, τt represents the smooth trend component, δt is the seasonal effect with periodicity S, and Rt is the remainder or residual. It is often assumed that the seasonal and remainder components have zero mean over a full period, ensuring identifiability of the individual components. From confirmed cases or deaths, ITS point estimates of the underlying time series yt can be obtained. Smoothing splines can then

be used to estimate the trend component τt, and the seasonal component δt can be derived by exploiting the relationship δt = yt − τt − Rt, assuming suitable properties for Rt (C. Brooks et al., 2018) (L. Daza-Torres et al., 2022).

9. Case Studies

Reliable forecasts of an epidemic's progression support public health planning. Basic epidemiological models cannot address temporally changing transmission and testing conditions or provide uncertainty bounds (Bracher et al., 2021). The introduced model predicts future COVID-19 cases and deaths based solely on the recent time series of cases and deaths. Model parameters drift to account for time-varying epidemic conditions while resulting confidence intervals reliably cover future observations (P. Hespanha et al., 2021).

The parameter estimation scheme is tested in two case studies that assess the model's capability to track rapidly evolving dynamics and its performance in both the first and second pandemic waves. The first case study focuses on the development of testing capacity in the USA during March to May 2020. Testing limitations during this phase led to an underreporting of the number of infected cases (Petropoulos et al., 2020). The second case study investigates COVID-19 in Italy from October to the end of 2020 as the second wave developed. The model accurately produces conditional forecasts of the trend and magnitude during this period

9.1. COVID-19 Pandemic

SARS-CoV-2 and its ensuing COVID-19 pandemic rendered, starting in late 2019 and early 2020, the world's first truly globalized health crisis of the modern age. It has been considered by a large number of epidemiologists as the most severe pandemic since the 1918 flu pandemic, yet one that can still be understood, given our knowledge of biology gathered in the 20th century or later. By 2021, the number of COVID-19 cases worldwide had exceeded 191 million, with about 4 million reported deaths.

Different countries adopted different epidemiological strategies. Some relied heavily on testing, tracing, and isolating; others managed to reduce the pace of infection, but only through a cycle of lockdowns; others let the infection spreading more or less freely within the population. The World Health Organization recognized that different models can predict different things and are designed for the different purposes of different users. More specifically, it distinguished between scenario projections, epidemic surveillance, response planning, and response monitoring.

9.2. H1N1 Influenza

H1N1 influenza (swine flu) has renewed interest in the field of infectious disease forecasting and in statistical methods for epidemic prediction. Debates in the United

States and elsewhere raised the need for the development of data and analysis methods able to produce short- and medium-term predictions suitable for policy prescription, public communication and public health planning. Despite different formulations, epidemic forecast models rely on many of the same mechanistic principles and the same classes of statistical approach. The global spreading of the H1N1 influenza originated before the official identification of the pandemic virus raised the concern of international organizations and policy makers. Only a handful of early estimates of the key epidemiological parameters were available prior to the dissemination of cases worldwide, and early empirical information remained quite limited during the first months of global expansion of the epidemic. However these few data were instrumental in defining the baseline conditions for epidemic modeling.

9.3. Ebola Outbreak

The 2014 Ebola outbreak in West Africa resulted in over 10,000 deaths in Sierra Leone alone, creating urgent demand for reliable forecasting tools to inform policy and healthcare decisions. The prolonged latent period and the evolution of the transmission processes due to behavioral changes and interventions complicated the task, constraining the choice of models suitable for capturing these dynamics without nonidentifiability issues (Frasso & Lambert, 2016).

Hierarchical model combinations have been proposed to bridge different modeling paradigms. Such hierarchical models combine the strengths of phenomenological, compartmental, and individual-based models through a statistical inference framework that links the latent variables across levels. Specifically, phenomenological and compartmental models operate at aggregate levels useful for trend characterization and scenario evaluation, while agent-based models simulate heterogeneous individual-level transmission crucial for spatial and mobility insights. This linkage capitalizes on the unique aspects of each paradigm to provide coherent epidemic insights of direct policy relevance across all scales (Viboud et al., 2017).

10. Challenges in Pandemic Forecasting

A range of statistical issues arise at different stages of the analysis when using complex stochastic systems models with multiple incomplete data sources in an evolving epidemic situation (Swallow et al., 2022). Data inconsistencies, including corruption and under-reporting, can be handled effectively when key error sources are known; modellers may use random effects or latent variables to account for individual variation across multiple data sources, and integrated models that combine various data streams represent an emerging approach. Developing sufficiently general methods is a significant challenge, especially as interventions (e.g., vaccination) and policy changes alter disease dynamics; shifts in the age distribution of cases at key points also affect the risk of hospitalisation and death, complicating interpretation. Reporting reliable

averages for large populations is problematic when epidemic trajectories remain asynchronous across regions, potentially biasing estimates; the sparse available data also often fail to support clear quantification of vaccine impacts on transmission and the role of different population groups. Assessing the information content of particular data streams about key parameters, incorporating geographic variations in data collection procedures and censoring mechanisms, and ensuring appropriate alignment between model complexity and data resolution are additional challenges. Furthermore, temporal aggregation complicates the balance between flexibility, timeliness and reliability in the interpretation of estimates, as it becomes more difficult to discriminate between real trends and noise; aggregation across demographic or social groups often conceals important trends, pointing to the need for methods that can accommodate inconsistencies between pooled data streams and produce more accurate and robust estimates.

10.1. Data Quality Issues

The Covid-19 pandemic has exposed major dashed expectations as to the quality of data available for appropriate regulatory decisions. The results of the analysis of Covid-19 data reflect the fact that these data are anything but simple to interpret and quite challenging to be used for accurate prognosis and prediction. Initial observations stated that a number of cases reported are subjected to a big number of errors which, unfortunately, has an impact on the data available and the statistical analysis of the epidemic.

The quality of any official statistics depends on the accuracy of the supplied data. This can be comprehended with the example of the overall mortality: data on COVID-19 deaths collected can constitute an overestimate if deaths are considered due to the sole COVID-19 infection, and the patient was instead affected by several other pathologies. In addition, underestimation can be a consequence of delays in obtaining data and errors in the record-keeping process of such information (Ferrari et al., 2023).

Several epidemiological modelling groups use statistical models of infectious disease to generate forecasts that inform the response to the COVID-19 pandemic in the UK. The models developed by the University of Cambridge MRC Biostatistics Unit, Public Health England, the University of Warwick, and the London School of Hygiene Tropical Medicine. Estimates for the effective reproduction number Rt highlight differences in bias and variability among models. A statistical model for multisource COVID-19 surveillance data uses symptom report data (NHS 111), compartments for convalescing and terminally ill individuals, and a bespoke numerical integrator for systems of ODEs. Simple scoring rules are applied to refine forecasts.

At the beginning of the pandemic nontargeted and inconsistent data collection occurred, resulting in many unconfirmed results and inappropriate public health decisions. Given the considerable amount of data accumulated, it is possible to look back and find ways

to recover this information globally and to develop more plausible and rigorous analysis protocols and integrated analysis models. Any data analysis is based on data that are never free of errors or inconsistencies, which can propagate in the statistical analysis process. A thorough knowledge of the data acquisition process and context is therefore always required. COVID-19 data quality analysis is considered a particularly important issue for future models and forecasting.

10.2. Model Uncertainty

Model uncertainty is an intrinsic element of epidemic modelling and encompasses errors in both observation and structural uncertainty. This latter type is often the dominant component. The dominant models used to inform responses to the COVID-19 pandemic in the UK—those developed by MRC Biostatistics Unit and Public Health England, the University of Warwick, the London School of Hygiene Tropical Medicine, and the University of Cambridge—tend to be deterministic; the only source of randomness is that introduced through the observation model. The consequence is that such approaches communicate uncertainty about data observation but cannot account for epistemic uncertainty about key parameters or model structure, nor can they treat that uncertainty consistently when simulating future scenarios. The scope of decision-making and stress testing required of policy advises requires the development of plausible scenarios, the projection of such scenarios through complex models, and the assessment of how responses perform when faced with these unknowns. A rigorous approach to quantify model-based uncertainty—one that does not rely on a single model calibrated with a fixed set of parameters—is consequently vital. Such methods are also consistent with the extensive literature that indicates that combining different response modelling frameworks results in improved forecasts (Petropoulos et al., 2020).

10.3. Ethical Considerations

Epidemiological forecasts are key tools for informing the public and supporting decisions during a pandemic. To improve the accuracy of these forecasts, information from a variety of sources can be considered, including the broad range of expert judgment, computer models, and human judgment. When multiple forecasts are available, combining them efficiently can make use of more information and expert opinion and reduce the risk of selecting the wrong individual forecast (W. Taylor & S. Taylor, 2021). Combining multiple forecasts often improves on the accuracy of the individual forecasts; when the forecasts to be combined are probability distributions, combining them is less well studied (E. Moore et al., 2021). Some approaches take the linear opinion pool as a basic model and improve on it by adjusting the tails or the tails as functions of the centre. A novel pandemic forecast combination method forms a combination based on the recent performance of each individual forecast. This approach can readily be updated as new forecasts become available, is computationally

inexpensive, and can be applied when only the central tendency and a single measure of spread of each distribution is known, as well as when the full predictive distributions are available.

11. Policy Implications

Forecasts of infectious disease spread remain integral for healthcare planning and government policymaking during pandemics. The Covid-19 pandemic illustrated that the characteristics of the virus often remain poorly understood during the early stages. Notably, transmission mechanisms and the effect of non-pharmaceutical interventions are uncertain initially, complicating efforts to design reliable forecasting models. To address these challenges, a template coupled with a probabilistic programming library was created to produce a flexible compartmental model that supports rapid development, accurate predictions, and the evaluation of policy interventions. The approach replicates the spread of Covid-19, incorporates under-reporting, and extracts posterior estimates for latent epidemic parameters (Mehta & Kasmanoff, 2022). The model thus provides key inputs for the optimization of governmental policy interventions. An extended study produced forecasts for confirmed cases and deaths in individual countries, confirming the adaptability of the model. The analysis supports early intervention and resource allocation strategies during the initial stages of an epidemic.

11.1. Public Health Interventions

Policy-makers implement public health interventions to reduce the spread of COVID-19 worldwide; such interventions are therefore a key factor of models. Several kinds of policy interventions exist. (1) Some policies affect epidemiological parameters, such as mask wearing (beta) and vaccination (mu). (2) Other policies act on mobility between regions, for example international border closures, and impact the network pseudo-distance matrix (Henrique da Costa Avelar et al., 2022). These two sets of interventions focus on disease spread rather than specific parameters, which may drift over time (as shown in Section 4). (3) Finally, lock-down policies may be used as a last resort.

11.2. Resource Allocation

In allocating resources to address an infectious disease outbreak, forecasts of incidence, rather than of deaths, are often most relevant. A forecast of incidence by day can be translated into a forecast of resource allocation for the relevant day or over the coming few days (Gerding et al., 2023). If interventions have a longer horizon or need to be reserved for predicted hot spots, it is also useful to evaluate forecasts over a longer period. Any evaluation method that mimics the uses to which forecasts are put would be particularly valuable. During the pandemic, much of the media coverage and working of planners revolved around predictions and forecasts of the IHME type; determining a data-driven method of converting a probabilistic forecast to a median projection might

constitute a valuable nugget of insight from the course. Throughout the pandemic, resources have been used inefficiently, and better probabilistic forecasting offers the possibility of substantial improvement (W. Taylor & S. Taylor, 2021).

12. Future Directions

Real-world data, such as that from a pandemic, are highly complex and challenging to analyze. For example, COVID-19 data originating from interconnected regions are influenced by complex regional dependencies, data distortion caused by changing epidemic prevention policies, weekday effects, and more. Common COVID-19 forecasting models cannot account for all these features, leading to relatively poor prediction performance. Statistical models equipped with a self-adaptive trend decomposition mechanism have been proposed, as applied to high-dimensional COVID-19 data from the 50 states of the United States. Empirical results demonstrate that the model can deliver accurate predictions and reveal the impact of the above features. With the availability of more high-dimensional COVID-19 data from various regions at multiple levels, these features will also be observable within each country or other smaller administrative regions, presenting ongoing challenges for forecasting models.

Upcoming public health crises of similar or larger scale may result in even more intricate data. The unfolding of the COVID-19 pandemic has demonstrated that SARS-CoV-2 is prone to accumulating mutations. The emergence and widespread transmission of several variants of concern have been associated with changes in the level of induced immunity and vaccine effectiveness. For a specific variant, such as the Omicron BA.1 sublineage, a significant decrease in vaccine effectiveness has been recorded. Nevertheless, statistical forecasting models have not yet incorporated the dynamics of antibody levels into their analyses. In this context, a combination of epidemic compartment models and statistical modeling has been employed to examine antibody dynamics. When the outbreak reaches its natural conclusion, a relationship between antibody titers and the decay rate of infected individuals becomes evident. Modeling future waves using this relationship yields accurate forecasts.

12.1. Integration of AI in Forecasting

Pandemic forecasting constitutes one of the most challenging domains in the field of forecasting. Artificial intelligence (AI) finds wide application in forecasting the ongoing propagation of the COVID-19 pandemic (H. Elsheikh et al., 2021). Research has made extensive use of statistical and mathematical methodologies to generate forecasts of COVID-19 spread. Models deployed across various countries demonstrated heterogeneous results. An Autoregressive Integrated Moving Average (ARIMA) approach was employed for forecasting in Pakistan, South Korea, and Japan. A hybrid model combining ARIMA with a wavelet-based approach predicted daily case numbers in India, South Korea, Canada, the United Kingdom, and France. Discrete wavelet-

ARIMA hybrids yielded forecasts for Spain, Italy, France, the UK, and the United States. Modified ARIMA variants, including the SutteARIMA and Kalman-filter-augmented methods, were utilized to project cases, deaths, and recov-eries in Spain and Pakistan. A comparative study assessed ARIMA, Support Vector Regression, ridge regression, random forest, cubist regression, and stacking-ensemble learning approaches applied to Brazil, identifying Support Vector Regression and ensemble techniques as the most accurate. The Gaussian spreading hypothesis informed models of epidemiological behavior in the United States, Germany, Italy, Spain, France, and Iran, underscoring the necessity of stringent control measures. Reduced-space Gaussian regression, integrating Bayesian systems with geographic information systems, facilitated projection of the U.S. outbreak trajectory. Finally, Susceptible-Infected-Recovered (SIR) models examined transmission dynamics in the twenty most heavily affected nations.

12.2. Improving Data Collection Methods

Incorporating the perspectives of case data, sewer virus concentration, and clinical data is pivotal to refining pandemic modeling strategies. Engaging a variety of data sources improves granularity and reliability, leading to better model performance (Jahn et al., 2022). During the early stages of the COVID-19 pandemic, limited infection data catalyzed a paradigm shift toward prioritizing data sources that are reliable, timely, and consistent (Rodríguez et al., 2022). Epidemiological modeling groups have increased reliance on statistical techniques, where robustness improves in tandem with the incorporation of diverse and complementary data streams (E. Moore et al., 2021).

13. Conclusion

The COVID-19 pandemic posed new challenges to forecasting and prediction. Although predictions are not a panacea, policymakers needed forecasts to guide their decisions. No statistical model can predict the long-term trajectory of a complex, dynamic system prone to wild shocks and changes, especially when data are sparse early in the evolution of the system. The integrated modeling approach described here combines statistical, machine learning, and epidemiological components. It produces short-term forecasts in the near term and generates scenario-based projections over a longer horizon. It uses a leading indicator, new hospitalizations, to improve forecasts of leading indicators, incident and prevalent deaths. Results from a counterfactual experiment highlight the impact of vaccinations and show the effect of increasing vaccination coverage in an earlier period.

Predictions of incidence and prevalence of new COVID-19 cases are required to generate vaccination and other scenario forecasts. The underlying COVGAP statistical machine learning modeling system produces accurate short-term forecasts despite the lack of a lead-lag relationship between new cases and hospitalizations or new cases and deaths. Ending the pandemic requires reducing infection rates. Therefore, daily reported new

cases of COVID-19 per 100,000 population are critical for further analysis and research. A multivariate spatio-temporal statistical machine learning forecasting model for new cases counts data is warranted.

References

W. Taylor, J. & S. Taylor, K. (2021). Combining probabilistic forecasts of COVID-19 mortality in the United States. ncbi.nlm.nih.gov

Petropoulos, F., Makridakis, S., & Stylianou, N. (2020). COVID-19: Forecasting confirmed cases and deaths with a simple time series model. ncbi.nlm.nih.gov

Mehta, S. & Kasmanoff, N. (2022). Compartmental Models for COVID-19 and Control via Policy Interventions. [PDF]

E. Moore, R., Rosato, C., & Maskell, S. (2021). Refining Epidemiological Forecasts with Simple Scoring Rules. [PDF]

L. Juul, J., Græsbøll, K., Engbo Christiansen, L., & Lehmann, S. (2020). Fixed-time descriptive statistics underestimate extremes of epidemic curve ensembles. [PDF]

L. Daza-Torres, M., A. Capistrán, M., Capella, A., & Andrés Christen, J. (2022). Bayesian sequential data assimilation for COVID-19 forecasting. ncbi.nlm.nih.gov

M. A. Bettencourt, L., M. Ribeiro, R., Chowell, G., Lant, T., & Castillo-Chavez, C. (2007). Towards Real Time Epidemiology: Data Assimilation, Modeling and Anomaly Detection of Health Surveillance Data Streams. ncbi.nlm.nih.gov

Sooknanan, J. & Mays, N. (2021). Harnessing Social Media in the Modelling of Pandemics—Challenges and Opportunities. ncbi.nlm.nih.gov

Tran, K. T., Son Hy, T., Jiang, L., & Vu, X. S. (2023). Multimodal Graph Learning for Modeling Emerging Pandemics with Big Data. [PDF]

Klein, B., C. Zenteno, A., Joseph, D., Zahedi, M., Hu, M., S. Copenhaver, M., U. G. Kraemer, M., Chinazzi, M., Klompas, M., Vespignani, A., V. Scarpino, S., & Salmasian, H. (2023). Forecasting hospital-level COVID-19 admissions using real-time mobility data. ncbi.nlm.nih.gov

Barreras, F., Hayhoe, M., Hassani, H., & M. Preciado, V. (2021). AutoEKF: Scalable System Identification for COVID-19 Forecasting from Large-Scale GPS Data. [PDF]

R. Biegel, H. & Lega, J. (2021). EpiCovDA: a mechanistic COVID-19 forecasting model with data assimilation. [PDF]

Chowell, G., Dahal, S., Tariq, A., Roosa, K., M. Hyman, J., & Luo, R. (2022). An ensemble n-sub-epidemic modeling framework for short-term forecasting epidemic trajectories: Application to the COVID-19 pandemic in the USA. ncbi.nlm.nih.gov

Zhang, P., Feng, K., Gong, Y., Lee, J., Lomonaco, S., & Zhao, L. (2022). Usage of Compartmental Models in Predicting COVID-19 Outbreaks. ncbi.nlm.nih.gov

Herriott, L., L. Capel, H., Ellmen, I., Schofield, N., Zhu, J., Lambert, B., Gavaghan, D., Bouros, I., Creswell, R., & Gallagher, K. (2023). EpiGeoPop: A Tool for Developing Spatially Accurate Country-level Epidemiological Models. [PDF]

Li, M., Dushoff, J., & M Bolker, B. (2018). Fitting mechanistic epidemic models to data: A comparison of simple Markov chain Monte Carlo approaches. ncbi.nlm.nih.gov

Rodríguez, A., Adhikari, B., Ramakrishnan, N., & Aditya Prakash, B. (2020). Incorporating Expert Guidance in Epidemic Forecasting. [PDF]

Swallow, B., Birrell, P., Blake, J., Burgman, M., Challenor, P., E. Coffeng, L., Dawid, P., De Angelis, D., Goldstein, M., Hemming, V., Marion, G., J. McKinley, T., E. Overton, C., Panovska-Griffiths, J., Pellis, L., Probert, W., Shea, K., Villela, D., & Vernon, I. (2022). Challenges in estimation, uncertainty quantification and elicitation for pandemic modelling. ncbi.nlm.nih.gov

Fintzi, J., Cui, X., Wakefield, J., & N. Minin, V. (2016). Efficient data augmentation for fitting stochastic epidemic models to prevalence data. [PDF]

Kandula, S., Yamana, T., Pei, S., Yang, W., Morita, H., & Shaman, J. (2018). Evaluation of mechanistic and statistical methods in forecasting influenza-like illness. ncbi.nlm.nih.gov

C. Brooks, L., C. Farrow, D., Hyun, S., J. Tibshirani, R., & Rosenfeld, R. (2018). Nonmechanistic forecasts of seasonal influenza with iterative one-week-ahead distributions. ncbi.nlm.nih.gov

Hammadi, L., Raillani, H., Mbaye Ndiaye, B., Aggoug, B., El Ballouti, A., Jidane, S., Belyamani, L., & Souza de Cursi, E. (2023). Uncertainty Quantification for Epidemic Risk Management: Case of SARS-CoV-2 in Morocco. ncbi.nlm.nih.gov

S. Hickmann, K., M. Hyman, J., & Y. Del Valle, S. (2015). Quantifying Uncertainty in Stochastic Models with Parametric Variability. [PDF]

Bracher, J., Wolffram, D., Deuschel, J., Görgen, K., L. Ketterer, J., Ullrich, A., Abbott, S., V. Barbarossa, M., Bertsimas, D., Bhatia, S., Bodych, M., I. Bosse, N., P. Burgard, J., Castro, L., Fairchild, G., Fuhrmann, J., Funk, S., Gogolewski, K., Gu, Q., Heyder, S., Hotz, T., Kheifetz, Y., Kirsten, H., Krueger, T., Krymova, E., L. Li, M., H. Meinke, J., J. Michaud, I., Niedzielewski, K., Ożański, T., Rakowski, F., Scholz, M., Soni, S.,

Srivastava, A., Zieliński, J., Zou, D., Gneiting, T., & Schienle, M. (2021). A pre-registered short-term forecasting study of COVID-19 in Germany and Poland during the second wave. ncbi.nlm.nih.gov

P. Hespanha, J., Chinchilla, R., R. Costa, R., K. Erdal, M., & Yang, G. (2021). Forecasting COVID-19 cases based on a parameter-varying stochastic SIR model. ncbi.nlm.nih.gov

Frasso, G. & Lambert, P. (2016). Bayesian inference in an extended SEIR model with nonparametric disease transmission rate: An application to the Ebola epidemic in Sierra Leone. [PDF]

Viboud, C., Sun, K., Gaffey, R., Ajelli, M., Fumanelli, L., Merler, S., Zhang, Q., Chowell, G., Simonsen, L., Vespignani, A., & Ebola Forecasting Challenge group, R. A. P. I. D. D. (2017). The RAPIDD ebola forecasting challenge: Synthesis and lessons learnt.. [PDF]

Ferrari, L., Manzi, G., Micheletti, A., Nicolussi, F., & Salini, S. (2023). Pandemic Data Quality Modelling: A Bayesian Approach. [PDF]

Henrique da Costa Avelar, P., del Coco, N., C. Lamb, L., Tsoka, S., & Cardoso-Silva, J. (2022). A Bayesian predictive analytics model for improving long range epidemic forecasting during an infection wave. ncbi.nlm.nih.gov

Gerding, A., G. Reich, N., Rogers, B., & L. Ray, E. (2023). Evaluating infectious disease forecasts with allocation scoring rules. [PDF]

H. Elsheikh, A., I. Saba, A., Panchal, H., Shanmugan, S., A. Alsaleh, N., & Ahmadein, M. (2021). Artificial Intelligence for Forecasting the Prevalence of COVID-19 Pandemic: An Overview. ncbi.nlm.nih.gov

Jahn, B., Friedrich, S., Behnke, J., Engel, J., Garczarek, U., Münnich, R., Pauly, M., Wilhelm, A., Wolkenhauer, O., Zwick, M., Siebert, U., & Friede, T. (2022). On the role of data, statistics and decisions in a pandemic. ncbi.nlm.nih.gov

Rodríguez, A., Kamarthi, H., Agarwal, P., Ho, J., Patel, M., Sapre, S., & Aditya Prakash, B. (2022). Data-Centric Epidemic Forecasting: A Survey.

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Chapter 13: Fuzzy Logic and Decision Making in Environmental Risk Assessment

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Abstract: Environmental risk assessment involves evaluating the likelihood and consequences of environmental hazards. However, the complexity and uncertainty inherent in environmental systems make traditional probabilistic models inadequate in many contexts. This paper explores the application of fuzzy logic as a powerful decision-making tool for handling uncertainty and imprecision in environmental risk assessments. Fuzzy logic, derived from fuzzy set theory, enables more flexible and human-like reasoning by allowing partial memberships and linguistic variables, making it especially suitable for modeling vague and incomplete data. We present the theoretical foundations of fuzzy inference systems and their integration into risk analysis frameworks. The methodology involves constructing rule-based systems using expert knowledge and membership functions, enabling qualitative reasoning in decision support. Several case studies are analyzed to demonstrate the effectiveness of fuzzy logic in environmental scenarios such as chemical hazard evaluations, water and air quality assessments, and construction risk management. Furthermore, this paper discusses hybrid models combining fuzzy logic with other computational techniques such as Bayesian networks and Analytic Hierarchy Process (AHP) for more robust assessments. The integration of stakeholder perspectives, ethical considerations, and policy implications is emphasized to enhance transparency and inclusiveness in decision-making. The research concludes that fuzzy logic offers a valuable and adaptable framework for environmental risk assessment, supporting better planning and management under uncertain and complex conditions. Its interdisciplinary nature promotes improved environmental governance and sustainable development strategies.

Keywords: Fuzzy Logic, Environmental Risk Assessment, Decision-Making, Uncertainty Modeling, Expert Systems

1 Introduction

Environmental risk assessment is intrinsically tied to an evaluation of hazard, vulnerability, and resilience; this assessment of risk endeavours to be realistic, objective,

precautionary, systematic and transparent. Such an assessment provides the basis for an effective risk management framework (Thi Thu Do et al., 2020). More specifically, environmental risk assessment is a systematic process that provides an appraisal of the potential harm a proposed project may cause to water, land, air, flora and fauna, with the aim of enhancing decision making. It strives to be precautionary and objective, yet it does not provide a precise prediction of what will occur, but offers a spectrum of credible scenarios. Because the environment is complex, there are inevitably gaps in baseline information, greater uncertainty about the impact, difficulties in defining significance and in quantifying the probability of impact, as well as a lack of historical precedent for major proposed development projects on-site. Many diverse interests, often contradictory, need to be considered, while many decisions remain value-based and qualitative even though context and emphasis may change. Eco-risk evaluation is conducted according to an explicit legitimate framework, which involves an incorporation of input from several disciplines; an integration of the consequences that may result; an acknowledgement of inherent uncertainties; and a provision of information for decision makers.

2. Fundamentals of Fuzzy Logic

Once initiated in the early 1960s, fuzzy set theory and fuzzy logic have provided the scientific community with a coherent theoretical framework for representing, evaluating and propagating uncertainty throughout hybrid systems dealing with human reasoning and perception. Over the last forty years the number of applications has continuously increased, influencing practice in such diverse fields as social and cognitive sciences, electronics, computer engineering, information technology, operations research and economics.

The general methodology of fuzzy logic was initially developed for designing intelligent machines, and the concept of a fuzzy controller was introduced to computer science simultaneously with the creation of what is arguably the first fuzzy inference system, the so-called linguistic synthesis of control. These alternative terms all refer to systems embodying the formal scheme known as the fuzzy inference model, which is a systematic methodology for mapping a given input into an appropriate output by modelling expert knowledge as a set of linguistic IF-THEN rules. The methodology consists of three distinct and fundamental parts: a rule-base made of a knowledge base and a database, a reasoning mechanism that implements the inference system, and a interface that allows the system to be connected to the outside world. The knowledge base holds the fuzzy IF-THEN rules provided by human experts, whereas the database contains definitions of linguistic variables in the rules by means of fuzzy sets; the reasoning mechanism combines rules and facts to obtain a meaningful output while the interface manages inputs and outputs necessary for the interaction between the system and its environment (Thi Thu Do et al., 2020).

3. The Role of Fuzzy Logic in Decision Making

Fuzzy logic is widely acknowledged as an effective means to emulate human reasoning and facilitate decision making in circumstances where input data are vague or imprecise (Humphreys et al., 2006). Throughout a wide spectrum of disciplines, fuzzy logic has long been employed to model uncertainty. Ample empirical evidence indicates that human cognition interprets all sensory stimuli and information in fuzzy (collection of due degrees) rather than binary (crisp and discrete) terms.

The essential feature of such an approach is the ability to manipulate fuzzy if–then rules. Given a specified set of input fuzzy membership function values, it is possible to compute a sensible output fuzzy membership function value. As a fuzzy system typically embodies a set of rules, each rule will generate an output fuzzy membership function as a consequence of the corresponding input membership function values. Hence, the first step involves inferring the logical sum of the rules, based on the possible output memberships, before defuzzifying to yield a crisp output. The Root-Sum-Square (RSS) method of inference is employed to combine the influence of all applicable rules, calculate the fuzzy centroid of the composite area, and determine the best weighted contribution of each firing rule (Hussain et al., 2006). Once the output membership function strengths for each output category have been established, defuzzification proceeds by integrating the inference outcomes and computing the fuzzy centroid of the output region. Specifically, the weighted strengths of each output membership function are multiplied by their associated centers, summed, and divided by the aggregate weight to produce a single crisp output value. Elevated membership values correspond to increased risk, while a negative sign indicates an advisement of ‘Don’t proceed.’

4. Risk Assessment Frameworks

Frameworks and Models for Risk and Safety Assessment. A generic framework and model to support managing risks related to variability and fuzzy uncertainties has been considered. A procedure based on questions–responses has been proposed to identify variables impacting decision-making. A meta-matrix analysis is proposed to identify relationships between these variables and assess their strength. The main purpose of the model is to aid decision makers in analysis for pre-active, reactive, and proactive decisions. Bayesian networks and influence diagrams have been chosen as the underlying mathematical tools of the established framework. Fuzzy integral, namely Choquet integral, is used for aggregation to present managers with concise information. While the illustrative example concerns decision-making with regard to an earthquake, the framework is general and applicable to other domains such as supply chain, food industry, banking, engineering, and medical fields. Future work will focus on applying this approach to real-world problems and developing computer applications based on this framework (Tchangani, 2011).

Construction Risk-Management Framework. Most current construction risk-assessment tools deliver unsatisfactory results because they rely on high-quality data—which are often limited, ambiguous or unavailable during the early project stages—due to inherent uncertainty. To resolve this, a holistic risk-assessment model, based on Fuzzy Synthetic Analysis (FSA), was developed among construction engineers, IT professionals and mathematicians. The model employs qualitative scales defined by triangular fuzzy numbers in pairwise comparisons, which captures vagueness in linguistic variables. An Analytic Hierarchy Process (AHP) risk-assessment model was created, and a pilot run demonstrated that it accelerated decision-making and ensured that resources were appropriately allocated to mitigate risks affecting project time, cost and quality. Quantitative approaches such as Fault-Tree and Monte-Carlo analyses can assist construction risk management; nonetheless, they require high-quality data—which are often unavailable in early project phases. Fuzzy logic, introduced by Zadeh in the 1960s, has been effectively applied to construction-duration management, cost estimation, risk management, safety, supply-chain management and earned-value management, thereby handling uncertainty and vagueness (Abdul-Rahman et al., 2013).

5. Fuzzy Logic Applications in Environmental Science

Fuzzy logic systems provide an effective approach to decision making under environmental risk and uncertainty. Unlike conventional methods such as probability theory and evidence theory, the fuzzy approach relies on fuzzy set theory to quantify the degree of membership of an element to a set. To date, numerous fuzzy logic applications have been reported in environmental problems including water quality evaluation and air quality management. Fuzzy reasoning processes can handle vague objectives capable of describing poorly defined goals and boundary conditions.

Since its introduction, the fuzzy approach has been widely applied to both engineering and social science problems. The rapid development of fuzzy systems has been driven by the realization that neither measurements nor process modelling can be exact for complex processes, and various uncertainties such as data incompleteness and randomness exist (Humphreys et al., 2006). Fuzzy sets, suggested by Zadeh, model the perception of human reasoning from imprecise information within a consistent mathematical framework. Unlike other techniques, fuzzy logic deals with imprecise data as the main feature of the various uncertainties rather than just the integration of randomness. Based on fuzzy set theory, a fuzzy system (or fuzzy inference system) is able to incorporate human experiential knowledge and reasoning capability to effectively control many types of ill-defined and highly nonlinear systems. As a result, fuzzy modelling continues to attract considerable research in many fields of science and engineering. Fuzzy models can be categorised in two main groups: one group models the system itself and one group models a plant, where the model output is used to control the process. Most reported fuzzy systems are linguistic models that use fuzzy logic to

describe system behaviour. For example, the supplier selection problem involves environmental performance assessment where linguistic terms are used to describe the importance of selection criteria. A concept of dynamic membership functions is therefore introduced into the evaluation process to significantly improve the adaptability of the evaluation system.

Rules used in fuzzy systems give the benefit of describing expert knowledge qualitatively and expressing this knowledge in fairly simple terms and simple analytic functions. Each control rule is a linguistic statement that relates the state of the system or process behaviour to the control action, such as "if emissions is high then suitability is adverse". Like rules, membership functions provide further opportunities to describe expert knowledge. A membership function describes the degree to which a given input belongs to a fuzzy set and varies from zero (no-membership) to unity (full-membership). In the supplier section system the variables pollutants and debt affect the output variable suitability. There are a number of membership functions for each variable spreading over the universe of discourse. The fuzzy logic system consists of a fuzzifier, a rule base, an inference engine and an output processor. The fuzzifier converts precise input values into fuzzy sets at the input level while the output processor converts the fuzzy set resulting from the inference process into a crisp output value. The inference engine seeks appropriate rules in the rule base and fires them in a way consistent with the adopted fuzzy implication. Each rule has a weight indicating the importance of the input in influencing the output and this weight is taken into account when aggregating the control actions within the output processor.

Fuzzy logic related techniques are extensively used for decision making in environmental sciences, especially in risk and safety assessment. Risk assessment (RA) and risk management (RM) for chemical processes have a great influence on hazard control, loss prevention and safety improvement in the oil and gas, chemical process and petrochemical industries. At present, guidelines and methods for RA and RM are still few and the application of RA and RM are even fewer. Hazard identification (HAZID) is a systematic technique for the identification of hazards of the chemical process. The techniques that are commonly employed in hazard studies include hazard-and-operability (HAZOP), failure mode and effects analysis (FMEA) and fault tree analysis (FTA). However, most of the techniques used in hazard studies are qualitative or semi-quantitative. Different studies apply fuzzy logic to the risk analysis of chemical processes. Fuzzy methods used for reliability analysis include fuzzy fault tree analysis (FTA), fuzzy failure mode and effects analysis (FMEA), fuzzy event tree analysis (ETA) and so forth. Hazard analyses that incorporate fuzzy logic appear in studies of fuzzy HAZOP, fuzzy HAZID, fuzzy fault tree analysis, fuzzy FMEA. Many studies apply fuzzy logic to the quantitative assessment of the risk of hazardous chemical processes. Fuzzy logic can be employed as part of an integrated approach for the semiquantitative

risk assessment of hazardous chemical accidents. The approach integrates a practical model for the estimating of toxicity and[]--concentration (PAC) curves and fuzzy layers with a composite risk indicator (CRI) for the assessment of the risk of hazardous chemical accidents. Another study presents an advanced fuzzy approach to safety performance assessment, which combines the employment of Dynamic Possibilistic-Certainty Distribution and also an Adaptive Neuro-Fuzzy Inference System. The combination of Dynamic Possibilistic-Certainty Distribution and Adaptive Neuro-Fuzzy Inference System can reflect the non-linearity phenomena and dynamic phenomenon of a real system with uncertainty (Thi Thu Do et al., 2020).

6 Comparative Analysis

Different approaches to design a fuzzy risk index for flammable and toxic releases were documented in a recent study (Thi Thu Do et al., 2020). The first approach applied a fuzzy weighting method to a conventional semi-quantitative risk matrix to evaluate the consequences, the likelihood, and the risk score. In the second approach, a fuzzy composite indicator method was proposed to aggregate a set of measured physical variables related to hazardous chemicals and hazardous zones. Eventually, two fuzzy risk indices were combined by an inference system in the third technique. A final fuzzy risk index was obtained, which can be used to assess and manage hazardous chemical accidents in process industries. All calculations related to fuzzy risk assessment were performed using the MATLAB® programming language (Jabbari et al., 2021). Fuzzy weighting and hierarchical analyses were executed with EXCEL software to determine the fuzzy weight associated with each risk factor.

7. Quantitative vs Qualitative Risk Assessment

Numerous studies offer insights into the differences between quantitative and qualitative risk assessment approaches and the role of fuzzy logic in bridging these distinct approaches. Quantitative risk assessment (QRA) methods systematically evaluate the likelihood, impacts, and risk of adverse events. QRA using fault tree analysis (FTA) typically assumes that failure events have crisp probabilities and are statistically independent, assumptions that often generate incertitude owing to unavailable failure data or failure dependencies. Expert knowledge can reduce data gaps but introduces imprecision and lack of consensus. Fuzzy set theory (FST), evidence theory, and Bayesian networks form one combined approach that characterizes different uncertainty classes, aggregates judgments from multiple experts, and updates prior beliefs in light of new evidence (Kabir & Yazdi, 2018). The resultant sensitivity analysis reveals critical fault tree events. During normal operations, numerous industrial hazard sources such as fire, explosion, toxic release, and vapor emission exist. These hazards may cause human injury or death, equipment damage, and environmental pollution. Industrial QRA hence supports decision making about safety and environmental aspects.

On the other hand, some researchers indirectly distinguish qualitative and quantitative risk assessment approaches through the use of fuzzy set theory. Such studies propose fuzzy qualitative risk assessment models that rely entirely on expert judgments and do not require additional risk data. They remain suitable for projects with limited information and yet incorporate features of quantitative models such as feedback and prediction capabilities (Abdul-Rahman et al., 2013). Similarly, FST applications combine fuzziness with hierarchy to prioritize risk sources. The resulting models effectively identify critical risks when risk sources are defined in linguistic terms and the data set is relatively large. Since FST goes beyond an either/or proposition, it captures more relationships and explains patterns better than binary sets. Many studies incorporate linguistic terms and FST into risk assessment to accommodate incompleteness, lack of information, linguistic ambiguity, and subjective judgments.

8. Integration of Fuzzy Logic in Risk Assessment Models

Environmental risk assessment, forecasting the likelihood of unwanted environmental events due to natural and industrial activities, still experiences uncertainty. Balancing risks with economic resources for remediation is problematic, as the precise probability and timing of damage remain unknown. Quantitative risk analysis employing probabilistic methods is hindered by data limitations and measurement errors. Fuzzy logic systematically incorporates human judgment and measurement uncertainty into risk assessment, yielding consistent, objective, and reliable outcomes despite limited data (Abdul-Rahman et al., 2013). Environmental risk assessment determines potential environmental harm, while hazard evaluation examines mechanisms leading to that harm; both rely on prior information often insufficient for analysis. Scientists typically employ either quantitative or qualitative criteria and models focusing respectively on numerical approaches considering likelihoods and magnitudes, or on using as much qualitative information as possible. Decision making under uncertainty is inherently non-probabilistic, involving vague assumptions, subjective reasoning, and semi-quantitative information, areas where fuzzy logic methodology can support the decision process. Complex risks from environmental and ecosystem changes necessitate enhanced techniques that transfer limited knowledge with minimal loss. The difficulty of risk assessment during early project stages makes the evaluation of risk mitigation strategies challenging. The proposed fuzzy synthetic model (FSM) addresses the lack of data and uncertainty.

9. Challenges in Environmental Risk Assessment

Environmental risk assessment continues to be challenged by two significant issues. Firstly, the paucity of a comprehensive environmental database constrains the development of effective risk-assessment models. Without adequate data, models face inherent limitations both in design scope and applicability of software, making it difficult

to identify hazardous events accurately and signal environmental quality concerns. Secondly, the intrinsic scarcity of information on certain hazardous events impedes quantification of related risks, thereby compromising the precision and reliability of predictive assessments. To enhance the analysis of environmental safety, further advancements in risk-assessment methodologies and the broader application of fuzzy logic are essential. Incorporating more elaborate indicators alongside fuzzy membership functions can refine assessments conducted through fuzzy inference systems and enrich probability density functions (Mysiak et al., 2008).

9.1. Data Uncertainty

Uncertainty plays a central role in environmental assessment, decision making, and policy. It is due to a lack of knowledge, the natural variability of the available data, the absence of statistical data, ambiguous and incomplete data, errors in measurement, and other reasons. Furthermore experts rarely give precise estimates about the state of the environment: seismic scenarios, water level, air quality, an epidemic outbreak, and so on. At the same time, an expert should provide as much information as possible using the most complete available model structures (Vicente Cestero et al., 2013). Many techniques involve the use of fuzzy sets to represent degrees of confidence associated with quantitative data and qualitative linguistic terms, to combine imperfect data into a decision support framework under uncertainty, and adapt the resulting recommendations to the required degree of confidence, thereby providing more realistic forecasts, mitigating risks, and improving decisionmaking under uncertainty (Mysiak et al., 2008).

9.2. Model Limitations

The fuzzy inference system (FIS) employed in the model operates as a black box for expert consultation, implemented using MATLAB Fuzzy-Logic Toolbox. This setup streamlines the coding process and enhances accessibility but imposes limitations on the flexibility and extensibility of the ordinary fuzzy-inference system (Azimi et al., 2018). Furthermore, approximate reasoning, which the model utilizes to solve complex problems, inherently involves a loss of precision (Thi Thu Do et al., 2020). Given that the model serves as a decision-support tool rather than a traditional expert system, efforts to maintain analytical rigor must be balanced against the pressures to improve prediction accuracy and speed. As such, the model offers a heuristic approach that replicates expert reasoning with reasonable accuracy and efficiency. The approximate reasoning method employed is designed to find a compromise between accuracy and speed in the certification process, preventing both a decline in decision quality and excessive computational delays.

10. Stakeholder Involvement in Risk Assessment

The input of multiple stakeholders is an important perspective to consider when conducting risk assessment, not only because it enriches understanding but also because the assessment process concludes with a decision that often involves multiple participants. Research on decision-making with fuzzy rules emphasizes efficiency in the face of both judgements expressed as interval sets and vague environmental states, as well as the presence of multiple decision-makers (Humphreys et al., 2006). For example, a hierarchical fuzzy system developed for supplier selection incorporates all relevant factors and their relative importance, allowing users to specify priorities in linguistic terms (Vicente Cestero et al., 2013). This approach reflects organizational decision-making preferences and integrates human priorities into the selection process. Similarly, in the chemical process industry, a suite of tools and regulatory documents addresses potential hazardous chemical accidents, supporting stakeholders in evaluation and management (Thi Thu Do et al., 2020).

11. Decision Support Systems for Environmental Risk

Decision support systems facilitate environmental risk assessments. They extend computer-aided systems to assess environmental risks for a given system through regulatory criteria and physical or chemical parameter estimates of individual releases at a site. These systems provide detailed estimates of environmental dispersion, individual exposure, and risk factors that can be used to make informed decisions on whether to proceed with a project or how to modify it to satisfy statutory or regulatory criteria or community standards. The systems include the capability to assess risks of chemical mixtures typically present in waste streams or released from stacks or ponds.

11.1. Design and Implementation

The framework consists of a fuzzy logic system for the risk assessment of environmental hazards. Its development involves the definition of fuzzy sets and fuzzy rules. An expert system is provided to allow all available knowledge on the risks related to environmental factors to be easily integrated. The model is designed to be as formally valid as possible, working both as a knowledge-based system and a scientific tool for decision support. Figure 10.1 presents one possible implementation for the integration of the model in a decision-making system.

The conception of the fuzzy system is as follows. The linguistic variables directly involved in the interaction are provided by expert knowledge as basis variables (MB = medium bound; ML = medium low; MH = medium high; P = positive; PS = positive small; PX = positive very small; Z = zero). A further linguistic variable, LX (linked to the definition of fuzzy rules and not connected to input data) represents the variation trend of pollutant path. It takes the values I = increase; D = decrease; N = maintain the

same level; for the sake of simplicity the support of I and D does not overlap. (Thi Thu Do et al., 2020)

11.2. Evaluation Metrics

Evaluation metrics provide essential tools for assessing diverse scenarios, including fuzzy multi-criteria evaluation and sustainability assessments (Jiménez Martín et al., 2016). Methods for fuzzy risk analysis and ranking fuzzy numbers support the quantification of uncertainties. Multi-criteria analysis, decision support systems and optimal ranking methods constitute key applications. Research concentrates on identifying properties for ordering fuzzy quantities and developing similarity functions to improve evaluation accuracy.

Various evaluation metrics for risk assessment in the chemical process industry are available. The methods include Layer of Protection Analysis, Fuzzy-based HAZOP studies and fuzzy multi-attribute HAZOP for gas wellhead facilities. Analysis models incorporate fuzzy-LOPA, hybrid fuzzy and probabilistic approaches for quantifying uncertainty, and FMEA-based risk analysis using fuzzy logic. Fault tree analysis methods, such as fuzzy fault tree analysis extensions, are employed for assessing fire, explosion and chlorine release risks. These techniques enhance safety and hazard understanding across industry processes.

12. Case Studies of Fuzzy Logic in Risk Assessment

Fuzzy logic's adaptability has been exploited in a range of exposure studies (Rezaei & Borjalilu, 2018). It has been combined with analytical network processes (ANP) to support dynamic occupational risk management (Hossein Chalak et al., 2022). Yet the most important applications of fuzzy logic have been devoted to environmental risk assessment – a field where the scarce amount and poor quality of available data can hardly be handled through conventional processing methods.In a concrete example, a fuzzy inference system (FIS) was designed and applied to develop a risk assessment model. The resulting approach was built on a fuzzy-regression for ordinal data (FORD) model, free of the restrictive assumptions about the sample size, normality, and co-linearity inherent to traditional methods used for risk-assessment purposes. The predictive performance of the model was tested in a real context, by making a comparison with the outcomes obtained through a distributed-lag linear model. The study confirmed that fuzzy systems provide a promising support for occupational health risk assessment.

Further demonstrative cases include: • The integration of fuzzy logic in a platform for arable crop risk assessment at a regional scale • The elaboration of a fuzzy Bayesian network (FBN) in support of monitoring and regulating exposure to contaminants in

coastal marine systems • The application of a fuzzy fault tree analysis (FTA) to the study of a landfill system.

13. Future Directions in Fuzzy Logic Research

Forecasts indicate that future research in fuzzy logic, machine learning, and decision-making will converge on the development of adaptive, model-free estimation techniques designed for uncertain, dynamic, and nonlinear systems, utilizing either fuzzy rules or neural computations. Further study should also focus on incorporating a variety of models and rapidly switching among them, rather than relying solely on model-free approaches. New methods are expected to enhance the extraction of information from non-linear correlational systems for decision-making purposes and to provide a more nuanced understanding of environments with limited information, thereby clarifying the reasons behind specific decisions (Chaudhuri et al., 2013).

14. Policy Implications of Fuzzy Logic in Risk Assessment

Fuzzy logic offers a new approach that could provide a principled understanding of the policy implications of risk assessment. It may complement traditional probability theory by framing the assessment problem in linguistic terms and guiding the mapping from empirical evidence to natural language expressions. The ‘‘fuzziness’’ inherent in the problem is either tolerated or embraced by returning fuzzy sets over precisely defined universes of discourse. Observed disentanglement of component and composite risks specifies the manner in which fuzzy theory can and should be applied.

The higher-order features unearthed by analysis of the accident-rate data—the linear log–log relation between the two parameters of the power-law distribution; the pattern by which the component risks relate to one another—bear on evaluation and subsequent treatment of the broader class of complex systems that defy precise analysis. Their policy implications range from the everyday to the spectacular. Supply-chain and transportation networks, critical infrastructures, ecological systems, food-chain and population dynamics, social networks, and terrorist group activity all fall within the ambit of complex systems. The log–log linear structure identified in the ratio of the power-law parameters indicates a means of characterizing individual components that is clearly intelligible within customary verbal and natural-language paradigms. The relative comprehensibility of the systems-wide pattern—formulated completely without recourse to numbers—explains why expert judgment has been able to construct remarkably effective working pictures of the cascading processes leading to rare catastrophic losses. What the public and their representatives require are tools for clarifying the boundaries, flow paths, and dependencies within, and the interrelationships among, the component parts of the complex systems of immediate concern to their lives and livelihoods.

“Fuzzy logic is a valuable tool for analyzing investment risks as a complex system and for easing the uncertainty embedded in the relevant information” (et al., 2019). The tool’s flexibility and robustness make it convenient for adaptation, qualification, and implementation within economic decision-making. When the fuzzy information can be presented in the form of well-defined membership functions, decision-relevant biases can be addressed early within the broader decision modeling before ensuing analyses. Subjectivity related to judgment considers the issues of linkage, scenario, and recognized quantitative outcomes obtained from the available investment-economy information. The modeling process proceeds truly in a spirit of complexity, combining fuzzy logics, uncertainty management methods, simple economic rules, and a few modifiers into a coherent framework capable of assessing the underlying information in the world of investment.370 Fuzzy Logic and Decision Making

The fuzzy approach is essential to macroeconomic scenario construction when vague information threatens to overwhelm the border of risk. The transition between stability and instability within macroeconomic systems eliciting multiple potential business outcomes is contained within the simplest formulation of the approach on investment risks. In the area of fuzzy assessment of risk, the objective approach of L. A.Gribbin (1993) finds the appropriate place in the ‘‘macro nature’’ of the world and its models. “Its area of application is associated with situations when proper universal risk function does not exist”. “Due to the imprecision of the reserve available investment-economy information and of the relevant qualitative indicators (when any of these imply the various and multiple range decisions) the particular approach has been extended considering multi-criteria and multi-valued fuzzy logics”.

While reflective of the ex post analysis undertaken, the resulting specification embodies the features of an ex ante decision-making tool for this class of problems. Iterative application of the formulation to the resulting list of decision-relevant-criteria results in well-defined weighting rules and scales of evaluation that link the natural-language input to the ultimately discrete material consequences of alternative courses of action. The approach employs only a modest number of criteria and only relatively simple operations on fuzzy sets readily represented by standard membership functions. The commitment of the analyst to the output of the formulation can be controlled at each point within the iterative chain of reasoning, thereby permitting the underlying belief system to be more clearly emulated. The fuzzy-logic formulation draws on components of much longer standing and wider applicability than the corresponding methodology based on formal probabilistic arguments, providing a familiar and congenial yet rigorous basis for narrative judgment about sources and impacts of risk.

“Fuzzy logic can be integrated with performance-based logistics and lean Six Sigma methodologies, and it can be used to analyze the failure of parts and the failure shootings of weapons” (Thi Thu Do et al., 2020) , thereby determining the capability and reliability

of a weapon system. Fuzzy logic is more effective for investigating the reasons for successes or failures after performing military missions—the exploration of root causes may be possible. Fuzzy logic as a formal and rigorous analytical approach can also be used to improve decision making in tactical logistics operations of naval organizations. Working as a management system and operator, emphasizing efficiency in activities that affect the quality of proceedings, fuzzy logic delivers a great tool for resolving the issues and problems faced during daily logistics operations at tactical level. Fuzzy logic can support the knowledge provided by experts, a specific method that enables the analysis of situations with data failures. The use of estimative tactics and their implementation make it possible to analyze the logistical situation, especially in the absence of detailed technical information, which can be difficult to acquire for experts. This capability has been particularly important during operations in Afghanistan, where the uncertainty of information and casuistic data has increased the need to better understand the situation and provide real-time solutions to logistic problems.

15. Conclusion

Fuzzy logic enables the use of a well-established mathematical structure capable of incorporating both quantitative and qualitative information in risk assessment models. The integration of fuzzy logic in environmental risk assessment provides a valuable framework for addressing uncertainties and enhancing the decision-making process. Fuzzy logic bridges the gap between quantitative and qualitative risk assessment methodologies, facilitating a more comprehensive and reliable evaluation of risks. It provides a framework that supports rapid decision-making and reasoning in complex environmental situations characterized by high uncertainty without compromising the relevancy and reliability of the analysis.

Environmental risk assessment is among the most significant applications where fuzzy logic contributes fundamentally to the assessment process. Fuzzy logic techniques enable the extraction of knowledge from both data and experts as well as the integration of this knowledge in an operational decision support system. Quantitative methods for risk assessment, which employ either deterministic or probabilistic approaches, are very effective only when all the parameters that influence the model are well understood. However, the information available for environmental risk assessment is usually incomplete and vague. A more general framework that includes qualitative information is required in this case. The framework supports mapping inputs into sets of decision rules and subsequently developing a fuzzy inference system that can compute a risk index based on the completeness of the available information.

The state of the art in environmental risk assessment indicates that the use of fuzzy logic could serve as an efficient tool for decision makers aiming at maximizing the utilization of available knowledge for performing preliminary assessment. The explored literature

demonstrates the intension to integrate fuzzy logic into environmental risk assessment practices, especially for tackling uncertainties, with many publishers conveying this philosophy. Adopting fuzzy logic in environmental risk assessment significantly improves the decision-making process under uncertain or incomplete information sources (Thi Thu Do et al., 2020) (Humphreys et al., 2006) (Jabbari et al., 2021).

References

Thi Thu Do, H., Thi Bich Ly, T., & Tien Do, T. (2020). Combining semi-quantitative risk assessment, composite indicator and fuzzy logic for evaluation of hazardous chemical accidents. ncbi.nlm.nih.gov

Humphreys, P., McCloskey, A., McIvor, R., Maguire, L., & Glackin, C. (2006). Employing dynamic fuzzy membership functions to assess environmental performance in the supplier selection process. [PDF]

Hussain, O., Chang, E., Hussain, F., & Dillon, T. (2006). A fuzzy approach to risk based decision making. [PDF]

Tchangani, A. (2011). A Model to Support Risk Management Decision-Making. [PDF]

Abdul-Rahman, H., Wang, C., & Lin Lee, Y. (2013). Design and pilot run of fuzzy synthetic model (FSM) for risk evaluation in civil engineering. [PDF]

Jiménez Martín, A., Carlos Martín Blanco, M., Pérez-Sánchez, D., Mateos Caballero, A., & Dvorzhak, A. (2016). A MCDA framework for the remediation of zapadnoe uranium mill tailings: a fuzzy approach. [PDF]

Jabbari, M., Gholamnia, R., Esmaeili, R., Kouhpaee, H., & Pourtaghi, G. (2021). Risk assessment of fire, explosion and release of toxic gas of Siri–Assalouyeh sour gas pipeline using fuzzy analytical hierarchy process. ncbi.nlm.nih.gov

Kabir, S. & Yazdi, M. (2018). Fuzzy evidence theory and Bayesian networks for process systems risk analysis. [PDF]

Mysiak, J., D. Brown, J., M. L. Jansen, J., & W. T. Quinn, N. (2008). Environmental Policy Aid Under Uncertainty. [PDF]

Vicente Cestero, E., Jiménez Martín, A., & Mateos Caballero, A. (2013). An interactive method of fuzzy probability elicitation in risk analysis. [PDF]

Azimi, S., Nikraz, H., & Yazdani-Chamzini, A. (2018). Landslide Risk Assessment by Using a New Combination Model Based on a Fuzzy Inference System Method. [PDF]

Rezaei, M. & Borjalilu, N. (2018). A dynamic risk assessment modeling based on fuzzy anp for safety management systems. [PDF]

Hossein Chalak, M., Kahani, A., Bahramiazar, G., Marashi, Z., Ivanov Popov, T., Dadipoor, S., & Ahmadi, O. (2022). Development and application of a fuzzy occupational health risk assessment model in the healthcare industry. ncbi.nlm.nih.gov

Chaudhuri, A., De, K., & Chatterjee, D. (2013). Solution of the Decision Making Problems using Fuzzy Soft Relations. [PDF]

MacGillivray, B. (2017). Characterising bias in regulatory risk and decision analysis: An analysis of heuristics applied in health technology appraisal, chemicals regulation, and climate change governance. [PDF]

Soltani, E. & Mirzaei Aliabadi, M. (2023). Risk assessment of firefighting job using hybrid SWARA-ARAS methods in fuzzy environment. ncbi.nlm.nih.gov

, G., Zvyagin, L., & Sviridova, O. (2019). Analysis of investment risks as a complex system using fuzzy logic and uncertainty management methods.

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Chapter 14: Mathematical Modeling of Air Pollution Dynamics in Urban Environments

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Abstract: A Urban air pollution, primarily driven by rapid industrialization, population growth, and vehicular emissions, poses significant threats to human health, ecosystems, and built environments. Among pollutants, particulate matter (PM) is particularly concerning due to its complex behavior and health impacts. Effective management of urban air quality demands reliable models that can analyze, predict, and inform mitigation strategies. This paper presents a comprehensive examination of mathematical modeling approaches to understand the dispersion and concentration of air pollutants in urban environments. The study explores deterministic models based on advection-diffusion equations, stochastic models such as SEIS frameworks for health impact analysis, and agent-based models simulating the behavior of emission sources. Emphasis is placed on mesoscale wind effects from urban heat islands, which significantly influence pollutant transport and vertical mixing. A two-dimensional Crank-Nicolson scheme is utilized to simulate pollutant dynamics under unstable atmospheric conditions. Comparative case studies from multiple cities demonstrate the model's applicability to real-world scenarios, revealing the influence of urban morphology and policy interventions on pollution distribution. The study also discusses model validation techniques, including sensitivity analysis and empirical comparisons with monitored data. In addition, the role of statistical and machine learning approaches in enhancing spatial and temporal resolution of exposure assessment is reviewed. The paper concludes with policy recommendations aimed at improving air quality through data-driven urban planning, regulatory reforms, and the adoption of reduced-complexity and fuzzy logic-based forecasting tools. The integration of empirical data, computational models, and regulatory frameworks offers a robust foundation for informed decision-making in urban air pollution management..

Keywords: Air Pollution Modeling, Urban Environments, Advection-Diffusion Equation, Particulate Matter (PM), Mesoscale Wind Dynamics.

Introduction

Acute PM pollution in urban areas results from rapid economic growth, population increase, industrial activities, and vehicle emissions, threatening human health, vegetation, water bodies, and property. Managing urban air quality requires reliable data on ambient PM concentrations across different zones. Monitoring involves continuous measurement of air quality and meteorological parameters, providing quantitative data on concentrations and deposition but only at specific locations and times. Modeling offers a comprehensive deterministic analysis of air quality issues, identifying sources and causes, and guiding mitigation strategies. Air pollution models are essential for assessing the significance of different sources and quantifying relationships between emissions and concentrations, including past and future scenarios. These models are crucial in regulatory, research, and forensic applications for effective pollution control. Most models balance physical accuracy with simplification, containing a degree of empiricism that limits their generality. As understanding of atmospheric processes improves, models incorporate less empiricism and become more broadly applicable (Chaitanya Kavuri, 2017). The level of air quality in urban centres is affected by emissions from vehicles. Reliable forecasting models would help administrators assess transportation policies. Physical models require numerous parameters, making them complex and difficult to assess. Recently, phenomenological approaches using fuzzy logic and algorithms focus on functional relationships between pollution sources and concentrations. A traffic model for Palermo is derived using data and fuzzy logic, validated over two years. This work aims to provide a reliable, user-friendly tool for urban pollution management (Ferrante et al., 2011)

2. Literature Review

Air pollution in urban environments has become a major concern as it is responsible for a significant number of premature deaths worldwide, especially in large urban centres. In view of this, there is a need to develop a reliable framework that can be used to model and understand the dynamics of the pollutant levels in urban areas. Mathematical modelling presents a useful tool for understanding the dispersion of pollutants, as well as for assessing the air quality of different urban cities. This chapter gives a detailed review of the various mathematical models that can be used for studying the dispersion of contaminants in urban areas.In general, air pollution occurs when any combination of solid, liquid and gas particles is introduced into the atmosphere. The concentration of pollutants can be impacted by changes in temperature and humidity. Urban areas are most affected by pollutant emissions due to human activities. Studies show that at least 7 million premature deaths per year are caused by air pollution, with urban populations accounting for the most affected group (Ulfah et al., 2017). Despite the high risk of urban

air pollution, an estimated one billion people are exposed to levels of fine particles that exceed the World Health Organisation (WHO) air quality guidelines. Due to these concerns, it is imperative to harness mathematical modelling to predict the concentration and dispersion of pollutants in urban environments. These models are capable of providing reliable information that is useful for government agencies to assess and predict pollution levels within cities. The models also play an important role in providing information on vulnerable areas within an urban setting, thereby establishing appropriate guidelines and regulations to maintain good air quality (Wai & K. N. Yu, 2023).A number of mathematical models have been developed for understanding pollutant dispersion under different atmospheric conditions. Under unstable atmospheric conditions the planetary boundary layer is expected to be shallow and turbulent, thereby impacting the vertical dispersion and mixing depth. In many urban regions under unstable atmospheric conditions the presence of mesoscale winds due to heat islands can have a significant impact on the distribution of air pollutants within the city. This often results in pollution circulation over the city and can lead to widespread high concentrations of pollutants at ambient levels. A two-dimensional advection-diffusion model can be used to study the effect of mesoscale wind fields on the dispersion and distribution of overall contaminant within the planetary boundary layer. The mesocale wind can be determined by solving the primitive equations for mesoscale flows and these are then used to compute the transport of pollutants using the advection-diffusion equations. The model can then be applied to a specific urban region to understand the effect of mesoscale winds on pollutant levels under unstable conditions. The advection-diffusion model uses the implicit Crank-Nicolson finite difference scheme for the numerical analysis of the overall concentration of pollutants in the atmosphere. Results show that at a fixed time of day, the concentration of the pollutants decrease with an increase in height. However, changes to wind speed and direction have a significant effect on the dispersion of air contaminants, and on the mixing depth. The intensification of the urban heat island following the rise in heating during daytime leads to the generation of mesoscale winds that increase the transport of pollutants both horizontally and vertically. This results in the enhanced concentration of pollutants in the city centre during the day, and the upward circulation of haze pollutants within the urban area. An increase in brightness temperature also leads to the emission of mesoscale winds that enhance the upward transportation of pollutants within the planetary boundary layer.

3. Theoretical Framework

Increase in PM is a sudden consequence of economic growth in some countries such as India, China, and Brazil. Intensive population growth, rapid development of industrial and commercial activities and a sharp rise in the number of automobiles over the years is the leading cause behind the increase in PM pollution in urban areas. Public health,

ecology and properties are seriously threatened by the poor air quality. Information regarding ambient PM concentrations, is a fundamental requirement in any strategy for the management of urban air quality. Improvement of the air quality can be achieved only through continuous monitoring and modelling. Once the possible origin of pollutants is known, appropriate corrective measures can be applied. Mon- itoring provides quantitative information regarding the degree of concentrations and deposition of different atmospheric pollutants but the data collected refer only to limited points in space and to the sampling time. Monitoring stations, in fact, can sample concentrations only at selected sites and times. Moreover, it is not possible to identify particles originating from different emission sources at the monitoring stations. Modeling, on the contrary, provides a deterministic description of the phenomenon of air pollution according to the emission sources, meteo- rological factors, physico-chemical transformations of airborne species and the conditions of the receptor environment.. Air pollution models have to provide a comprehensive theoretical and mathematical framework for assessing the significance of the various pollution sources and for quantifying the relationship between emissions and concentrations of airborne species at a given location and time. Source apportionment, source inventory, regulatory studies, research activities and forensic investigations can be conducted on the basis of data generated by the models. Most air pollution models include all relevant physical aspect but, at the same time, embed empirical elements, so that their results are only locally applicable and not extrapolable to different scenarios (Chaitanya Kavuri, 2017).

A two-dimensional mathematical model, based on the advection-diffusion equation, is presented in order to analyze the transport and diffusion of under the effect of mesoscale wind as an effect of urban heat islands. The model is solved numerically using the implicit Crank-Nicolson finite difference scheme under stability-dependent meteorological parameters involved in large-scale wind, mesoscale wind, and eddy diffusivity. The main objective is to investigate the distribution of air pollution by numerical simulation of the advection-diffusion model. Unstable atmospheric conditions are assumed. The results have been analyzed for the dispersion of air pollutants in an urban area in the downwind and vertical direction. The purpose of this research is to investigate pollutants dispersion under the effect of mesoscale wind using advection-diffusion equation. Wind strength determines the movement, the mixing and the spreading of the pollutants and also the contamination level in surrounding areas. Wind speed determines how pollutants are initially mixed and irregularities in wind speed and direction influence the pollutants' dispersion. Urban heat islands appear to increase haze pollution and promote upward circulation, so that the air pollution is more severe (Ulfah et al., 2017).

The level of air quality in urban centres is affected by emission of several pollutants which primarily arise from vehicles. Hence it is important to develop reliable forecasting models which provide a means of assessing different transportation policies. Further controlling strategies becomes very difficult if adequate traffic information. Physical models require many parameters regarding the emission and characteristics of vehicles as well as their routes i.e. they need to be very detailed. These parameters make the model cumbersome, whereas an exact solution in many cases is not feasible. Recently, phenomenological approaches which start from analysing functional relationships between the sources of pollution and the concentration levels, appear to be a most promising route. Among these approaches, a major role are played by those based on fuzzification of the phenomenon which are often supported by genetic or neuronal algorithms. A traffic model for Palermo is therefore derived on the basis of a fuzzification of the phenomena and validated on the basis of two years of data. This offers a reliable, easier tool for the management of urban pollution; the analysis presented in this work leads therefore to a new approach to the problem of urban air quality.

3.1. Mathematical Foundations

Air pollution models are an important component in efforts to assess the significance of various sources and to establish the relationship between emissions and air concentrations. These models become indispensable regulatory, research and forensic tools of analysis for past or future scenarios. The art of modeling is the extraction of the key physical aspects, and the elimination of the irrelevant details. The accuracy and the complexity of the models depend on the specific applications that they are designed for. Most practical models contain empirical components which determine their degree of generality and their reliability.

3.2. Key Variables in Air Pollution

Air pollution is generally a discontinuous field—a continuous field consisting of distinct particles from different sources. Various physical, chemical, and biological processes result in a highly complex mixture of gases and particulates of various sizes and compositions. To estimate concentrations at different locations and times, air pollution models have been extensively developed to establish the dispersion of pollution (Chaitanya Kavuri, 2017). Controlling air pollution in urban environments and understanding the dispersion of pollutants demand the development and implementation of effective urban air pollution dispersion models (Shi et al., 2021). Two essential variables must be known to estimate urban air pollution levels: population and weather conditions.

4. Modeling Approaches

Ambient air quality encompasses a diverse range of pollutants originating from multiple sources within a given area. Pollutants contributing to air quality degradation include carbon monoxide (CO), nitrogen oxides (NO x), sulphur oxides (SO x), volatile organic compounds (VOCs), and a family of particulates with both organic and inorganic components. Although monitoring ambient air quality delivers useful information on geographical location and time variation, it cannot ascertain pollutant sources (Chaitanya Kavuri, 2017). Models capable of determining the contributions of different emission sources thereby provide a valuable investigative tool. Air quality models, whether stochastic or deterministic, straddle the spectrum from straightforward data fitting to detailed system description. The latter depends naturally on a thorough understanding of processes controlling system development and sufficient information to quantify these effects. Routine monitoring presently affords insufficient spatial information to underpin this approach; however, current studies aim to utilize sparse data intelligently to obtain relevant information. Brief historical reviews of modelling exercises pre-2000 are provided by Steyn and McKendry (1996) and Wilkening (1999). The relatively small modelling effort in urban areas should not be understood as a reflection of a lack of interest. It seems more reflective of the complexity and nonlinear interactions present in urban environments, which are challenging to account for.

Mathematical approaches to air pollution resulting from transport in urban areas have attracted attention only recently. Physically based models, which require detailed parameters on vehicle fleets, microclimatic conditions, and driving behaviors for accurate predictions, often become too complex and their parameters challenging to quantify (Ferrante et al., 2011). Consequently, phenomenological approaches focusing on observed relationships between pollution sources and local concentrations have gained popularity. Analytical models incorporating fuzzy logic, genetic, or neuronal algorithms have increased in acceptance. An empirical traffic model developed for Palermo, based on 1997 observations and validated over two years, offers a robust and simplified tool for urban administrators and transport engineers. Using air quality data to estimate traffic flows on city roads provides an alternative method, comparable in reliability to traditional traffic models.

4.1. Deterministic Models

Mathematical models are useful to study how pollutants behave when new sources of air pollution are introduced or emissions change . They are essential tools in environmental monitoring, management, and assessment of air pollution . The perfect air pollutant concentration model would predict concentrations based on emissions, meteorological

conditions, location, and time with total confidence . Simulating air pollution provides information about pollutant spread, pollution levels, and estimation . The main physical processes in pollutant dispersion are advection and diffusion; advection involves wind transporting pollutants, while diffusion involves particle movement from high to low concentration caused by turbulence .

4.2. Stochastic Models

In the field of air pollution modeling, stochastic models are particularly valuable for investigating the complex relationships between pollution levels and population dynamics such as respiratory infections. Air pollution is a widely recognized and rapidly growing environmental hazard. A stochastic SEIS (susceptible-exposed-infected-susceptible) framework captures the dynamics of respiratory disease transmission affected by air pollution. The methodology involves parameter estimation from collected data followed by a model fitting process. Time-varying environmental factors, human activities, inflow rates, and clearance rates are each represented by appropriate functions. Change points in these functions are identified using a Bayesian estimation framework. Results reveal that intervals between switches in pollution severity are lengthening, indicating a progressive deterioration in air quality; this is especially evident in recent years during which periods of high pollution have surpassed the winter heating season. The analysis further suggests a concurrent decline in both air quality and the environment's self-regulation capacity (He et al., 2018). Clearly, stochastic models are a powerful tool for describing the intricate interactions among air quality, seasonal variations, and population behaviors.

4.3. Agent-Based Models

Agent-based models simulate the behaviour and interactions of autonomous agents to assess their effects on the system as a whole (Ghazi et al., 2019). The MAESPA model emphasises the effects of complex vegetation elements on particle dispersion, assuming a continuous emission source and comparatively simple traffic activity (Ghazi et al., 2019). A multi-agent based simulation can be combined with classic modelling tools for greater insight. Regulation rules can be computed according to how much the agent participates in pollution levels, with regulation having a big influence on pollution control. Cooperation between agents helps reduce pollution levels and affects pollutant evolution. The current modelling system accounts only for point emission sources. Future developments include adding continuous sources such as roads and predicting additional pollutants. A Geographic Information System (GIS) interface may be incorporated to enhance visualisation.

5. Data Collection and Analysis

Severe particulate matter (PM) pollution in urban areas in India primarily results from rapid economic growth, increasing population density, expansion of industrial and commercial activities, and rising vehicle emissions (Chaitanya Kavuri, 2017). Increased pollution levels jeopardize human health, degrade ecological systems, and threaten cultural heritage and private property.

The availability of reliable data on ambient PM concentrations at a range of urban sites is crucial to effectively managing air quality. Monitoring of air quality typically involves measurements of PM levels and meteorological parameters, relating to specific locations and given times, providing a quantitative data set of the pollution status, but not aiding in the identification of pollution sources. Air pollution modeling offers a more comprehensive view by analyzing the emission sources, meteorological influences and chemical transformation that govern the concentration distributions. Models form the basis for strategic planning of air pollution reduction and enable assessing the significance of potential emission sources and evaluating the effectiveness of possible control measures, and hence have become important tools for regulatory and research purposes.The core of air pollution modeling is the representation of the essential physical aspects while omitting irrelevant details. All models depend on specified initial and boundary conditions and all include some empirical or semi-empirical elements, such as parameterizations and closure terms, which become more sophisticated as the understanding of atmospheric processes increases.

5.1. Air Quality Data Sources

Air pollution has long been a subject of scientific scrutiny, with a focus on understanding its sources and effects. Acute PM pollution in urban areas is caused by rapid economic expansion, population growth, industrial activities, and increased automobile use. Monitoring and modeling are essential for managing urban air quality. PM pollution monitoring involves continuous measurement of air quality parameters and meteorological factors but only describes conditions at specific locations and times. PM pollution modeling provides a comprehensive analysis of sources, causes, and potential mitigation measures, helping assess the significance of different sources and the effectiveness of pollution control strategies. Air pollution models are critical for quantifying the relationship between emissions and concentrations, and are used in regulatory, research, and forensic applications. The essence of air pollution modeling is to capture key aspects of reality while simplifying details, and models vary in accuracy and capability based on their level of empirical assumptions (Chaitanya Kavuri, 2017). Air pollution is the greatest environmental health risk worldwide, with fine particulate

matter (PM2.5) having the largest health impact. Efforts to reduce PM2.5 are challenging due to the complexity of atmospheric and emission systems. Air quality models and decision support tools are essential for designing policies to improve air quality. Mechanistically detailed models like chemical transportation models (CTMs) are expensive and often unavailable at urban levels, leading to the development of reduced-complexity models (RCMs) such as InMAP. InMAP uses a variable spatial resolution grid and has a global urban version to estimate high-resolution PM2.5 exposure in densely populated areas. Policymakers often lack detailed information on the sources of ambient PM2.5 pollution within their cities, such as contributions from local versus external sources. Previous studies have provided broad-scale data suitable for national or regional analysis but limited urban-level insight. This study uses InMAP to assess 96 global cities, estimating contributions from 12 emission sectors inside and outside city boundaries to primary and secondary PM2.5 concentrations. It also evaluates model performance and discusses future improvements, providing critical data where limited information previously existed (W. Tessum et al., 2022).

5.2. Statistical Analysis Techniques

Air pollution modeling offers a deterministic framework for air quality analysis that evaluates the influence of emissions, meteorological conditions, chemistry, and transport processes, which is essential for guiding mitigation strategies. Models provide a structured means for source-receptor assessment and for quantifying relationships between emissions and concentrations that seldom emerge directly from field measurements. Regulatory, research, and forensic applications rely extensively on predictive models to interpret and extend the network of physical observations (Chaitanya Kavuri, 2017).

The myriad models that attempt to replicate air quantity are designed to simulate the physical reality of the atmosphere. They aim to allow for wide-ranging sensitivity analyses, thereby furnishing insights into the effects of changing emissions, land use, transport systems, or meteorological patterns. This capacity for exploratory analysis is valuable because direct field experiments to probe these variables are usually impossible. The ability of a model to elucidate such relationships, however, demands a certain abstractness; if a model is forced to reproduce observations with excessive accuracy, the dominant empirical elements tend to fix a particular solution and preclude broader generalization. Remaining uncertainties typically become concentrated in these phenomenological aspects, which might eventually be replaced by formal descriptions as the understanding of atmospheric processes advances.

Statistical and machine learning models offer complementary approaches to air quality modeling. Statistical models, which emphasize interpretability, furnish estimates of uncertainty that describe inferential reliability and enable model diagnosis. Machine learning methods, in contrast, prioritize prediction accuracy to identify important risk factors and formulate hypotheses concerning complex relationships (J. Berrocal et al., 2019). They can efficiently capture nonlinear effects when trained in data-rich environments, although they generally do not provide parametric inference. For exposure assessment in health-related applications, where individuals with health data often have sparse or irregularly available pollutant concentrations, several approaches have been developed to estimate air pollution on finer spatial and temporal scales than the monitoring data. These methods include geostatistical techniques such as kriging, spatial statistical models incorporating output from air quality models into their mean structure, linear regression models employing GIS covariates as predictors, and machine learning techniques including neural networks and deep learning.

The appropriate selection among these approaches depends on the modeling goals and data availability. Statistical and machine learning methods fit spatial statistical models to measured pollutant concentrations that leverage inputs from chemical transport models along with covariates that influence air pollution levels. Because each statistical model differs in its construction, the scientific issues it addresses, and the context in which it should be implemented, working knowledge of the air pollution context is essential to deploying the correct approach. Different classes of spatial statistical models have traditionally been developed for separate settings and modeling objectives, raising questions about their suitability and adequacy for exposure assessment.

6. Case Studies

A comprehensive understanding of air quality in urban environments requires consideration of both meteorology and functional properties of the area. The composition of trace species in urban air depends on emissions, photochemical reactions, removal processes, and transport of species in and out of the urban air. Rapid photochemical reactions result in strongly nonlinear processes, creating challenges for understanding the mechanisms leading to concentration and deposition values (G. Prinn & B. Cohen, 2009). Predictions of air quality now often come from models tailored to a specific urban area for which data on emissions, meteorological conditions, and air quality exist. Urban-scale transport is usually modeled with a regional-scale model of approximately 100 km in horizontal extent, with a uniform grid of approximately 3 km resolution over the urban area itself (Blake Cohen, 2010). A one-way nested grid allows the dispersion and transport from the urban-scale model to be fed into the regional-scale model, providing some downwind urban plume growth in the regional-scale model through the chemical

and transport routines. The air quality model CAMx is the state of the art in urban-scale 3D models and includes many processes leading to accurate predictions of urban-scale concentrations and surface deposition of chemically and physically important trace species.

Urban-scale threats to air quality are significant due to concentrations of population and the related concentration of anthropogenic emissions. Urban-scale source apportionment and forecasting information about these concentrations can be highly useful for air quality management and planning of clean-up activities (Chaitanya Kavuri, 2017). This information, however, cannot be easily obtained from measurements in space and time. A full urban-scale model provides sufficient detail and robust results for a variety of realistic weather conditions, making it a valuable tool for support of forecasting, planning, and regulation of air quality subject to the direct impact of emissions from within the urban domain. The metamodel provides urban-scale air quality information efficiently and with traceability deriving from the underlying comprehensive model CAMx.

6.1. City A: Modeling Results

The Daysimeter records daylight data relevant to chronobiological investigations; its raw data is field-calibrated against the fluorescent standard Calibration Jar and later calibrated against the D65 standard. Urban air quality is a major concern worldwide, prompting extensive research into urban pollutant dispersion with models of various complexities. Air pollution modeling is vitally important for understanding pollution and finding solutions. Land Use Regression models are becoming popular for estimating air pollution concentrations, but their accuracy depends on the properties of the monitoring network. The model's application in different urban environments is then discussed. Both high-resolution and intermediate-resolution simulations of NO2 concentrations are conducted. The effects of different emissions inventories and urban canopy properties on model performance are explored. Highly resolved traffic emission data have little impact on model performance in either city, while intermediate-resolution NOx emissions extracted from a local inventory improve results for the London domain only. Topographic orographic forcing also affects NO2 concentrations appreciably in London; neglecting this process leads to an overestimation of NO2 concentrations of about 5%.

6.2. City B: Comparative Analysis

Air pollution predictions for City B form the basis for a comparative analysis with City A. Vehicular emissions remain the dominant source of pollutants, particularly within street canyons where the impact is most severe and diminishes with increasing distance

from the road. Urban morphology significantly affects the spatial distribution of pollutants: street canyon aspect ratio and building group shape emerge as critical parameters. Deep and narrow canyons tend to accumulate higher pollution levels; conversely, increased building height promotes better air circulation and reduced pollutant concentration. Additionally, the shape of building groups influences pollution distribution patterns in the vicinity of urban complexes, generally leading to decreased concentrations.

6.3. City C: Policy Implications

The case of City C demonstrates how a simulation model can be used to evaluate the relative impacts of alternate local, national and international policy actions on urban-area air pollution. The model focus in this city is PM-2.5 air pollution, a group that of particular concern because of its significant adverse health effects (United States Environmental Protection Agency, 2019). Although certainly not of the same magnitude as economics, health, or the environment, the current focus on air pollution in the wake of the COVID-19 outbreak has brought attention to air pollution's sensitive linkage with other concerns.

Inputs to the simple PM-2.5 emission model include urban-area population data from The World Bank (2019), per capita GDP from the United States Census Bureau (2020), purchasing power parity conversion factors from the Global Economy (2020), national carbon emissions data from the Global Carbon Atlas (2020), carbon emissions exclusion of commercial (International Air Transport Association, 2019) and domestic shipping activities (International Council on Clean Transportation, 2018), and a least-squares log-log regression of the 38 cities for which reliable PM-2.5 data were available from the World Health Organization (2018). The focus centers on evaluating the cumulative effect on air-quality outcomes of different levels of travel activity in a city, an emissions factor that tends to be significantly affected by government policies.

7. Model Validation

Wherever numerical procedures are employed, model validation is compulsory for overall control. Usually, equations representing processes like dispersion, photo-chemical transformations and aerosol dynamics are solved separately. A realistic description of all physical and chemical processes remains an open problem. Therefore, several simplifications are made to reduce mathematical equations to an acceptable level of complexity, achieving useful accuracy. For validation, the Peters-Besson scheme is applied directly (Chaitanya Kavuri, 2017).

7.1. Validation Techniques

Validation of an air pollution model implies the evaluation of its ability to predict pollutant concentrations over a wide temporal and spatial domain. Time series of modelled pollutant concentrations are compared with corresponding measurements at the position of air-quality monitoring stations. Validation of an air pollution model is performed through extensive comparisons with one or more monitoring stations. Chapter 11 presents a systematic approach for full model validation (Chaitanya Kavuri, 2017).

Validation of a modelling system usually starts by testing the model applied in a simple, idealised way in the situations for which it was developed and then the complexity is increased stepwise. For instance, an atmospheric dispersion model may be validated by comparing modelled pollutant concentrations with measurements taken from a single small source in relatively simple or well-known meteorological conditions, such as dispersion of smoke from a chimney stack under known hourly wind conditions or dispersion from an axisymmetric flow source in a large wind tunnel. The model should then be able to predict more complex situations, such as the combined pollution impact of the smoke from different chimneys over extended areas and severe atmospheric turbulence. The objective of validation is to ascertain whether a model is capable of producing results that are sufficiently accurate in comparison with measurement data. It is very difficult to quantify ‘‘sufficiently accurate’’, since it depends on several factors, such as the used methodology and the severity of the applications. Later sections concentrate on describing the most important techniques of validation relevant to traffic–street–urban areas.

For detailed model validation, it is often necessary to make use of specialised statistical tools.

7.2. Sensitivity Analysis

Sensitivity tests investigate the robustness of the metamodels when exposed to different input conditions. Alterations to the base-case inputs—such as enhanced emissions of NOx, CO, or VOCs, adjustments to temperature, and increased emission levels—account for differences between urban regions, temporal variations, and unusual situations. Non-linear responses arise in ozone formation at high NOx concentrations, secondary organic aerosol production, sulfate aerosols, and VOC oxidation; these effects are reflected in the concentration of formaldehyde. Each metamodel was executed with 50,000 randomly sampled input parameter sets.

8. Policy Recommendations

Analysts reportedly confirmed that achieving adequate source control—such as reduced emissions from significant emitters—would negate the necessity for future air-quality controls for an additional two or three decades (Janene Fincher, 2007).

A systems model facilitates examination of whether, once emissions return to 1973 levels and controls are subsequently lifted, the system would exceed air-quality standards necessitating the reestablishment of controls. Temporal patterns also present potential insights: control managers are unlikely to maintain constant control levels indefinitely. Rather, they would tend to reduce controls after attaining desired emission reductions, engendering oscillatory behavior as emissions temporarily fall before controls are relaxed. Implementing a gaming mode—wherein managers periodically interact with the model and adjust policies—could further simulate real-world decision-making. Spatial dynamics may prove critical for understanding phenomena such as pollution hotspots and urban sprawl induced by policy interventions. Incorporation of actual emission trends and an expanded suite of control measures—including seasonal restrictions—would likely enhance realism. Several variables remain insufficiently developed or lack feedback mechanisms; for example, the impact of overcrowding on development density has yet to be integrated. Additionally, current formulation omits changes in residential land disturbance and associated costs throughout the simulation. Enrichment through additional mass-transit options—already included in prior frameworks—would also be beneficial, especially under policies promoting transit use as an emissions mitigation strategy.

8.1. Regulatory Frameworks

Air pollution is a complex phenomenon with detrimental effects on human health, the environment, and property. Economic growth, increasing population, industrial activities, and vehicle emissions have caused acute pollution problems in numerous urban areas (Chaitanya Kavuri, 2017). Consequently, understanding and controlling pollution levels has become a pressing challenge for governments, researchers, and engineers worldwide.

Air pollution regulatory programmes have been established in most countries, creating a social and political context within which research must operate. These policies impose increasingly stringent requirements on the quality and type of information to be developed. Because reliable forecasts of the effects of alternative pollution control strategies are not generally available, these regulations frequently have the consequence of prohibiting emission increases. Such restrictions may be overly conservative and

unnecessarily costly. To address this challenge, an important goal of air pollution research is to develop methods to translate these regulations into a mathematically well-posed problem that can be dealt with effectively and to create reliable modelling and forecasting tools capable of assessing the consequences of different control strategies and suggesting courses of action that satisfy the multi-pollutant air quality criteria. Various mathematical models describing the dispersion of pollutants from one or more sources has been developed during the last decades. The goal of these investigations is to provide a reliable forecast of the temporal and spatial evolution of pollutant concentrations, which could be used to design strategies for the control of pollution levels.

The Danish Euler Model (DEM) is a state-of-the-art model used in many countries worldwide to forecast air pollution episodes (P. Chernogorova & G. Vulkov, 2016). DEM consists of a set of PDEs describing the behaviour of chemical species formed in the atmosphere after emission of primary pollutants from different sources. The main physical processes taken into account are advection, diffusion, chemical reactions, emissions and deposition. To improve the accuracy and the efficiency, operator splitting techniques are often applied. However, the resolution of each of the resulting sub-problems obtained after operator splitting presents considerable computational challenges because of the size of the related dynamical systems.

8.2. Public Health Considerations

The negative effect of air pollution on public health is an acknowledged concern, particularly the physiological response to particulate matter (PM), whose implication in cardiovascular, respiratory, and visibility problems is now firmly established. PM is reported as micrograms per cubic meter, so the level should according to standards not exceed 35 μg/m3 (the hourly average), but actual levels often lie above this, a report from 66 monitoring stations in Taiwan observed median values of slightly above 37 (Deb & S. Tsay, 2017). PM may consist at any time partly of particles emitted directly and partly of particles formed in the atmosphere from gaseous emissions such as sulphur dioxide, nitrogen oxides and organic gases. The conversion rates depend in a complex way on regional and seasonal factors and must therefore be estimated by spatio-temporal models.

9. Future Research Directions

Urban air pollution is a critical threat to human health, vegetation, wildlife, and property (Chaitanya Kavuri, 2017). The growing concern surrounding air quality and atmospheric processes has led to increasing demands for reliable prediction models and efficient mitigation measures. Despite widespread pollution monitoring, comprehensive

understanding and forecasting remain elusive. Computational modelling of ambient air quality has proven successful in representing key physical and chemical processes occurring in the atmosphere. Atmospheric models are widely used to simulate the dispersion, transformation, and removal of pollutants in the ambient atmosphere and to predict the resultant air pollution levels at locations of interest. The lack of reliable data on particulate matter concentrations within the various zones of Rourkela makes it difficult to gauge the extent of the problem and construct an appropriate regulatory framework to address air quality. Monitoring involves the continuous measurement of air quality and meteorological parameters, but data can only be obtained at specific locations and times. Moreover, the source of pollution cannot be identified from monitoring data alone. Modelling, on the other hand, can provide a more comprehensive view of the problem by providing guidance on the sources of pollution as well as the influence of meteorology and chemical changes.

The air quality model considered is capable of simultaneously simulating the effects of transport, dispersion, chemical transformation, and removal processes that determine the ambient concentrations of a wide range of air pollutants. Air pollution models have considerable value in addressing problems related to urban air quality. A highly cost-effective alternative to costly and time-consuming field experiments, these models enable an initial assessment of source contribution, a quantification of the relationships between emissions and ambient concentrations, and an evaluation of the relative effectiveness of various control measures. At the core of a model is the representation of the main physical and chemical processes, which tends inevitably to be complex and detailed, especially when very high accuracy is required. A large number of air pollution models have been developed, each model differing from the others in terms of both methodology and complexity. Most models include empirical elements whose contribution decreases as knowledge and understanding of atmospheric processes improve. Several installations in Rourkela attract an enormous number of people who comprise the Rourkela metropolitan area. The modelling approach for addressing such problems is to treat the total Rourkela area as comprising several subareas within or downwind of which a number of sources exist. The main aims of the model are to provide a reliable estimate of the ambient air pollution level in each such zone and to provide a quantitative assessment of the relative contribution of different sources. By providing such information, the model facilitates the formulation of potential control strategies, in addition to highlighting the areas most at risk and hemispherically detected air pollution level in zones such as education, commercial, residential, and mixed zones during peak hours.

9.1. Emerging Technologies

Acute PM pollution in urban areas of a developing country results from rapid economic growth, increased population, industrial and metallurgical activities, and vehicular emissions, especially during special events. Managing urban air is challenged by the absence of reliable information about ambient concentrations in different activity zones. Continuous monitoring at fixed locations captures air quality and meteorological parameters, providing a localized and temporal snapshot. Models present a deterministic picture of air quality, elucidating the air pollution problem and identifying sources and reasons behind high pollutant concentrations, including emissions and meteorological processes. Consequently, models are necessary for effective mitigation strategies. Air pollution models assess whether a particular set of sources is significant and quantify the complex relationships between emissions and ambient concentrations, rendering them essential for regulating pollution, assessing source importance, quantifying cause-and-effect, forecasting air quality, supporting design and research, and aiding enforcement and permitting. Modeling air pollution entails selecting physical aspects important to the problem to be modeled while omitting irrelevant details. Various models may be employed depending on the desired accuracy and capability to analyze causes of high pollutant concentrations. Most models incorporate empirical elements, but the degree of empiricism diminishes as understanding of atmospheric processes improves, enhancing generality (Chaitanya Kavuri, 2017).

Particulate pollution-induced health effects are well documented, and a total economic loss of USD 2.4 billion per year is estimated from PM10-induced premature death and chronic respiratory diseases. Vehicular emissions constitute the main source of atmospheric particulates in cities not directly influenced by industrial emissions. A simulation model for urban air pollution is urgently needed for practical use, which would benefit megacities like Hong Kong. Plume dispersion in the urban canopy layer (UCL) is determined primarily by building-induced flows and heterogeneity in building heights, causing asymmetries in plume structure. Gaussian dispersion models such as AERMOD and ADMS-urban describe urban effects in a simplified manner, while computational fluid dynamics (CFD) models resolve the mean wind and turbulent flow field more accurately but are computationally demanding and typically focus on neutral flow. Machine learning (ML) techniques are increasingly employed for predicting regional-scale air pollution, often outperforming traditional models such as Gaussian dispersion, Kalman filtering, nonlinear regression, and time series. Various algorithms including artificial neural network (ANN), least absolute shrinkage and selection operator (LASSO), long short-term memory (LSTM), k-nearest neighbours (kNN), random forest (RF), and support vector machine (SVM) have been evaluated with differing predictive accuracy. The importance of meteorological data in prediction is well evidenced. However, limited research applies ML models to neighborhood-scale PM10 dispersion within compact-city UCLs. The study investigates whether a recent ML

technique can efficiently provide accurate neighborhood PM10 predictions in such environments. The ML model is trained on past PM-reference and meteorological monitoring data, with predictions compared to experimental measurements and CFD simulation results, which are more physically accurate but computationally intensive (Wai & K. N. Yu, 2023).

9.2. Longitudinal Studies

Longitudinal data arise when a single individual is observed over time, such as the amount of pollution on a particular day recorded repeatedly. Historical data gathered over an extended period form the basis of many environmental and economic studies (Deb & S. Tsay, 2017). These data enable analysis of dynamic properties, forecasting of future trends, and assessment of the impact of fitted models on policy. To analyze such data, City air pollution data often encompass measurements recorded hourly or daily for several consecutive years. Analyzing such time series aids in understanding long-term dynamics, determining future concentration levels, and designing intervention strategies.

10. Conclusion

Urban air pollution presents an increasing health risk, potentially harmful even at moderate levels. Integrated investigations into urban pollution can be conducted quantitatively using mathematical and numerical techniques (Chaitanya Kavuri, 2017). The scanned area represents a two-dimensional horizontal section of the atmospheric boundary layer integrating continuum field techniques; the unit volume element is sufficiently large while maintaining a proper characterization of the system's microstructure (Wai & K. N. Yu, 2023). Diffusion is treated microscopically at the molecular scale, with the interaction of pollutant particles addressed via a modified Langevin equation (Ferrante et al., 2011). The georeferencing system, relative to which all emitted particle paths are reconstructed, coincides with local cartesian coordinates on the ground. The analysis pertains to periods characterized by the absence of precipitation and thermal inversion conditions and is temperature dependent. The model confirms traffic pollution as the dominant emission source at sites denoted by low altitudes, with atmospheric parameters indicative of the absence of rain and inversion situations..

References

Chaitanya Kavuri, N. (2017). Source Apportionment and Forecasting of Aerosol in a Steel City - Case Study of Rourkela.

Ferrante, P., Lo Bosco, D., Nicolosi, S., Scaccianoce, G., Traverso, M., & Rizzo, G. (2011). Obtaining Traffic Information by Urban Air Quality Inspection.

Ulfah, S., Bekoe, C., & Atta Owusu, B. (2017). ADVECTION-DIFFUSION MODEL WITH TIME DEPENDENT FOR AIR POLLUTANTS DISTRIBUTION IN UNSTABLE ATMOSPHERIC CONDITION.

Wai, K. M. & K. N. Yu, P. (2023). Application of a Machine Learning Method for Prediction of Urban Neighborhood-Scale Air Pollution. ncbi.nlm.nih.gov

Shi, Y., Kai-Hon Lau, A., Ng, E., Ho, H. C., & Bilal, M. (2021). A Multiscale Land Use Regression Approach for Estimating Intraurban Spatial Variability of PM(2.5) Concentration by Integrating Multisource Datasets. ncbi.nlm.nih.gov

He, S., Tang, S., Xiao, Y., & A. Cheke, R. (2018). Stochastic modelling of air pollution impacts on respiratory infection risk.

Ghazi, S., Dugdale, J., & Khadir, T. (2019). Modelling PM10 Crisis Peaks Using Multi-Agent based Simulation: Application to Annaba City, North-East Algeria.

Ghazi, S., Dugdale, J., & Khadir, T. (2019). Modelling Air Pollution Crises Using Multi-agent Simulation.

W. Tessum, M., C. Anenberg, S., A. Chafe, Z., K. Henze, D., Kleiman, G., Kheirbek, I., D. Marshall, J., & W. Tessum, C. (2022). Sources of ambient PM(2.5) exposure in 96 global cities. ncbi.nlm.nih.gov

J. Berrocal, V., Guan, Y., Muyskens, A., Wang, H., J Reich, B., A. Mulholland, J., & H. Chang, H. (2019). A comparison of statistical and machine learning methods for creating national daily maps of ambient PM$_{2.5}$ concentration.

G. Prinn, R. & B. Cohen, J. (2009). Development of a Fast and Detailed Model of Urban-Scale Chemical and Physical Processing.

Blake Cohen, J. (2010). Urban-scale impacts on the global-scale composition and climate effects of anthropogenic aerosols.

Janene Fincher, S. (2007). Evaluating the benefits of a systems approach to particulate matter air pollution management.

P. Chernogorova, T. & G. Vulkov, L. (2016). Numerical solution of a parabolic system in air pollution.

Deb, S. & S. Tsay, R. (2017). Spatio-temporal models with space-time interaction and their applications to air pollution data.

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Chapter 15: Role of Mathematics in Human Language Patterns and Computational Linguistics

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Abstract: Mathematics plays a foundational role in understanding the complexities of human language, both structurally and functionally. This paper explores the deep interconnection between mathematical concepts and linguistic structures, emphasizing the ways mathematics facilitates the modeling, analysis, and interpretation of language. Formal language theory, automata, and algebraic structures underpin the syntactic and semantic frameworks that define human communication. Tools such as lambda calculus, Bayesian inference, and Markov models support computational processes that mirror human cognitive functions in language comprehension and production. Furthermore, mathematical linguistics intersects with machine learning, natural language processing (NLP), and information theory, enabling machines to process language with increasing sophistication. The Chomsky hierarchy and dependency parsing exemplify how mathematical structures mirror linguistic hierarchies. Formal and probabilistic models bridge theoretical linguistics with practical applications, including speech recognition, machine translation, and text mining. Mathematics also provides robust frameworks for investigating ambiguity, complexity, and evolution in natural languages. Through semantic networks and network theory, the relational nature of language is captured quantitatively. Importantly, the paper underscores the interdisciplinary nature of mathematical linguistics, drawing from physics, biology, and computer science to advance understanding. It highlights ongoing challenges, such as language ambiguity and computational limitations, while pointing to future directions in AI-driven language modeling. Ultimately, the paper demonstrates that mathematics is not merely a tool but a language itself—one that complements, structures, and reveals the intricacies of human linguistic expression.

Keywords: Mathematical Linguistics, Computational Linguistics, Formal Language Theory, Natural Language Processing (NLP), Syntax and Semantics Modeling

Introduction

Humans naturally employ the mechanisms of language to describe real-world phenomena. Mathematics similarly serves as a description of abstract structures, the real world, the universe, and even itself (Esterhuizen, 2008). As an archaic step in cultural evolution, mathematics emerged from attempts to describe and solve real-world phenomena. Physicists employed mathematics in attempts to comprehend the physical structure of the universe, and engineers applied them to practically construct artificial structures. Some areas of pure mathematics deal with abstract structures that have no known physical counterpart, yet some of these abstract structures can be modeled physically. Mathematics can describe itself in the form of metamathematics, which provides a detailed analysis of the structure of mathematics and its syntax. Some theories suggest that language may have enabled the emergence of another uniquely human cognitive function: mathematics. The human mind's mathematical competence is closely tied to language, and it is speculated that mathematical development presupposes the possession of language skills. A finite set of words and a finite set of numbers enable an infinite variety of meaningful combinations that are subject to a finite set of rules. Language is the only technology we explicitly require in order to think, argue, and express ourselves, which allows the speculations of different language patterns locating different patterns of thought to be taken seriously.

2. Mathematical Models in Linguistics

Mathematics plays a pivotal role in the study and analysis of human language patterns; sophisticated linguistic categories cannot be accurately modelled without mathematical tools. Such models enable the comprehension of both singular linguistic facts and the overarching structural patterns of language, thereby facilitating pro-fessional analysis and interpretation of linguistic data. Consequently, branches of linguistics such as semantics and syntax adopt mathematical methodologies to validate their analytical frameworks. Linguistics and mathematics are commonly regarded as "twins," two intellectual disciplines exhibiting striking congruence in conceptual constructs and methodological approaches (Esterhuizen, 2008). Unlike physics or chemistry, where content is closely bound to experimental data, mathematics is fundamentally conceptual, rooted in pre-existing notions and accessible to a priori investigation once formal axiomatic foundations are established. In mathematical linguistics, the system of axioms is predicated on the set of semantic categories formulated by linguists, thus providing the conceptual framework from which logical consequences are deduced.

In the quantitative analysis of literary styles, mathematical techniques prove invaluable. Mathematics enables the rigorous definition and characterization of abstract structures,

qualities, or patterns, allowing complex phenomena to be conceptualized with precision, clarity, and the elimination of ambiguity—qualities essential for the development of computer models of the world. Overview of Mathematical Linguistics can be found in "Linguistics + Mathematics = Twins".

2.1. Statistical Models

Language models (LMs) are statistical constructs designed to assign probabilities to sequences of words or other discrete symbols. Both count-based n-gram models and neural LMs can be unified within a single framework that formulates a set of probability distributions across the vocabulary, controlled by dynamic mixture weights. This unified approach facilitates the development of hybrid models that amalgamate count-based and neural LM features, resulting in enhanced performance (Neubig & Dyer, 2016). Statistical models emphasizing word-based translation and word-level alignment constitute the foundation of the majority of contemporary statistical machine translation systems. Alternative methodologies are documented extensively in the literature. The advent of statistical and mathematical techniques has profoundly influenced fields such as computational and quantitative linguistics, embedding them within the exact sciences. Successors of these pioneering approaches increasingly disseminate their outcomes through accessible online platforms (Junczys-Dowmunt, 2008).

2.2. Algebraic Structures

An axiom is a string of symbols with intrinsic meaning only in the context of all derivable formulas of an axiomatic system. According to incompleteness, every sufficiently powerful axiomatic system contains undecidable formulas, making a final axiomatization of mathematics impossible. Mathematics is often seen as reducible to set theory within axiomatization, as every statement or proof can be formulated as a set-theoretic expression. Mathematical linguistics studies mathematical structures and methods important to linguistics. It emphasizes the internal organization of linguistics, frequently focusing on phonetics, phonology, morphology, syntax, and semantics, which develop through hierarchical structures of stable recurrent items. Chomsky formulated models of linguistic structure based on finite-state automata, context-free grammars, and context-sensitive grammars, which relate under the heading of generative capacity. These contributions underpin much of formal language theory in computer science. Natural sciences also play a role in language communication, encompassing psychology, physiology, physics, and acoustics to interpret speech from brain to sound waves and back (Esterhuizen, 2008).

Mathematical equations with the same solution set can exhibit different surface structures yet share the same deep structure. By observing certain properties, mathematicians transform equations analogously to how linguists follow grammatical rules. Zepp identifies mathematics as a register possessing a unique vocabulary, which can cause confusion for students due to meanings that differ from everyday language. The mathematics register also severs the link to external context, rendering written language self-contained and precise. Formal written language is a hallmark of mathematical activity. Recognizing the nature of language and its similarity to mathematics benefits educators and students. Parallels exist between natural language and mathematics in notation, symbolism, and structure. In language, elements and actions correspond to numbers and operations. Combining elements in accordance with rules forms coherent expressions, with infinitely many possible sentences and equations. Mathematical symbols facilitate communication; although developed from necessity, many students struggle to grasp their conceptual meanings, which may contribute to math anxiety (Shafer, 1992).

3. Formal Language Theory

The features of human language have been examined within the realm of formal language theory, which addresses common rules of a universal grammar governing the generation of syntactic structures (Witzany, 2011). Such theory elucidates language evolution and relates to a perceived inner logic of nature amenable to mathematical analysis. Universal Grammar emerges as a mechanism underpinning language acquisition, posited as an innate rather than learned faculty. Correspondences exist among languages, grammars, and machines: context-free languages are generated by context-free grammars, implementable via push-down automata, whereas context-sensitive languages require context-sensitive grammars. The semantic dimension initially comprises an incidentally developed sign sequence that acquires significance through selection processes. These signs adhere to natural laws governing neural architecture, thereby reflecting the natural laws expressed by the language of mathematics.

Formal methods facilitate the discovery of language universals, employing two primary procedures: investigating dimensions and principles driven by communicative function, and developing explicit formal languages characterized by defined syntactic categories (Otto Samuelsdorff, 1977). The objective is to render linguistic statements as precise and verifiable as those in the natural sciences, enabling comparisons of diverse grammars within a unified rule framework. Accordingly, syntactic rules incorporate semantic functions, and categories depend on elements' communicative roles. Montague demonstrated that algebraic systems combined with categorial grammar afford a flexible description of any natural language, treating syntax, semantics, and pragmatics as

branches of mathematics. He devised two formal languages, one specifying the lexicon, syntactic classes, and rules necessary for unambiguous interpretation.

Formal language theory provides a framework for quantifying the complexity of computational problems and algorithms (Tecumseh Fitch & D. Friederici, 2012). It originated in the work of Turing and others, constituting a foundational pillar of the theory of computation, alongside computability and problem complexity. The theory underpins numerous practical software tools and everyday concepts, such as search functions embedded in operating systems. The discussion commences with regular expressions—which are equivalent to finite-state machines—and appear in search functions like DOS's dir command or UNIX's ls command. These facilities enable pattern matching within extensive databases by employing syntax that includes wildcards (e.g., the "*" character) to match arbitrary sequences of characters. Regular expressions thus constitute a powerful basis for search, replacement, and related operations in many computer programs.

3.1. Grammar and Automata

The sequence structure of the genetic code may be studied by the classical informatic approach. A similar procedure is applied here to human language. Languages, grammar and machines are interrelated: context-free languages are generated by context-free grammars which are implementable by push-down automata. Context-sensitive languages are generated by context-sensitive grammars. Nucleic acids are arranged according to the molecular syntax of this language (Witzany, 2011).

Comparative linguistics compares words across languages, forming linguistic families and hypothesizing ancestral languages. An alternative approach focuses on morphology and word construction with a state-machine model. Word groups that are phonetically, semantically, or pragmatically related are each associated with a formal language and alphabet using finite automata to decide membership (M Prabhu & Midye, 2023). Panini's system of sounds is employed to construct a phonetic map whose symbols serve as states in the state-machine representation. The distance between words on the phonetic map is measured to gain further insight.

3.2. Chomsky Hierarchy

The linguistic parallels to abstract machines are best illustrated by the Chomsky hierarchy introduced in the 1950s by American linguist Noam Chomsky. Initially assuming that the structure of any natural language could be modeled as a formal grammar, Chomsky formulated models based on finite-state automata, context-free

grammars, and context-sensitive grammars. These models were investigated in terms of their generative capacities, which refer to the kinds of strings or sentences they can produce. Since their inception, these types of models have been extensively employed to represent the hierarchical structures found in natural language, despite their differing capacities to capture linguistic nuance (Esterhuizen, 2008).

4. Probability and Language

A significant development arose from efforts to analyse the probabilities of different words following specific words or occurring in certain contexts. If a particular word is followed by certain words more frequently than expected by chance, the latter are designated as "predictive probability candidates" for the first word. This approach tackles the potential infinity of continuations by reasoning in reverse from the projected start point rather than forwards. Similar concepts in probability theory address the likelihood of sequences of events occurring, a principle that can be applied to sequences of words (Esterhuizen, 2008).

4.1. Bayesian Models

Bayesian approaches for quantitative data analysis have become increasingly widespread within the psycholinguistic community. It has become relatively straightforward to fit complex Bayesian models due to increased computing power and the emergence of probabilistic programming languages. Packages such as brms and rstanarm enable users to specify models using formulae similar to those employed with the lme4 package; the estimation and sampling procedures are, however, implemented in Stan. For researchers more comfortable with frequentist models, these R packages provide an approachable gateway to Bayesian modeling. Some benefits of employing Bayesian methods concern the specification of the random structure. Models including random-slopes parameters with several grouping factors may have convergence issues when fitted with lme4; Bayesian models tend to converge easily or may predict unrealistically high correlations among random effects in the frequentist framework (Nicenboim & Vasishth, 2016). In addition, Bayesian modeling offers the possibility to move beyond the linear model. For example, shifted log-normal hierarchical models can be utilized for reaction times, whereas ordered probit hierarchical models are suitable for ratings. Meta-analyses and Bayesian cognitive modeling constitute promising avenues for applications in psycholinguistics.

4.2. Markov Models

The task of assigning a probability to each sentence, where grammatically correct sentences receive higher probabilities than incorrect ones, is known as language modeling. A language model is typically represented as a vector of parameters, which can be estimated using a training algorithm such as expectation-maximization to determine the parameters that maximize likelihood on a corpus of well-formed sentences (Majewsky, 2017). An n-gram language model bases the probability of a word on the previous n−1 words, estimating probabilities from relative frequencies in a training corpus.

The bigram model, a special case with n=2, estimates the probability of the next word conditioned on the previous word. This model can represent just the vocabulary and a two-dimensional matrix of transition probabilities. Variable-length n-gram models and approximations thereof enable the use of longer contexts within memory and computational constraints. N-gram models are commonly employed in autocorrect systems and predictive keyboards. Hidden Markov models (HMMs) generalize n-grams by incorporating hidden states that influence the emission probabilities of words, making them especially useful in part-of-speech tagging and related tasks. The Baum-Welch algorithm provides an expectation-maximization approach to train the parameters of an HMM from data.

5. Mathematics of Syntax

Mathematics has played an underlying yet significant role in the development of ideas about human language and how we use it. Beyond its theoretical significance, the use of mathematics as a practical tool to process language has advanced the prospects for increasingly sophisticated and user-friendly applications for humans to interface intuitively and effectively with computers. Examples include the use of mathematical principles in analysing quantitatively the patterns people use in determining descriptions of the world and spelling out syntactic rules of language, all which underpin the development of models for human-computer dialogues. Encoding human knowledge in complete and rigorous mathematical form, including that surrounding human language usage, remains an ambition. Ultimately the expression of utterances mathematically would make possible a model of dialogs and a dialogue-management system enforceable by a computer to support intelligent information exchange in one-on-one human-computer interactions.

5.1. Tree Structures

Trees are a widespread representational device in both linguistics and evolutionary biology. Phylogenetic trees, or phylogenies, express relationships among species, and

many mathematical methods have been developed to infer these trees for related species. The resulting phylogenies allow researchers to reconstruct the evolutionary histories of the species concerned. Language families have traditionally been depicted as trees; however, the methods for building these are considerably less formalized. Consequently, techniques for constructing evolutionary trees could serve as valuable tools in historical linguistics.

Languages and species exhibit striking parallels. Both categories are difficult to define, manifesting primarily at the population level, where classification often proves arbitrary or ambiguous. For example, artificial selection has greatly amplified and modified naturally occurring variation within species to yield markedly different breeds of domesticated animals. Chihuahuas and Great Danes remain classified as the same species despite pronounced differences. Similarly, many English dialects differ so profoundly in phonology and syntax as to be mutually unintelligible on first encounter, yet all share a common orthographic system. Social and political factors likewise influence language distinctions, as they may affect biological species delineations. Early classification systems distinguished species primarily by morphological characteristics. Charles Darwin pioneered the evolutionary interpretation of taxonomic hierarchies and championed the use of trees to represent them (vanCort, 2001).

5.2. Dependency Parsing

Dependency parsing constructs syntactic parse trees that describe the grammatical relationships between words (Jaf & Calder, 1970). Dependency parse trees are built over direct relations between tokens; a token depends on another token, as opposed to the ROOT. Based on the dependency relation formalism, projective trees satisfy the property that arcs between tokens do not intersect when the tokens are arranged in the linear order of the sentence, while non-projective trees contain intersecting arcs. Dependency parsing for Chinese adopts the principle that DG only accounts for surface syntactic dependencies while more complex functional and semantic dependencies can be managed by control mechanisms (Yeung Tom Lai & Huang, 1994). Recognition and parsing of linguistically adequate dependency grammars is NP-complete (Neuhaus & Broeker, 1997).

6. Mathematical Semantics

Assuming a language consists of sentences, each of which can be represented as a sequence of words, where each word belongs to a finite set of word classes, a sentence is represented by a sequence of pairs of words and word classes: (w(1), c(1)), (w(2), c(2)), ... (w(N), c(N)), in which the jth word of the sentence is w(j) and its word class is

c(j). Mathematics, particularly formal and cognitive geometry, offers an approach for mapping the symbolic mathematical language of semantics onto natural language. The f model, encompassing three levels of mental representation—conceptualization (C), formulation (F), and articulation (A)—provides a framework for this mapping. Conceptualization defines the target input on the C level, formulation produces a semantic structure represented via mathematical semantics on the F level, and articulation transforms this structure into an output vector on the A level (Esterhuizen, 2008). Mapping from the conceptual to the formulation level can be achieved using cognitive geometry through relations such as the Kuhn, Chew, Chew*, and Akton relations, which are derived from a directed network of mathematical-design world variables within the natural language domain.

Symbol Sequences and Components

Consider the set W of symbols. A symbol sequence s of length |s| is defined as a sequence of symbols s(1), s(2), ..., s(|s|), where each s(i) ∈ W for i ≤ |s|. A symbol-component t of s is similarly a sequence t(1), t(2), ..., t(|t|), where |t| ≤ |s| and each t(j) ∈ W for j ≤ |t|. A component t of s is a component such that t occurs as a consecutive subsequence within s; formally, there exists an index u ≤ |s| - |t| + 1 such that t(j) = s(u + j - 1) for all j ≤ |t|. “Occurs in s” abbreviates “is a component of s.”

Linguistic Structures: Kernels and Shells

The concept of an n-linguistic structure involves sequences of n pairs of symbol sequences arranged cyclically. For each i from 1 to n, consider symbol sequences K(i) and S(i), with the notation indicating that K(i) and S(i) are components of certain cycles formed by concatenating these sequences in a specified order. These arrangements yield a framework for distinguishing between different configurations—notably alternating and stacked n-linguistic structures—which can be represented using a diagrammatic notation referred to as a Y-sentence. In this configuration, K-symbols constitute a “kernel,” while S-symbols form a “shell.” Mathematics thus provides novel tools for applying formal and computational geometry to study the semantic domains of natural language (Shafer, 1992).

6.1. Lambda Calculus

Lambda calculus serves as a formalism for the definition of effective computability and the specification of effective procedures (Esterhuizen, 2008). It can be thought of as a model of computation or a programming language, not dissimilar to the Turing machine model. Lambda calculus originated from the work of Alonzo Church, who introduced it

in the 1930s as part of an effort to formalize the notion of effective computation. It functions as a simple formal programming language designed to specify effective procedures.

Lambda calculus also provides a foundation for formal semantics in terms of function-argument relationships. It offers a means to specify precise semantics for programming languages. Furthermore, the lambda calculus functions as a model of computation that is (mathematically) equivalent to the "Turing machine" model.

The Lambda Calculus defines a language that is extremely simple, yet surprisingly expressive and flexible. Lambda-expressions are constructed from variables according to three (recursive) rules. When used as a programming language, the lambda-calculus is typically augmented with assignment, sequencing, and a conditional construct. It is common to further extend the language by allowing a definition construct and a facility for local scoping of variables. Such an augmented language is often referred to as the "applied lambda calculus".

6.2. Model Theory

Model theory, as a branch of mathematical logic, contributes to mathematical linguistics by defining the interpretation of formalized linguistic objects within an axiomatic system. Such interpretation involves assigning a set-theoretic construct from a hierarchical universe to a formula in a formal language, thereby associating truth-values with linguistic statements organized as axioms and theorems within that system (Esterhuizen, 2008).

7. Computational Models of Language

Mathematical linguistics bridges the sphere of linguistic inquiry with formal methods. While both linguistics and mathematics prenatally rely on intuition, mathematics welcomes quantification, and formulates linguistic intuitions stringently in the process of theory construction. Turning from historical origins to linguistic modelling, the field is exemplified by Haskell's plinth and Frege's foundational work on sense and reference.Language processing without comprehension and production is of no practical use. Computer science is therefore concerned with facsimilating linguistic and psychological accounts of production and comprehension processes. The computer makes it possible to specify large sets of linguistic rules with their interactions and interdependencies, while parsing models that allow for structural ambiguities are experimentally tested on large corpora.

OLED as a new light source of the next generation has gained considerable attention as a promising candidate for a large-area and highly efficient light source applied for full color flat panel displays or solid state lighting. In order to improve the performance of OLEDs, several methods have been proposed: (i) development of new light emitting materials, (ii) device structures, and (iii) increasing the out-coupling efficiency. Especially, the realization of full color flexible displays for the next generation display has been focused on flexible OLEDs on plastic substrates. The nonlinear quantum theory of open systems must be one of the best theories that can describe the physical properties of OLEDs, which can be modeled by a fully quantum-mechanical approach. As one of the successful approaches, dissipative space has formulated the quantum theory of open systems. The theory has been successfully used to interpret luminescent and conductive properties of complexes or molecules in various materials, including liquid, solid, and powders.

7.1. Natural Language Processing

Efforts to mechanise natural language date back to the 1950s and remain difficult and challenging. Progress has accelerated dramatically in the last ten years (Schöneberg & Sperber, 2014). Natural Language Processing (NLP) is a powerful machine-learning approach to semiautomatic speech and language processing, applicable to mathematics. Well-established NLP methods must be adjusted for the special needs of mathematics, in particular for handling mathematical formulae. A mathematics-aware part-of-speech tagger demonstrates the adaptation of NLP methods for mathematical publications. The tools developed are used for key-phrase extraction and classification in the database zbMATH.

Mathematics describes the real world, abstract structures, and itself. It originated to describe and solve real-world phenomena and is used in physics and engineering. Pure mathematics deals with abstract structures, some of which model physics. Mathematics also describes itself through metamathematics. Some researchers suggest that language is fundamental to human cognition and that mathematical structures are linked to language. The finite number of words and symbols on hand enable the generation of an infinite number of sentences and mathematical ideas. Language facilitates thinking, reasoning, and expression, and different languages may influence thought patterns (Esterhuizen, 2008).

7.2. Machine Learning Approaches

Content analysis of scientific publications is a useful task for scientific information services. In the digital age, machine-based methods such as graph analysis tools and

machine-learning techniques have been developed for this purpose. Natural Language Processing (NLP) is a powerful machine-learning approach to speech and language processing, which can be applied to mathematics. The well-established methods of NLP have to be adapted for the special needs of mathematics, particularly for handling mathematical formulae. A mathematics-aware part of speech tagger has been developed, and NLP methods have been adapted for mathematical publications. These tools are used for key phrase extraction and classification in the database zbMATH (Schöneberg & Sperber, 2014). A great deal of work has been done demonstrating the ability of machine learning algorithms to automatically extract linguistic knowledge from annotated corpora. Very little work has gone into quantifying the difference in ability at this task between a person and a machine (Brill & Ngai, 2001).

8. Mathematical Linguistics Applications

The relevance of Linguistics to Mathematics is chiefly revealed by an overview of significant linguistic applications of mathematics. Mathematical linguistics, computational linguistics, and the mathematics of language can serve as an initial framework. Mathematical linguistics focuses on the mathematical description of the properties of particular languages or general linguistic principles (Esterhuizen, 2008).Computational linguistics, which overlaps considerably with mathematical linguistics, relies on quantitative descriptions of language or linguistic phenomena rather than qualitative ones. The mathematics of language, on the other hand, concerns mathematical abstractions of natural language independent of particular content and is intimately linked with formal language theory or automata theory. Other applications include aiding in the search for an ideal semantic metalanguage, supporting the design of writing systems and typefaces, conducting phoneme surveys, modeling syntax, illustrating principles of information theory, and studying literary style, authorship, and reception.

8.1. Information Theory

Information theory is a mathematical theory of communication devised by Claude Elwood Shannon. The theory provides the underlying framework for a quantitative linguistics. The phenomenon of human language communication can be viewed from different perspectives, leading to various mathematical models. One perspective investigates how humans understand individual sentences, involving theories of phonology, morphology, syntax, automata, formal languages, and semantics, primarily using discrete, non-quantitative models. The other perspective examines how sentences are chained into texts and discourse, analyzed through quantitative linguistics or corpus linguistics, which has not yet established a comprehensive mathematical framework.

Influenced by probabilistic modeling, mathematicians such as Shannon have contributed concepts that underpin the field.

Information theory is guided by deductive principles. It prescribes a discriminative process of uncertainty reduction, whereby communication reduces a receiver's uncertainty about a message using a code designed to maximize discriminability while minimizing signaling costs. Unless the way natural languages converge on shared probabilistic models can be explained—models that define information in human communication—the analogy between language use and information theory remains largely meaningless. The distributional structure of personal name systems across languages closely aligns with information theory predictions, and appears to evolve socially to meet communicative challenges posed by incomplete human codes. Studies have shown a reliable association between word frequency and length, supporting the idea that natural language resource allocation is influenced by informativeness.

Mathematics serves as a tool for investigating language and genetic codes, and as a depiction of the material reality to which both belong, including the Universal Grammar (UG) that all languages share. Formal-language theory not only explains the evolution of human language but also underlies UG—which determines the rules of syntactic structures. Noam Chomsky's concept of Universal Grammar represents the inner logic of nature, linked to neuronal networks in the brain that operate according to natural laws. These laws can be analyzed mathematically. Languages, grammar, and machines correspond: context-free languages are generated by context-free grammars and implemented by push-down automata, whereas context-sensitive languages are generated by their respective grammars. The natural laws governing the universe are expressed mathematically. The semantic aspect of language involves sequences of signs that acquire significance through natural selection, with linguistic signs influenced by the brain's neuronal architecture (Dębowski, 2011) (Ramscar, 2019) (Witzany, 2011).

8.2. Network Theory

Network theory is recognized as a key discipline for the study of the relational nature of human language at all levels (semantics, syntax, morphology and phonology) (V. Solé & F. Seoane, 2014). From a semantic point of view, network building consists of eliciting a series of proto concepts (usually relying on some blog or dictionary) that are associated to other concepts as linked nodes. These semantic relations such as isa, part-whole or opposition determine connections to other concepts which play the role of nodes. Mental concepts (perceived as units of thought) emerge from such interconnected relationships. Semantic networks exhibit a scale-free, small-world topology in which most elements—usually linguistic units—are highly specialized—i.e., they have a small number of

links—and few have a very high connectivity. This arrangement is well suited to account for the widespread presence of polysemy in languages, given that heterogeneity combined with very short average path lengths facilitates rapid association between one or more meanings of the word and the neighborhood. From a global perspective, language complexity and universality can also be captured through network analysis. Core universal patterns appear as key building blocks of human language organization. Statistical studies show that universal network traits influence the dynamics of language communication and evolution. Those patterns have to be ingrained at a neural level—i.e. neural assemblies reflect universal traits—imposing relevant physical constraints on language. Once those restrictions are set, the eventual emergence of ambiguity and polysemy owes its presence to the relentless drive for increased communication efficiency.

9. Challenges in Mathematical Linguistics

Mathematical linguistics faces formidable hurdles similar to those encountered in the axiomatization of mathematics itself. At a formal level, an axiom is merely a string of symbols that only acquires meaning in the framework of all formulas derivable within a given axiomatic system. Hilbert's program aimed to establish a firm axiomatic foundation for all mathematics, yet Gödel's incompleteness theorem proves that every sufficiently powerful axiomatic system contains undecidable formulas, rendering a definitive axiomatization impossible. Although mathematics is often conceived as set theory formulated within some axiomatic system, permitting the expression of every statement or proof as a set-theoretic formula, the ambition of a completely axiomatized mathematical linguistics remains elusive (Esterhuizen, 2008).

Mathematical structures and methods relevant to linguistics constitute the primary concerns of mathematical linguistics. The discipline's internal organization often mirrors that of general linguistics, encompassing traditional subdivisions such as phonetics, phonology, morphology, syntax, and semantics. The fundamental conceptual framework, particularly the concept of hierarchical structures composed of stable recurrent elements, originated chiefly in the analysis of phonological and morphological phenomena. Chomsky introduced models corresponding to finite-state automata, context-free grammars, and context-sensitive grammars or unrestricted rewriting systems. The interrelations among these models are examined under the notion of generative capacity, which serves as the foundation of formal language theory in computer science.

9.1. Ambiguity in Language

Ambiguity is a fundamental property of language, thought, and reasoning. Certain phenomena exhibit high levels of ambiguity, complicating analysis. As certain categories grow larger, they tend to absorb outlying members from smaller categories. Slang tends to acquire almost all the outlying members of a language, particularly ephemeral language, whose force and impact on thought and meaning are staggering. Mathematical objects may be difficult to specify; they exist indifferent to our desires and normal modes of thought. Elements tend to be absorbed unpredictably, and elements frequently oscillate between categories. One hundred years ago, most new scientific papers, including those on linguistics, could be addressed to individuals, and personal handwritten letters were a medium holding a majority. Currently, even an unassigned student accumulates dozens or hundreds of e-mails weekly, many requiring leading figures' attention, a multiplication that had become almost exponential ten years ago. Mathematically, this indicates that the number of messages multiplying at an exponential rate will soon surpass all known systems' capacity. It is more convenient to talk about “ambiguity” than “am¬biguities,” as numerous language and thought types group with multiple subjects and predications, and many each associate with several related types. In the language of sets, it is challenging to maintain a one-to-one correlation between such pairs; another one-to-one restriction is to limit the same element to appear in only one pair. Lambrp (1973) stated, “If a string Babylon is found in a language, then (1) Babylon by itself, (2) Babylon and the next word, and (3) Babylon and one or more preceding words will also be found in the corpus.” These conditions frequently resemble similar but less likely conditions of contiguous sub-strings. A two-element sequence would have every 2-element sub-string occurring at least once; a strict sequence of 2 elements would mean that every two-letter sub-string occurs. High ambiguity is a major means of information storage, whereas low ambiguity relates to high information. (Esterhuizen, 2008)

9.2. Complexity of Language Models

Language remains an extraordinary trait of the human species; a sophisticated model of complex signals organized in time that conveys explicit meaning and allows coordination and communication among members of society. Beyond a direct survival function, the use of language also allows people to express feelings and the way in which they perceive the world, and is crucial for the development of abstract ideas. Transcript language facilitates the evolution of civilization and culture, which strongly depends on the ability to understand and share concepts with others. This makes language the most profound cultural artifact and a key factor in human development (Stanisz et al., 2024). Language is a complex structure shaped by the interaction of individual components; a multifaceted phenomenon that typically attracts the interest of a variety of disciplines, each with its own focus, theoretical foundations, techniques, and goals. Because no single discipline can comprehensively understand the broad scope of human language, it is crucial to

preserve bridges that guarantee a healthy exchange of ideas to drive progress in each contributing research field. When considering the wide range of potential disciplines, mathematics and physics are well suited to collaborate with traditional fields as the level of abstraction and the analytical capabilities they offer can be applied to human language with great effect.

The complex-system approach incorporates concepts, tools, and models from statistical physics and offers a set of ideas, methods, and also interdisciplinary space in which any field dealing with complex systems, including quantitative linguistics, can fit. Language is conceptualized as a complex system where a large number of interacting elements organize solely or mainly by their mutual interaction. As a complex system, it displays properties such as hierarchical structures of different scales, long-range correlations, fractality, and the occurrence of power laws. Terminology and methodology from statistical mechanics, stochastic processes, multifractal analysis, and network theory are generally used for describing human language from a complex-system viewpoint.

Despite the high phenomenological complexity of human language, related quantitative studies are practically nonexistent. Bridging quantitative linguistics and complexity research remains very challenging and constitutes a truly open problem. Quantitative information obtained by statistically analyzing the structure of language and its dynamics is at the heart of many contemporary quantitative linguistic studies and carries fundamental motivation to investigate the observed properties in terms of underlying processes. Quantitative characterization of language evolution is difficult and rarely attempted but imperative for advancing our understanding of communication by human language. Interdisciplinary thinking is crucial for a broad and deep insight into the multifaceted phenomenon of human language. Language is connected to human civilization and has a decisive impact on global development that is already at the stage of directed intentional engineering with timely and increasing importance that is expected to grow further. Quantitative investigation focused on uncovering fundamental casual relations and efforts to formulate elementary theoretical principles of natural language equip contemporary linguistics and language technology with a firm and testable analytical basis. Quantitative research aimed at discovering new laws and patterns present in language with applications to language technologies represents a breakthrough in our understanding of human language. Recognizing quantitative aspects, the organization of natural languages offers the implication that the complexity and diversity of all aspects concerning natural languages should originate from a small number of quantitative patterns. The potency of a single organizing principle behind this complexity opens a new set of challenges about democratization, equality, and human development. Research aimed at discovering hierarchies of language models and at relating different models to universal laws represents a crucial step in this direction.

10. Future Directions in Research

As the interplay between human language and mathematics continues to be studied and revealed, the breadth and depth of the relationship between the two domains encourages ongoing and future investigation. The relationship between next-word probabilities and human brain activity shows the involvement of information processing in language comprehension. The parameters of language models consistently exhibit correlations with those in brain networks, suggesting that consistent representation of brain networks is an intrinsic property of language-comprehension processes in the human brain. Successful forecasting of brain activity from a small number of model parameters further indicates that these parameters contain important information related to the language-comprehension process that is embedded in the brain's physiological activity. Despite the discovery of inherent correlations between the representations of brain networks and the parameters of sophisticated language models, the full interpretability of these parameters remains elusive. Future research should thus aim to unravel the exact information comprehended by the human brain and captured by the model parameters.

10.1. Interdisciplinary Approaches

Human language is not only a complex and inspiring human phenomenon but also a subject attracting multidisciplinary mathematical studies (Esterhuizen, 2008). The fields of physics, mathematics, biology and computer science contribute certain useful concepts, models and tools to the investigations of the origin, evolution and dynamics of language. The efforts of theoretical linguists also inspire new mathematics, physics and statistical methods, observation and experiments have indicated certain regularities and patterns in human languages.

10.2. Advancements in AI and Language

The growth of internet-based content over the past few decades has been massive. The vast information storehouses on the web have invigorated research in information retrieval, information extraction, data mining and natural language processing. For example, many Web services rely on information extraction technologies to improve retrieval experience and connect users with related content in a more meaningful way. As a result, there is a growing need for automated procedures that aid individuals in locating and navigating appropriate materials by content. The focus here, however, is not on information retrieval per se, instead of this challenge, the language content of Web pages is studied and the question of whether one can identify, purely based on the content of a web page, the language in which that page is written is addressed. There are many applications for such a tool. Search engines and tools for organizing or labeling web

pages would gain a valuable feature if they were able to determine the language of the documents they process (Esterhuizen, 2008).

11. Case Studies

Mathematics plays a pivotal role in the study of human language patterns. This connection is evident when analyzing written textual communication where, under certain circumstances, disturbances to preexisting or conditioned language patterns manifest as combinations and permutations of mathematical structures. Consequently, spontaneous language behaves as a state vector with evolving state coefficients. When this formalism is applied to docs by various authors, it becomes apparent that spontlog, or spontaneous language, is multifaceted with either too few or too many degrees of freedom. Both characteristics are exploitable in the analysis of human language patterns (Esterhuizen, 2008). For instance, knowledge of the mathematical foundations that underpin language patterns has been shown to enhance the financial ratios of companies in the USA by up to 20% behind the scenes. This effect is even more pronounced when applied to large volumes of data, such as that handled by governmental institutions. Similar analyses also extend to human language where it is believed that human thought processes are communicated instantaneously through speech to multiple listeners. As a result, a single speaker who addresses multiple listeners simultaneously will effectively be generating multiple-state configurations.

11.1. Language Processing Systems

The rise of computers has had a vast influence on our lives and especially on linguistics. One of the many branches of linguistics that have benefited from computer technology is natural language processing. Natural language processing is a bright new field in linguistics that almost exclusively depends on mathematics, and the aim of this chapter is to highlight the ways in which mathematics and computer programming help linguists refine the understanding of linguistics and language in general. A natural language processing system is one of the few linguistic models that has been successfully implemented in programming. Although the idea has been around for some time, the implementation aspect has only gained momentum within the last couple of years. To fathom the usefulness and variety present in the natural language processing field, it is important to first comprehend what a natural language processing system actually does.

A natural language processing system is a program that receives natural human language as the input and returns some type of response based on that input. The goal is to provide the system with enough competence to supply a satisfying and logical response for any sentence of reasonable length and complexity. The system consists of five components:

a decoder, an interpreter, an evaluator, an output generator, and a feedback generator. The flow of information is mainly linear starting with the decoder, which receives the initial input and provides the other components with the function words, the content words, and the general structure of the sentence. The interpreter then takes that information to discover the specific meaning of the sentence and to link the different parts together. Based on these findings, the evaluator generates a set of responses, which will later be refined by the output generator to a single output. The feedback generator creates questions and suggestions that are used to clarify parts of a confusing sentence. The first stage of a natural language processing system consists of the decoder, whose task is to separate a sentence into its constituent groupings and labels and to determine the type of sentence. The information provided to the decoder is an initial sentence, which can either be typed into the system by the user or be provided by a file supplied to the interpreter. This dependency of components is the reason the decoder only provides the other modules with a sentence and never receives any.

The decoder starts out by dividing the input into words and separating those words that are clearly marked as function words. This means that punctuation or any other form of direct marking is used to determine if a word is a function word or not. The remaining function words go through a second separation process, where the program decides if the remaining function words belong to the same group or not. This separation process occurs before the assignment of binding information, parts of speech, or ELAG (EBL active grammar) tags (Esterhuizen, 2008). Once the remaining function words have been teased apart, the composition stage takes over in an attempt to regroup some of these words.

11.2. Real-world Applications

Mathematical linguistics, formal language theory and computational linguistics have important real-world applications. Natural language processing is used in information extraction in electronic monitoring of newspapers and the World Wide Web, reading machines for the blind, scanning for credit card fraud, and so on. Understanding the basic principles of language is also relevant to the challenge of getting robots to interact usefully with human beings.

Consider a crime reporter who tracks down the occurrences of various individuals on the World Wide Web and other data sources. Instead of simply locating mentions of the role of a person, it might be necessary to know whether the person is speaking about the role, or if it appeared in a direct quotation, or was just casually mentioned by the author without the person really expressing that viewpoint.

Because the primary source of information for language technology applications comes in the form of large collections of unstructured or semi-structured documents, text mining and knowledge discovery in databases are potentially valuable techniques in many problem domains. There are numerous sub-tasks within Natural Language Processing, and most realworld applications require a combination of these varied tasks and analytical methods in order to generate useful results. Existing solutions are often composed of a combination of technologies and modules from different sources, whereas a single platform is desirable to provide a robust flexible environment for the rapid development of applications (Esterhuizen, 2008).

12. Conclusion

Human language and psychology are complex phenomena whose underlying mechanisms remain largely unknown. Recent theories, linguistic and non-linguistic, have enhanced understanding, yet much complexity remains to be explained. Mathematics offers essential tools that underpin much of scientific investigation (Esterhuizen, 2008). In particular human language, the argument is developed that analytical language is dependent on the logarithm and that all human regression is logarithmic. The processes are described by which non-human communication transforms into language with syntax, and is consequently related to the logarithm.

References

Esterhuizen, H. L. (2008). Linguistics + Mathematics = twins.

Neubig, G. & Dyer, C. (2016). Generalizing and Hybridizing Count-based and Neural Language Models.

Junczys-Dowmunt, M. (2008). Wprowadzenie do metod statystycznych w tłumaczeniu automatycznym.

Shafer, K. (1992). Learning Mathematics as a Language.

Witzany, G. (2011). Can mathematics explain the evolution of human language?.

Otto Samuelsdorff, P. (1977). On describing determination in a Montague grammar.

Tecumseh Fitch, W. & D. Friederici, A. (2012). Artificial grammar learning meets formal language theory: an overview. ncbi.nlm.nih.gov

M Prabhu, S. & Midye, A. (2023). Linguistic Analysis using Paninian System of Sounds and Finite State Machines.

Nicenboim, B. & Vasishth, S. (2016). Statistical methods for linguistic research: Foundational Ideas - Part II.

Majewsky, S. (2017). Training of Hidden Markov models as an instance of the expectation maximization algorithm.

vanCort, T. (2001). Computational Evolutionary Linguistics.

Jaf, S. & Calder, C. (1970). Deep Learning for Natural Language Parsing.

Yeung Tom Lai, B. & Huang, C. (1994). Dependency Grammar and the Parsing of Chinese Sentences.

Neuhaus, P. & Broeker, N. (1997). The Complexity of Recognition of Linguistically Adequate Dependency Grammars.

Schöneberg, U. & Sperber, W. (2014). POS Tagging and its Applications for Mathematics.

Brill, E. & Ngai, G. (2001). Man [and Woman] vs. Machine: A Case Study in Base Noun Phrase Learning.

Dębowski, Łukasz (2011). Excess entropy in natural language: present state and perspectives.

Ramscar, M. (2019). Source codes in human communication.

V. Solé, R. & F. Seoane, L. (2014). Ambiguity in language networks.

Stanisz, T., Drożdż, S., & Kwapień, J. (2024). Complex systems approach to natural language.

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Chapter 16: Simulation and Control of Infectious Disease Spread Using Compartmental Models

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Abstract: Understanding and controlling the spread of infectious diseases is vital to public health planning and intervention strategies. This paper presents an in-depth study of compartmental models—such as the SIR (Susceptible-Infected-Recovered), SEIR (Susceptible-Exposed-Infected-Recovered), and SIS (Susceptible-Infected-Susceptible) frameworks—to simulate and analyze the dynamics of disease transmission. These models are grounded in mathematical epidemiology and provide a simplified but effective representation of real-world infectious disease progression. The simulation of compartmental models using differential equations allows for predictive analysis of infection peaks, reproduction numbers (R_0), and potential epidemic outcomes under various scenarios. The study emphasizes the significance of parameter estimation, such as contact rate and recovery rate, and their impact on the model's accuracy. Control strategies such as vaccination, quarantine, isolation, and social distancing are also examined by incorporating them into the basic models, allowing for an assessment of their effectiveness in reducing disease transmission. Real-world case studies, including outbreaks like COVID-19 and influenza, are simulated using these models to illustrate their practical relevance and policy implications. The paper also discusses the integration of data analytics and computational tools for improving model reliability and real-time forecasting. Challenges in data availability, parameter uncertainty, and model limitations are acknowledged, suggesting directions for future research in hybrid and stochastic modeling.Overall, the paper underscores the critical role of mathematical modeling in understanding epidemiological trends and guiding evidence-based public health interventions.

Keywords: Compartmental Models, Infectious Disease Simulation, SIR and SEIR Models, Epidemiological Control Strategies, Mathematical Epidemiology.

Introduction

The modeling and simulation of infectious disease spread and the development of effective control policies constitute a fundamental challenge with wide-reaching implications. Compartmental (population) disease models continue to serve as core constructs that support the formulation of more refined models and inform decision-making regarding mitigation and intervention strategies. A diverse range of mathematical approaches exists for simulating infectious disease propagation and the dynamics of susceptible populations, each suited to particular scenarios. Central to these methodologies are the compartmental model and differential equation approaches, both of which can incorporate stochastic and deterministic elements. Other prominent techniques include the multi-agent approach and betweenness methods. The remainder of the manuscript concentrates on the compartmental model, which, while widely used, is often presented in a cursory manner in the literature.

2. Overview of Infectious Disease Models

Infectious disease modelling aims to represent and predict epidemic dynamics in different societies, studying transitions between health statuses and absorbing the effects of individual-level characteristics and population mixing properties. The choice of model depends on the characteristics of the population and disease, intervention implementations, available data, and required accuracy (Campillo-Funollet et al., 2021). Compartmental models simplify, grouping individuals into time-dependent compartments, such as susceptible, infected, and recovered (SIR) and susceptible, exposed, infected, and recovered (SEIR), and have been widely used since the early work of Kermack and McKendrick (Zachreson et al., 2022). Due to the high dimensionality of these systems and the scarcity of statistical information for parameter estimation, computational approaches complement analytical studies.

Compartmental models are popular for their tractability and small parameter space; their ordinary differential equation (ODE) derivations enable analysis tools and facilitate numerical investigation, but the specification of transmission and recovery processes limits their flexibility and realism. Model assumptions about disease dynamics, for example an exponential distribution of generation intervals, may disagree with empirical real-world evidence. Moreover, the same ODE system can describe distinct diseases with different transmission pathways (Campillo-Funollet et al., 2022) , necessitating phenomenological interpretation. Additionally, the homogeneity of the population fails to account for properties such as age, immunity level, co-infections, or asymptomatic cases, which affect the infection rate; spatial and social mixing heterogeneities influence transmission rates as well. In the classic Kermack-McKendrick formulation, the population is splitting into the time-dependent classes of susceptible, infectious and removed, with a total population size that remains constant. The model concentrates on

the evolution of the susceptible and infectious proportions of the population, driven by the rates of transmission and removal. The extent of an epidemic and other key quantities, such as the basic reproduction number R_0 and the exponential growth rate, may be also calculated and used for forecasting and assessing the impact of the control strategy.

2.1. Compartmental Models

Compartmental models are among the most commonly used frameworks for modeling infectious diseases in epidemiology. These models divide a population into compartments or states, with transition between compartments mediated by different parameters. Over time, compartmental models have been enhanced by coupling them with complex networks that capture the heterogeneity of interactions, with diffusion processes that account for mobility patterns, and by considering behavioral factors that influence the acceptance of interventions. Recently developed models consider the early detection and isolation of infectious individuals through testing and contact tracing to slow transmission, exploring the effect of limited testing resources on epidemic control (Campillo-Funollet et al., 2021). In addition to the well-known epidemic transition occurring when the basic reproduction number exceeds one, a second transition arises that depends on the system's maximum detection capacity. When the reproduction number surpasses a critical value linked to this capacity, the disease spreads freely. This framework helps determine the detection resources and confinement measures needed to control outbreaks and can be adapted to more detailed compartmental models.

Most commonly, compartmental models are solved as initial value problems for systems of ordinary differential equations. In contrast, observed data often resemble a boundary value problem: some dependent variables are observed at specific times without knowledge of initial conditions. Reformulating the classical Susceptible-Infectious-Recovered system in terms of the number of detected positive infected cases at different times yields a boundary value problem. Existence and uniqueness of a solution can be established, and a numerical algorithm enables its approximation.

At the other end of the computational complexity spectrum, models explicitly consider the state and behavior of every individual. Compartmental models treat the population as an ensemble of indistinguishable entities of each compartment. The Susceptible-Infectious-Recovered model specifies time-dependent infection rates, determined by the current numbers of susceptible and infected individuals, at which single susceptible entities become infected and single infected entities recover, respectively. Such models are sufficiently simple to be evaluated, simulated, and fit to data with relatively small computational effort (Zachreson et al., 2022). Two pervasive critiques question the faithfulness of these assumptions to real-world transmission. The first relates to the

underlying dynamics. Empirical data indicate that the actual generation interval distribution (interpreted as the distribution of time to transmission) of most diseases differs from the exponential distribution inherent in Susceptible-Infectious-Recovered and related compartmental models, suggesting that the dynamics are often incorrectly modeled. The second critique focuses on assumptions of individuals' epidemiological states. Complex, multiscale social systems feature multiple sources of heterogeneity in susceptibility, infectiousness, and contact patterns that compartmental models neglect by treating large numbers of entities as homogeneous (Lamata-Otín et al., 2023). Attempts to incorporate non-Markovian characteristics into these systems rarely address underlying heterogeneities in state or edge attributes. The simplicity that defines the strengths of compartmental models simultaneously limits their capacity to accurately represent detailed epidemic processes that unfold on networks or within populations consisting of interacting subpopulations exhibiting heterogeneity in terms of contact, demography, or behavior.

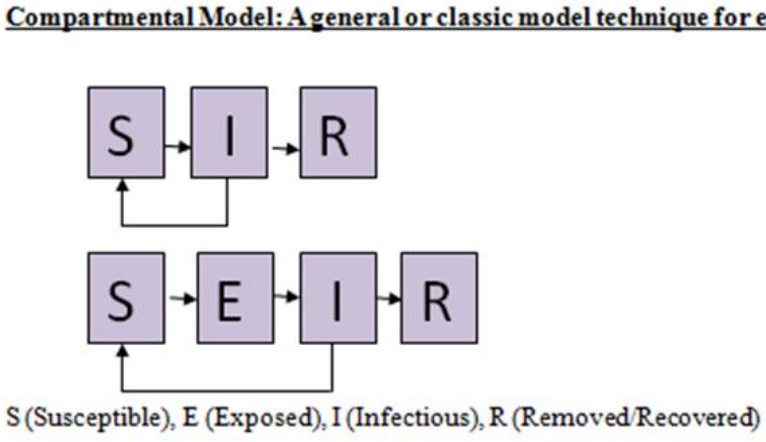


Fig.1. Compartmental Models in predicting COVID-19 outbreaks

2.2. Agent-Based Models

Agent-based models (ABMs) simulate events at the individual-agent level, where agents are autonomous entities operating under a set of rules that dictate their actions and interactions with other agents and their environment. Represented as individuals, organizations, or broader entities such as nation-states, agents can perform simple movements or engage in complex behaviors including social interactions and information searching (Hunter et al., 2018). ABMs track the states and locations of each agent over time, enabling the study of spatial and spatio-temporal patterns often inaccessible to compartmental models. Their capacity to incorporate complex agent-

level dynamics makes ABMs a valuable complement to simpler population-level models (Doussin et al., 2021). The computational expense of ABMs is an important consideration in model selection and design: detailed analyses of spatial spread or super-spreader events favour ABMs, while demographically stratified local spread can often be adequately captured using compartmental models.

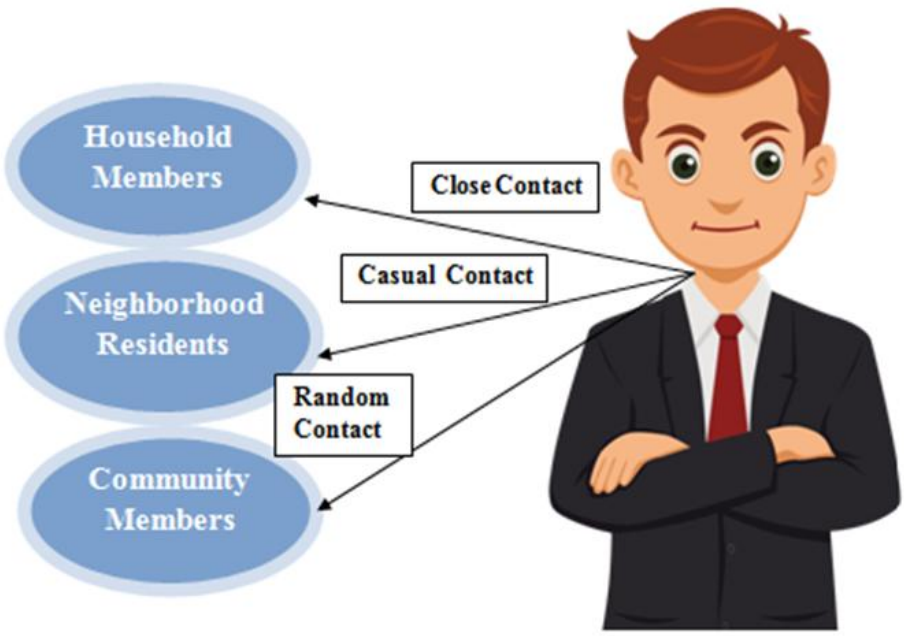


Fig.2. Agent Based infectious Disease Model.

2.3. Network Models

Directly associating a unique link to each contact leads to the concept of networks, where individuals are represented as nodes and their contacts as edges (C. Miller et al., 2011). Networks can be constructed to capture the interaction structure of an urban system, encompassing both static features such as the spatial distribution of metropolitan areas and dynamic characteristics like changing daily travel patterns. Epidemiological models can then be deployed on these networks to generate time series data for infectious and susceptible populations (Zachreson et al., 2022).

Network models with compartmental structures have been used extensively, and more generalized approaches are being developed. While variations of the SEIR framework have been applied to network models, during the mid-eighties the Kermack–McKendrick

equations offered an alternative to the SEIR models. Network models have also successfully described the spread of SARS in Hong Kong, as well as other diseases.

Building network models requires substantial effort over time, along with extensive empirical information and high computational resources;. The resulting models, although more realistic, are often less efficient and less interpretable than metapopulation formulations based on compartmental systems of ordinary differential equations since they involve large-scale simulations. Variations of the SEIR model have proved helpful by providing features sufficiently accurate to assist medical professionals in understanding the evolution of an epidemic and identifying the most effective control strategies (Carlson, 2016).

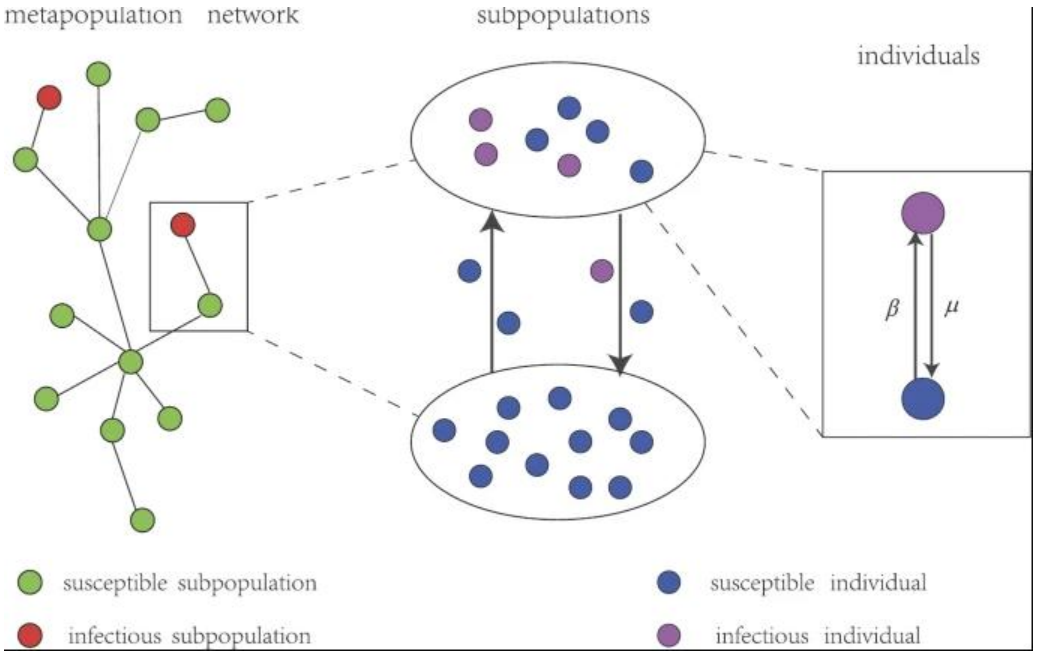


Fig.3. A metapopulation network model of SIS infections with individuals' mobility. (Shanshan F, and Zhen J. 2018)

3. Mathematical Foundations

Infectious diseases propagate as infected individuals transmit a disease to susceptible individuals, who become infected themselves. Mathematical formulations of infectious disease spread typically consider only the susceptibles, infectious, and recovered (immune) individuals within a population. Thus, population members exist in one of three "compartments:" susceptible, infectious, or recovered (Campillo-Funollet et al., 2021).

The movement of population members between each compartment is described by a system of first-order ordinary differential equations. The governing differential equations and initial configurations define an initial value problem that can be solved numerically by standard time integration and root-finding methods.

Compartmental models are popular in the mathematics of epidemiology for their simplicity and wide range of applications. Although typically solved as initial value problems for a system of ODEs, the observed data are often akin to a boundary value problem because some dependent variables are observed at given times, but the initial conditions are unknown. To address this, the classical SIR system has been reformulated in terms of the number of detected positive infected cases at different times. The existence and uniqueness of a solution to the derived boundary value problem have been proven, and a numerical algorithm to approximate the solution has been presented.

3.1. Differential Equations

Compartmental models are characterized by a set of compartments tracking the number of individuals in each state of infection. When movement of individuals between compartments depends solely on the number of individuals within each compartment, the dynamics may be described by a system of ordinary differential equations (ODEs). The models may contain a susceptible population (S) at risk of infection, an exposed population (E) that is infected but not yet infectious, an infected population (I) that is actively infectious, a recovered compartment (R) that is immune to further infection, and a death compartment (D) that has died from the disease (Grave & L. G. A. Coutinho, 2020). The control then consists of the movement of individuals between compartments, which may be manipulated to reduce the overall number of infections or deaths (Campillo-Funollet et al., 2021).

3.2. Stochastic Processes

Stochastic methods provide a means to describe the behavior of epidemic models without invoking stationarity assumptions. One approach is to conceptualize an epidemic as either a discrete or continuous-time Markov chain, which are both formulated under the assumptions of constant force of infection and the sojourn times in compartments described by exponential distributions (Hernandez-Suarez et al., 2022). Developing an understanding of these Markov chain epidemic models is important because simulation algorithms for sophisticated stochastic epidemic models are typically formulated in terms of the underlying continuous-time Markov chains (J.S. Allen, 2017).

Another class of stochastic epidemic models gives the number of individuals in each compartment as a system of random variables satisfying a system of stochastic equations. Such systems are usually taken as stochastic differential equations or ordinary differential equations perturbed with noise, but they can also be normalized set-valued Markov processes as well. Several aspects of epidemic dynamics can be studied with such models, including steady-state fluctuations around deterministic equilibria of the

model, extinction times, the problem of statistical inference, and epidemic shape and duration.

4. Key Compartmental Models

Compartmental models serve as a robust mathematical framework for simulating the spread of infectious diseases. Generically, such a model divides a population into groups (or compartments) distinguished by their disease status: susceptible, diseased, recovered, etc. Transitions between compartments are represented by an underlying continuous-time Markov process. The most straightforward variant is the Susceptible-Infectious-Removed (SIR) model, in which persons begin in the Susceptible group and are transferred to the Infectious then Removed groups as a result of illness. The model assumes that each person remains in the removed group permanently. This framework can be further elaborated to accommodate more disease-specific considerations; for instance, a Susceptible-Exposed-Infectious-Removed (SEIR) model adds an intermediary Exposed group for persons in the disease incubation period who have not become infectious.

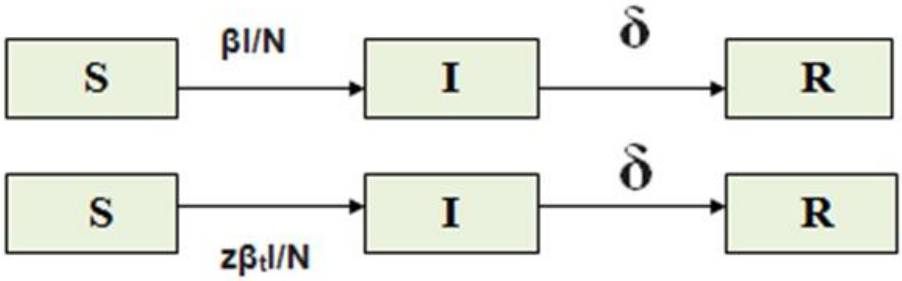
Assigning values to model parameters that is reflective of the real-world location and disease under study produces a probabilistic simulation of the disease spread in that particular situation; the resultant data are instrumental in epidemiological studies. When a control input vector is defined also, for instance representing the number of administered vaccines or the extent of imposed travel restrictions, the model can be interpreted as a state-space model for the underlying stochastic dynamic system, thereby lending itself to analysis and control via the arsenal of optimal control theory.

4.1. SIR Model

The SIR compartmental model provides one of the simplest frameworks for describing disease spread through a population. Individuals are assigned to three classes: susceptible (S), infected (I), or recovered (R). At the beginning of an epidemic, the population typically contains a few infected individuals and a remainder that is susceptible, with no one recovered. Susceptible individuals may then acquire the infection through contact with an infected individual; infected individuals later recover; and recovered individuals remain immune. The process continues until no infected individuals remain and the epidemic abates (Hollister, 2018).

The approach follows the construction of a SIR compartmental model by considering the temporal variations that alter the count of individuals in each class. Many fast-moving diseases are well suited to the SIR model. In mathematical terms, a fixed population that has never been affected by the disease is considered. Only interactions between susceptible and infected individuals move people from the susceptible to the infected compartment. After entering the infected compartment, each individual

proceeds through the disease. Individuals who have recovered are considered immune and do not transition back to the susceptible compartment (Wilkinson & Roper, 2020). The assumption of immunity is a reasonable one for many diseases of interest, such as influenza. Formally, the model considers a population of size N composed of the three groups (S, I, and R) for which S + I + R = N at any given time. The central assumption is that the population through which the disease spreads is well-mixed. While real populations include heterogeneities in contacts, the simple continuous SIR model nevertheless approximates a model which includes heterogeneous contacts and fits various datasets well.



Classical & Modified SIR Model

Fig.3. The classical SIR model was fitted to observed total (I total), active (I) and removed (R) cases of COVID-19 before lockdown to estimate the basic reproduction number. Transmission coefficients are β and z.

4.2. SEIR Model

The SEIR (Susceptible, Exposed, Infected, Removed) model, an extension of the SIR model, incorporates an additional compartment, exposed, representing the incubation period of the disease. Formally, the population is divided into four compartments, and the total population at time t is given by:

$$N(t)=S(t)+E(t)+I(t)+R(t), \quad (1.2)$$

where S(t) is the number of susceptible individuals who are free of the disease and might be infected, E(t) denotes the number of exposed individuals who are infected but in the latent period of the disease, I(t) is the number of infectious individuals who have the disease and are capable of transmitting it to susceptible individuals, and R(t) denotes the number of recovered individuals who have either recovered from the disease and acquired immunity or died of the disease. The SEIR models prove to be more appropriate for infectious diseases with an incubation period (Kounchev et al., 2020).

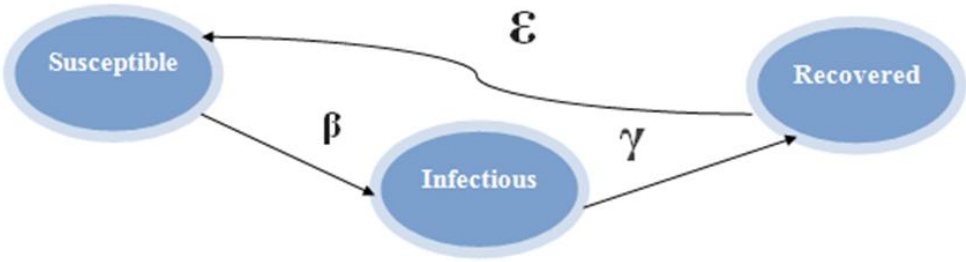


Fig.4. SIRS model. The infectious rate, β, controls the rate of spread which represents the probability of transmitting disease between a susceptible and an infectious individual. Recovery rate, $\gamma = 1/D$, is determined by the average duration, D, of infection. For the SIRS model, ε is the rate which recovered individuals return to the susceptible statue due to loss of immunity.

4.3. SIRS Model

The SIRS compartmental model is an extension of the SIR model, with the added feature that the "Recovered" population eventually loses immunity to the disease and becomes "Susceptible" once again. This is a particularly realistic model for infectious diseases that have recurrent outbreaks in the same population—such as cholera, typhus, and influenza. In the model, the rates of change for each compartment are calculated as follows:

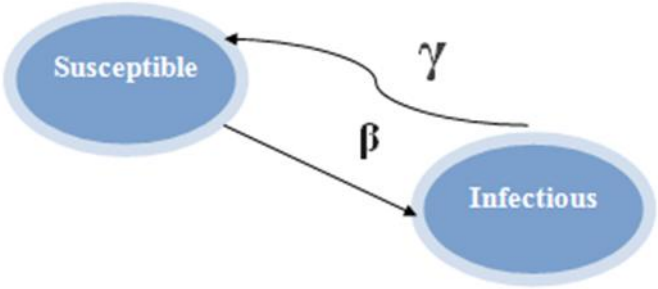
$- dS\ dt = -\beta SI + 1\ \tau\ R - dI\ dt = \beta SI - \gamma I - dR\ dt = \gamma I - 1\ \tau\ R$

where S, I, and R are the simulated counts in the Susceptible, Infected, and Recovered compartments, respectively. The transition rate constants β (effective infection rate), γ (recovery rate), and 1 τ (loss of immunity rate) are estimated from empirical data. The SIRS model is widely utilized by national health services and pandemic-modelling authorities to inform quantitative decisions on infectious disease management and screening. (M Jenkins, 2015)

4.4. SI Model

The SI model consists of two compartments: susceptible and infected. The model assigns different transmission rates to asymptomatic and symptomatic individuals, screening rates for these cohorts, and a maximum quarantine capacity. The system begins with a demographic comprising all susceptible individuals. The population subsequently diverges along separate branches, corresponding to those who become symptomatic and those who develop an asymptomatic infection. The two branches evolve at different rates with the initial condition of all individuals susceptible (Campillo-Funollet et al., 2021).

The infectious rate, β controls the rate of spread which represents the probability of transmitting disease between a susceptible and an infectious individual. Recovery rate, γ = 1/D, is determined by the average duration, D, of infection.



$$\frac{dS}{dt} = -\frac{\beta SI}{N}$$

$$\frac{dI}{dt} = \frac{\beta SI}{N} = \beta I\left(1 - \frac{I}{N}\right)$$

Fig.5. SI-SIS model for disease spread, where N=(S+I) is the total population.

5. Model Parameters and Estimation

Compartmental models rely on parameters used within state transition functions to capture the transmission dynamics of infectious diseases. Compartmental models generally limit the number of adjustable parameters in order to balance model complexity and fidelity, and solely or primarily rely on public health data. The availability, error characteristics, and temporal resolution of public health data influence the number of states that can be constrained simultaneously. As the number of compartments that are constrained by data increase, parameter uncertainty decreases. Once a model structure and regime have been selected, model parameters are estimated using statistically principled procedures to gain quantitative descriptions of regime and transition dynamics.

The SIR model describes three compartments: susceptible (S), infectious (I), and removed (R). The dynamics can be described by a system of nonlinear ordinary differential equations that depend on two parameters, β and γ. This system of equations can be rewritten as a discrete-state, discrete-time state-space model via the forward Euler method. The susceptible compartment includes all individuals that are vulnerable to the

infection in question, while the infectious compartment accounts for active cases. Individuals move from the susceptible compartment into the infectious compartment through interactions with infectious individuals characterized by the quadratic term βSI, where β reflects the average daily number of distinct interactions and the transmission probability.

The parameter β can vary over time due to interventions such as lockdowns, mask mandates, and vaccinations (Robinson et al., 2023). The time-varying effective reproduction number R_t incorporates the effect of declining susceptible individuals as the outbreak progresses and is given by R_t = R_0 S / N. The basic reproduction number R_0, which describes the average number of secondary cases caused by a single infected individual in a susceptible population, is given by the product of the transmission rate and the infectious period (Chowell, 2017).

5.1. Transmission Rate

The transmission rate is a critical parameter in the study of infectious diseases. Compartmental models such as the susceptible-infected-recovered (SIR) model provide a valuable framework to simulate and understand disease transmission. In these models, the transmission rate governs the flow of individuals between compartments, modulating the epidemic's evolution.

For example, SEIR variants have been applied to the COVID-19 pandemic. These models include compartments for the susceptible (S), exposed (E), infectious (I), and recovered (R) populations. The effective transmission rate β captures the speed of dissemination; transmissions occur when susceptible individuals contact exposed or infectious individuals. Incorporation of time-varying perturbations, inferred from mobility data, enables studying influences such as lockdowns and reduced social mingling. An accurate estimate of β is therefore crucial for reliable predictions (Jing et al., 2021). Even if typically considered constant, complex scenarios require a transmission rate dependent on societal behavior, intervention measures, and time.

5.2. Recovery Rate

The recovery rate parameter, γ, quantifies the average fraction of infected individuals who recover in a time interval. It is essentially the inverse of the average disease duration and thus represents the recovery rate per unit time. For instance, in the context of COVID-19, the disease duration after symptoms appear is approximately 11 days, corresponding to $\gamma = 1/11 = 0.09\ \text{day}^{-1}$ (Campillo-Funollet et al., 2021). The recovery rate is a fixed parameter that does not depend on the susceptible, infected, or recovered populations. Its value is determined by the characteristics of the specific disease and remains constant throughout the epidemic.

5.3. Contact Patterns

In population modelling, the interaction of different subgroups is reflected in what is usually called a transmission or contact matrix. For directly transmitted infections such

as influenza, a contact matrix estimates the average number of contacts per day between individuals of group j and individuals of group l. The more contacts, the more chances an infection can spread. The driving element of urban disease spread is human activity.

The patterns of urban travel and contact are actually very complex society-wide interaction patterns and the terms L j,l and r j,l in the above equations for X l (t) and Y l (t) are closely related to the classical two-dimensional trip matrix that indicates the trip counts in a city between all pairs of urban districts or neighborhoods. These large trip matrices specify in detail the movement of thousands or millions of people over the entire urban space. However, only the marginal relations of the movement of people originating from sector j against the movements of people going to sector l are important in the concept of epidemic spread. More precisely, any taboo is contained in the row total L j,l =M j and the column total r j,l =S j of the trip matrix and describes the movement pattern of the population. These marginals M j and S j show the importance of the sector j as a place of origin and destination.

6. Simulation Techniques

Simulation of the dynamic model can be achieved using discrete-time or continuous-time methods. In discrete-time simulation, a time step t is selected and the number of individuals who leave and enter each compartment at that time step are calculated. The time step must be sufficiently small to prevent the number of departures from exceeding the number of individuals currently in any compartment. However, discrete-time simulation is often complicated by the difficulty of computing the number of infectious individuals at the current time step.

Continuous-time simulation relies on numerically integrating the governing differential equations rather than iteratively increasing the time. Both approaches provide consistent solutions.

An important distinction between integral and differential equation formulations is the ease of parameter modulation. The parameters of the integral equation can be changed arbitrarily throughout a simulation at no additional cost, allowing reaction to external factors. Such flexibility requires considerable effort in the differential formulation, where parameters are fixed constants. Discrete-time simulation can help circumvent this obstacle. However, the integral equation model is not suitable for investigating the effect of acquired immunity or vaccination since these introduce additional compartments not easily represented by a simple memory kernel.

6.1. Discrete Event Simulation

Discrete simulation of an epidemic compartmental model involves the stochastic evolution of individuals or groups among compartments (Campillo-Funollet et al., 2021). Simulation is usually interpreted as an algorithm for numerically solving a compartmental model that involves the approximation of continuous variables, such as the population ratio in a compartment, by a discrete variable, such as the number of

people in the compartment (Nakamura et al., 2018). For an epidemic model, classical simulation algorithms approximate the continuous variables of a compartmental model using discrete values that simultaneously correspond to the discrete nature of population movements (Hernandez-Suarez et al., 2022).

6.2. Monte Carlo Methods

A new Monte Carlo (MC) framework accompanies an epidemic SIR model, with an additional $SIRS$ variant where recovered individuals regain susceptibility (E. Aiello & A. A. da Silva, 2002). Explicit spatial components link to epidemic modeling. The Dynamical Monte Carlo (DMC) method simulates Markovian processes with explicit connections. Thorough comparisons use the deterministic Runge-Kutta mean field approach and stochastic Euler methods on two space-dependent systems. The stochastic framework calls into question the deterministic physicochemical approach traditionally applied to epidemic processes by physicists and mathematicians. Large-population compartmental equations mismatch simulated and empirical results for finite populations, and uncertainties achieve research focus. Twenty months of Zika surveillance data provide a study period during which affection permanence is discarded completely, with no recurrence assumption either. Robust parameter estimation applies uncertainties more systematically to covariance matrices, achieving better performance with smaller datasets than classical least square approaches (Nakamura et al., 2018). The invariant event-following method converts any compartmental generalized model into a fully defined stochastic system with widely applicable control policies (Hernandez-Suarez et al., 2022). All dwelling-time distributions admit realistic descriptions commonly rejected by traditional algorithms. A straightforward description accounts for differential transition rates on input/output compartments, with no computational overhead. Descriptions remain deterministic due to finite differences, and predictions adopt the exact distribution of compartment times concurrently.

7. Control Strategies

A series of interventions termed control strategies were considered for the simulation before applying control to the COVID-19 dataset. Unit step functions were used to demonstrate the effect of the control strategies on the spread of the disease. The model allowed for population movement between states, and the matrices A and B were time invariant for the duration of the simulation. The states S, E, I, and R captured the dynamics of people affected by the COVID-19 pandemic. The B model matrix incorporated the control measures applied to the system. As the simulation displayed chaotic behavior at certain times, the PeSSonal dataset was used for calibrating the model parameters.

In practice, the load disturbance elements D1, D2, and D3 are time variant. Control was applied to the Milan dataset, where it was active from March 31 to April 20, 2020; after this period, the disturbance was considered zero. An output feedback control loop employing the state vector S was implemented to restrict the number of susceptible individuals.

7.1. Vaccination Strategies

Vaccination remains one of the most effective tools available for the control of epidemic outbreaks (Tao et al., 2018). A control approach to an outbreak may rely on a vaccine or other protective agent being distributed according to a prescription that is functionally dependent on the current observed state of the pathogen trajectories.The choice of such a control law involves a trade-off between how broadly and quickly to disseminate the countermeasure and the time at which to begin distribution. A simple compartment model that captures the spatially constrained and density-dependent nature of vaccination responses is presented. For a given amount of vaccination effort, vaccinating large, densely populated areas takes longer than reaching a small, sparse cluster. Delays due to logistical constraints are incorporated in an agent-based simulation of disease spread through a population with an adjoining partial differential equation describing the spatiotemporal evolution of vaccination effort.Disease dynamics are represented with an agent-based model (ABM), in which spread is simulated as a series of individual infectious contacts between susceptible and infected agents. The ABM setup allows for straightforward incorporation of the PDE vaccination component and provides a direct means of assessing the effectiveness of delay-mitigating vaccination prescription policies. Methods and analyses focus primarily on a single, widely distributed dose of a fixed budget. Given a limited stockpile and a spatially constrained vaccine rollout, an intermediate optimum emerges that balances earlier vaccination begins with wider final coverage. The ABM–PDE setup can be generalised to more complex and realistic scenarios, including multiple doses, non-spatially constrained vaccination campaigns, variable agent mobility, and distinct agent epidemiology and mobility populations.

7.2. Quarantine Measures

The importance of quarantine measures in pandemic control has been underscored by the catastrophic consequences of the COVID-19 pandemic (Lamata-Otín et al., 2023). Since pharmaceutical interventions often require time for development and implementation, non-pharmaceutical interventions, notably quarantine and testing, play a crucial role, particularly at the outset of an outbreak or in cases involving vaccine-resistant pathogens with no effective treatment (Chatterjee et al., 2023). The compartmental approach, including models such as SIR, SIRD, and SIQR, aids in the analytical investigation of epidemic outbreaks and the evaluation of governmental reactions (Öz, 2022).

7.3. Social Distancing

Social distancing has been enacted to mitigate the spread of COVID-19 (Fliess et al., 2022). Many authors adopt the classic epidemic SIR model, where the infection rate is the control variable. Its differential flatness property provides simple formulas for open-loop scenarios, useful for decision makers.

The social distancing strategy is formulated as a dynamic law that depends on the point prevalence and allows for the incorporation of socio-behavioral factors (Cabrera et al., 2021). The SIR-type model considers the culturally induced heterogeneity of the social response to social distancing, distinguishing between contact and non-contact cultures. Contact cultures relate through close personal distance emphasizing physical contact; they are found in Southern Europe, Latin America and Arab countries. Non-contact cultures manifest when individuals keep further distance from each other, avoiding physical contact; they are found in North America, North Europe and Asia.

The modeling of contact patterns and cultural norms clarifies the heterogeneous social response to social distancing and assists in finding optimal feedback control strategies. Social studies provide information on the average distance between susceptible and infectious individuals useful for identifying social patterns. Empirical evidence shows that the probability of infection decreases with distance according to a Power Law. Population behaviour linked to social and cultural characteristics offers useful ecological and epidemiological information. The effect of contact frequency, duration and distances between households on disease dynamics plays an important role in the spreading of respiratory infections. The distance is inversely proportional to the infection probability and social contacts decrease with age. A uniformly distributed distancing behaviour within populations grouped by culture is assumed due to technical simplicity and lack of more accurate data.

8. Case Studies

The SIR model has been especially well-studied and widely used in epidemiology. These ordinary differential equations describe the dynamics of the portion of a population that is susceptible (S) to an infectious disease, currently infectious (I), or that has been removed or recovered (R).

In the 2021 COVID-19 pandemic, a problem arose in fitting SIR models to case data. Epidemiological data about the epidemic evolve over time and take the form of an initial value problem. In contrast, SIR models are formulated as an initial value problem. An initial condition for the number of infected individuals is required in order to obtain a solution at all later times. The initial conditions for the susceptible and removed variables, as well as the initial infectious population size, are generally unknown. Only a few observations of the infected population's size are available. These observations define a boundary value problem.

(Campillo-Funollet et al., 2021) showed that a unique solution of the new observational model exists and described numerical algorithm for solving it.

8.1. COVID-19 Pandemic

The COVID-19 pandemic is modelled using the compartmental SEIQR framework, which accounts for the transmission of SARS-CoV-2 from an infected to a susceptible individual who works within a vertical system of infection compartments. The SEIQR model comprises Susceptible, Exposed, Infectious, Quarantined and Recovered populations, where the Quarantined population represents individuals who are under isolation and do not infect others. The model accounts both for asymptomatic carriers and for a recurrent infection configuration in which a recovered individual can become infected again. Several parameters are involved: Substantial progress has been made to address the complexity of the COVID-19 pandemic using a system of fractional equations, leading to predictions of multiple wave spikes (ElHassan et al., 2023). The pandemic is modelled through the five SEIQR states from Susceptible to Recovered by means of fractional ordinary differential equations and a Monte Carlo approach (Calleri et al., 2021). The SEIQRS model is tested against data from March to September 2020 in Jordan, showing consistency with the number of cases and highlighting the relevance of both asymptomatic carriers and recurrent infections. Low-cost face masks such as surgical masks and N95 respirators can reduce the COVID-19 infection case numbers by up to 70%.

8.2. Ebola Outbreak

The current Ebola outbreak in West Africa started from a 2-year-old boy infected by a bat. Ebola spreads through human-to-human transmission via contact with bodily fluids of infected individuals and contaminated surfaces. Healthcare workers are frequently infected during treatment. Airborne human-to-human transmission has not been demonstrated. Diagnosis without laboratory testing is difficult because symptoms resemble those of flu, malaria, or typhoid, and progression includes diarrhea, vomiting, hemorrhage, and abdominal pain. The incubation period ranges from 2 to 21 days, averaging 8–10 days. The fatality rate is approximately 50%, with case fatality rates ranging from 25% to 90%. Epidemiologists employ contact tracing to contain the virus, focusing on individuals with direct contact with infected persons, combined with symptom monitoring and avoidance of crowding. Isolation is necessary to interrupt transmission, but deciding whether to quarantine exposed individuals is challenging. Quarantine restricts movement of healthy people exposed to the virus, whereas isolation separates infected individuals. The World Health Organization does not recommend bans on travel or trade, as closing borders hampers outbreak control efforts. The WHO and CDC recommend isolating infected individuals and self-monitoring by exposed persons. To understand the virus's widespread transmission and the impact of preventative behaviors, a mathematical model employs nonlinear differential equations for analytical and numerical analysis (Sug Do & S. Lee, 2016).

Ebola is a deadly virus that attacks healthy cells and replicates within a host's body. Discovered in 1976 in Central Africa, recent outbreaks have affected West African countries. Early symptoms include fever, headache, joint and muscle aches, sore throat, and weakness. Later symptoms encompass diarrhea, vomiting, stomach pain, hiccups, rashes, bleeding, and organ failure. External and internal bleeding usually marks a fatal progression. Initial human transmission occurs via contact with an infected animal's bodily fluids. Subsequent spread primarily results from contact with blood and secretions through direct contact or contaminated surfaces (Rachah & F. M. Torres, 2017).

8.3. Measles Resurgence

Measles is a highly contagious infectious disease caused by the measles virus (MeV). The virus has only infected humans throughout history, and no other natural reservoir has been identified. Thanks to an effective, inexpensive vaccine, the World Health Organization (WHO) raised the goal of stopping the measles virus circulation in 1997. Despite the mass vaccination efforts in the 1960s, cases exploded in many States of the USA in the 1980s and 1990s. The measles attack rate has dropped significantly in the Americas during the past decade, mainly because of improved vaccination coverage in select regions. A mass vaccination campaign in 1994 drastically reduced new cases in Southern Brazil, leading to very few or no reported cases per year afterward despite a reduced anti-MeV immunity.

Extensive research has already been conducted on the modeling of the measles virus spread. The analysis of the interplay of outbreak attack rate and post-outbreak delay to the next epidemic has been estimated for countries throughout Europe. It demonstrated the interplay between deficits of routine childhood vaccination in the 1990s and the overall decline in susceptibility to measles in Europe. Furthermore, it offers a framework for interpreting serosurveillance data in the context of the control of the disease.

9. Data Collection and Analysis

Data quality has long been recognized as lacking in infectious disease epidemiology (S. Koopman et al., 2001). Yet high-quality data, including not only reliable incidence or prevalence reports but also the social and geographical context of epizootics, are essential for realistic modeling approaches. Ideally, species-based surveillance needs to be linked to pathogen-based surveillance for meaningful biological understanding and targeted disease control. Unfortunately, at both a general and specific level, data on epizootics of emerging diseases remain relatively unstructured and consequently difficult to analyze (Efstathiadis, 2022).

9.1. Epidemiological Data Sources

Epidemic modelling is a tool with which the progression or outcome of an epidemic can be analyzed readily under different control policies such as vaccinations, quarantines, lockdowns, use of face-masks, pharmaceutical interventions, etc. When such models

emulate a real-life situation accurately, they become a convenient means for decision-making.

Compartmental models are a popular type of models where the population is divided along health criteria in such a way that everybody in the population occupies a compartment that corresponds to their health status. In most epidemiological situations individuals move along a series of compartments to describe the complete progress of the disease and the subsequent treatment. Most compartmental models in the literature turn out to be Markovian in the sense that the time spent by an individual in each compartment follows an exponential distribution. This raises doubts whether some particular models based on this assumption incorporate the dynamics of the disease realistically, since the probability of recovery is assumed to be independent on time already spent sick. The restriction to Markovian dynamics hinders their acceptance by decision-makers, since waiting times in real problems are often known to behave differently from exponential distributions. There is only a handful of algorithms to address this problem available in the literature (Efstathiadis, 2022). The extensive waiting and computational times required by the existing proposal make it also very inconvenient for real-time forecasting. A novel approach that simulates stochastic epidemic models efficiently allowing sojourn times in compartments to follow any distribution is introduced (Hernandez-Suarez et al., 2022).

9.2. Statistical Analysis Techniques

The construction of epidemic models is dictated by the particular phenomenon under study. Here we focus on a class of models that reproduce the propagation of a single micro-parasite pathogen in a population of constant size, divided into groups or compartments according to the type of interaction that individuals have with the pathogen. The population of each group is represented by a time-dependent variable indicating the number of individuals, and the aggregate state of the population at a given time is represented by a vector of variables. Transition rates govern the transfer of individuals from one group to another, expressed in terms of the state-vector. The rates constitute the building-blocks of the resulting set of ordinary differential equations. These models remain simple and adequate in most cases, and historically paved the way for the later development of more sophisticated models with one or more of the following ingredients: time-dependent rates, population heterogeneity, stochasticity, and uncertainties (Nakamura et al., 2018). Also of general applicability is the strategy of dividing the total population into two distinct classes to describe the influence of social aspects, such as adherence to social distancing practices.

Statistical analysis techniques have been developed to determine groups of model parameters from epidemic data. For a deterministic model, data from one or several epidemic episodes can be used. For a stochastic model, both biological and statistical uncertainties are relevant, so that information from epidemic simulations is also required to determine parameters in a confidence region. Small sets of parameters can be examined effectively, but complexity growth provides an incentive for the development

of proper statistical methods with wider scope and efficient handling of uncertainties. Basic quantities can be studied through numerous epidemic models. As an example one can consider the basic reproduction ratio R0, which measures the potential of an infection to generate secondary cases throughout the next generation of infectious individuals. R0 can be computed through the next-generation method, applied in deterministic as well as stochastic systems.

10. Model Validation and Sensitivity Analysis

Proper validation is the last and critical stage in any modeling project. The main objective is to determine whether the model accurately represents and predicts the real-world situation it intends to mimic. Forecasts should span days to several months to be applicable for most decision support and planning purposes. A model's efficiency is gauged not only by its ability to replicate historical data but also by exhibiting reasonable volatility that encompasses a range of potential outcomes (Combrink, 2016). Individual-based and agent-based models, which capture the attributes, behaviors, and interactions of individuals through complex non-linear processes, require particular attention to predictive validity, especially given their increasing use in epidemic planning and policy-making (Hyder et al., 2013). Calibration is an essential step in model development; however, it does not eliminate all uncertainties, as some inputs may remain uncalibrated or suffer from data scarcity. These factors underscore the necessity for thorough uncertainty quantification alongside sensitivity analysis to identify key drivers of variability and understand the dependence of forecasts on uncertain parameters (Lu & Borgonovo, 2023). Sensitivity analysis methods include one-at-a-time input variations, one-way sensitivity functions, and scenario analysis. One-at-a-time sensitivity analyses examine changes in model output when varying individual inputs from a base case to alternative sensitivity cases. Such analyses are crucial for assessing model robustness and guiding the interpretation of results.

10.1. Validation Techniques

One of the fundamental challenges in the field of mathematical epidemiology involves the design of strategies to efficiently control the spread of a disease. Government intervention often requires a delicate balance between limiting the transmission of the disease and maintaining the normal operation of society, economy and services. Mathematical models of epidemics play a crucial role in this process by predicting the impact of different mitigation strategies on the evolution of the epidemic and assisting policy makers in deciding on appropriate measures. Given the diversity of models currently available, appropriate validation is required before any model can be used for making quantitative projections and informed decisions (Campillo-Funollet et al., 2021).

Due to the scarcity of data related to COVID-19 spread in the initial phase of the pandemic, simple models such as the standard Susceptible-Infectious-Recovered (SIR) framework have proven very helpful. The reason is that highly detailed models usually require extensive information about initial conditions, parameters and the epidemic

environment, which neighbouring models continuously update to take the evolving epidemic into account. Hence, SIR-like compartmental models are often developed and preferred because they strike a balance between complexity and tractability, enabling them to incorporate the main features of an epidemic within a manageable framework (Lamata-Otín et al., 2023).

10.2. Sensitivity Analysis Methods

Sensitivity analysis is a fundamental tool in the evaluation and understanding of simulation models of epidemics. In essence, it is the study of how variation in the output of a quantitative model can be apportioned to different sources of variation in the inputs of the model. The main result of a sensitivity analysis is a set of sensitivity measures, which quantify how much a specific source of variation only contributes to the observed response variation. They have two key desiderata:

1. Representativeness: Both the analysed sources of variation and the target response must be defined clearly and comprehensively without missing important phenomena. 2. Interpretability: The strength of the relationship between inputs and output can be quantified accurately and conveniently through a proper sensitivity index that can be interpreted easily by users.

The purpose of sensitivity analysis is threefold: (i) to identify the input features—parameters, distributions, variables, combinations, interactions, etc.—that drive the variability of the output or its uncertainty; (ii) to determine the ranges of variation of the input features to which the output is sensitive; and (iii) to understand how the output depends on each input feature when all the others vary. A sensitivity-analysis exercise takes as inputs the target output, the uncertain input in which one is interested, and their probabilistic dependence to compute a measure of the selective influence of one given input on the output (Lu & Borgonovo, 2023).

11. Ethical Considerations in Disease Modeling

Mathematical epidemiological models possess widely recognized predictive capabilities, accommodating even multiple model formulations of diverse origins (Zachreson et al., 2022). The adoption of such models is often linked to ethical considerations that play a critical role in influencing policy decisions. For instance, specific advanced economies selected policies aimed at shielding vulnerable people while permitting younger, less vulnerable groups to become infected, intending to reduce disruptions to the system. Nonetheless, these strategies produced higher numbers of infections, hospitalizations, and deaths compared to nations enforcing more stringent interventions (Sinha, 2022). Consequently, letting the disease spread to attain herd immunity may not effectively protect vulnerable populations in the long term.

The modeling framework can be extended beyond the basic SIR model by including compartments such as the exposed category, leading to the SEIR model. This augmentation better captures disease progression, particularly for COVID-19, and

thereby enhances the accuracy of projections. Additionally, differentiating between symptomatic and asymptomatic infected individuals is vital for understanding and modeling the effects of rapid detection and isolation on controlling the epidemic.

11.1. Public Health Ethics

A behaviour-based health policy framework can be used to predict and contain the spread of infectious diseases such as smallpox and Ebola haemorrhagic fever, motivating workshop designs to determine optimal responses. The adoption of health policies generates social behaviour that influences the course of an epidemic, and the framework aims to predict the interplay between public health policies and human behaviour throughout the outbreak. Models incorporate a health policy game to evaluate the pay-off between competing policies such as vaccination and quarantining. A multi-scale simulation framework clarifies spatial and temporal characteristics of a pandemic and the effects of control policies. Epidemiological trends are analysed using different network models that represent individuals and their contacts during the outbreak. The framework integrates demographic and geographical datasets with population-level information. The resulting behaviour-based health policy network model assists decision-makers in the determination and implementation of effective policies. A pre-analysis framework supports network-based epidemic simulations for students and researchers to analyse disease-spread patterns, predict transmission dynamics and evaluate public health policies. Geographic information systems assist the evaluation of control measures through visualisation of their spatial influence (Kurahashi & Terano, 2015) (Huang et al., 2010).

11.2. Privacy Concerns

Many countries implemented movement restrictions to reduce in-person interactions and delay the epidemic peak (Zachreson et al., 2022). Fig. 11.9 illustrates the resulting flattening of the epidemic curve and the postponement of the outbreak, effecting a reduction in the basic reproductive number, R0. To determine the optimal relaxation of these restrictions, models incorporate economic flows into the transmission model, facilitating an assessment of the trade-off between public health and economic impacts.

To make treatment, isolation, or vaccination policies more implementable, models often integrate movement patterns, as individual movements primarily drive infection spread (S. Koopman et al., 2001). In addition to government-imposed restrictions, working-from-home policies1 typically voluntary and self-regulated at the global network scale1 also affect contact rates and can delay symptom onset in densely connected social networks. Closing public venues or limiting their occupancy effectively reduces contact rates, although such policies are costly and may not fully compensate for increased interpersonal interactions in other settings, such as private gatherings. These effects can be incorporated into models through appropriate adjustments. Simulations using realistic, graph-based data compactly capture contact heterogeneity (Günther et al., 2022). Unlike homogeneous and metapopulation models, graph-based data account for

repeated contacts and explicit social groups, leading to markedly different disease outcomes starting from the same initial conditions. Therefore, individual movement profiles cannot simply be replaced by demand or flux matrices without introducing significant systemic error.

Dynamic contact network models derived from high-resolution GPS trajectories yield synthetic, user-level contact trajectories essential for direct study of disease transmission processes. The lack of such user-level mobility data hampers epidemic modeling and forecasting, raising urgent privacy challenges. By integrating differential privacy with randomized response, a plausible deniability mechanism, these challenges can be addressed. This approach supports users1 policy search while preserving location and trajectory privacy, enabling the use of fine-grained GPS data for simulating epidemic outbreaks and spatial 6temporal processes.

12. Future Directions in Disease Modeling

Recent outbreaks of infectious diseases have accelerated the development of mathematical models. Analyses of communicable diseases often employ compartmental models, which divide the population into mutually exclusive groups according to their disease status and describe the flow between compartments using differential equations. Compartmental models provide substantial insight into the dynamics of disease spread. Variation in the compartmental structure and more accurate parameter estimation contribute to improved forecasting (Zhang et al., 2022). Future developments may embrace multiscale modeling paradigms, including tactics such as the equation-free approach (I. Siettos & Russo, 2013).

12.1. Integration of AI and Machine Learning

Recent advances in machine learning are increasingly coupled with traditional equation- or agent-based epidemic simulators, enabling fast approximations, real-time forecasting and the estimation of hidden epidemiological parameters through well-established statistical techniques. Several machine-learning approaches to pandemic modelling have gained prominence during the COVID-19 pandemic. Bayesian optimisation and deep learning accelerated an agent-based simulator of London, enabling the rapid exploration of intervention policies in response to the evolving pandemic. Compartmental metapopulation models were transformed into neural networks, providing a fast, scalable and accurate infection forecasting algorithm with greater predictive skill than conventional methods. To better capture long-term behaviours, another study proposes digital twins of a modified SEIRS model built with a combination of bidirectional long short-term memory networks and generative adversarial networks that maintain the epidemiological interpretability and generality of the original model without the restriction to the dynamical equations; the architecture is data-agnostic and transferable across towns, ensuring applicability to a broad range of different scenarios (Schroeder de Witt et al., 2020) (Doussin et al., 2021) (Quilodrán-Casas et al., 2021).

12.2. Real-Time Data Integration

The inclusion of real-time data acquisition also plays a fundamental role for modeling and pandemic monitoring. From 1 January 2020, the John Hopkins University launched a resource for aggregating and visualizing data on Covid-19 cases . Starting from week 2 in 2020, the NOVELCOVID API developed by Petter Anderson has provided information about the state of the pandemic, both at the national and world level, on cases, tests, hospitalizations, fatalities, and vaccination rates.

Compartmental models describe the dynamics of infectious diseases. The classical deterministic SEIR model splits the population into four compartments: susceptible, exposed, infectious, and recovered. The exposed compartment includes individuals who carry the virus in a latent form without symptoms, which is crucial for understanding virus spread (Kounchev et al., 2020). The infectious compartment consists of individuals who are actively spreading the virus; most show symptoms or are asymptomatic. To simulate general stochastic epidemic models, the Poisson algorithm allows any distribution for sojourn times, overcoming the unrealistic exponential sojourn time assumption in Markovian models (Hernandez-Suarez et al., 2022).

13. Challenges in Modeling Infectious Diseases

Most epidemic models are able to reproduce a set of empirical, physiological or clinical constraints, but not every architecture can fit the data because the model structure imposes hard constraints on the solution (Turinici, 2020). The distribution of transit times from one compartment to another may mandate a variable number of intermediary states; additionally, a non-linear relationship between time-dependent measures of compartment sizes may indicate the necessity of structural refinements that consider groups of heterogeneous individuals. Classical compartmental models also rely on hypotheses about disease dynamics that default to the law of mass action, thus supposing that illness progresses according to average rate equations (Zachreson et al., 2022). Yet real transmission often departs from such assumptions, with empirical generation interval distributions rarely being exponential, which undermines the compatibility of natural history assumptions with the model's governing equations. Extensions such as the generalized SIR framework or the SEIR model are congruent with the governing equations but introduce additional parameters. The assumption of homogeneous mixing is an important limiting case in metapopulation models because the X–Y interaction term depends on local contact patterns, and these may be strongly non-homogeneous due to social clustering and population mobility.

13.1. Data Limitations

A major difficulty associated with compartmental epidemiological modelling lies in the availability of data. Model parameters typically correspond to sociological or biological quantities that must be obtained independently for the model to be fully descriptive. In principle, only the initial compartment sizes can be obtained from population censuses. Other parameters, such as infection and recovery rates, are typically determined by

fitting the model to data. Often, experiments must be designed to be model-specific, because data are seldom directly transferable between different models and diseases.

Most available epidemiological data, both contemporary and historical, are time series describing the dispersal of the disease among the population. These records contain information about the number of affected individuals (daily, weekly, or monthly) and are employed to determine model parameters and initiate simulations. On the other hand, clinical trials provide data on biological characteristics ((Campillo-Funollet et al., 2021)).

A macroscopic description of epidemic transmission is given by temporally varying concentrations of the primary compartments: susceptible, infected, infectious, recovered, and so on. These concentrations vary from one clinical trial to another and differ from the corresponding data obtained during the epidemic. If epidemiological models are to be relied upon, it is therefore imperative that they be capable of incorporating both types of information. Such models would not only be applicable to a variety of diseases without modification but could also contribute significantly to the design of the clinical trials themselves.

From Figure 13.5 it is clear that the sampling points obtained during the COVID-19 clinical trial investigated here are unsuitable for the determination of the average temporal evolution of the viral load at the scale of the population. Consequently, some mechanism to incorporate information extracted from the standard epidemiological data is warranted ((Turinici, 2020)).

13.2. Model Complexity

The past decade has witnessed the introduction of new families of compartmental epidemic models with large numbers of compartments and transmissible states. Although a variety of techniques and software exist to simulate models of a given architecture, there is a lack of general tools that enable investigators to select the architecture most appropriate for a particular application. Models proposed to describe the propagation of an infectious agent in a host population must be capable, after adjustment of their parameters, of reproducing the available data. While the role played by the fitting procedure in this respect is well understood, the impact of the model architecture on the ability to reproduce data is often ignored. Deterministic compartmental models account for many epidemic applications and therefore constitute a framework of choice for the development of general methods.

The architecture of a compartmental model establishing how compartments connect through transitions strongly constrains the shape of solutions. Given a set of observations, it is natural to ask whether there exists a model architecture consistent with the data. Two situations are explicitly addressed. First, the distribution of transition times from a given compartment either into a unique or into several possible compartments may impose the number of intermediary states. This problem typically arises in the context of nonlinear dynamics. Second, there may exist (nonlinear) relations between

time-dependent measures of compartment sizes indicating the need for structuring, which consists in unfolding a given compartment into a collection of homogeneous sub-populations with heterogeneous characteristics (Turinici, 2020).

14. Conclusion

Compartmental models for epidemiological processes generally classify individuals into populations according to their current role in the disease cycle. The simplest of these models, the SIR (susceptible-infected-recovered) formulation, describes two populations (susceptible and infected) characterized by a time-dependent transmission rate (Zachreson et al., 2022). Such models remain popular over a century since their conception due to their relative simplicity (especially, availability of semi-analytical fitting methods) and operational convenience. One fundamental critique concerns the commonly adopted assumption of an exponential distribution for the generation interval, which lacks empirical support for many diseases, including influenza, measles and SARS-COV-2—the characteristic infectious and latent periods often vary non-exponentially. More realistic descriptions are available through more general formulations, but require a larger set of parameters, which remain challenging to characterize from available data. A second critique concerns the very limited range of population heterogeneity that such models can take into account. Models are frequently formulated under a simplifying assumption of homogeneity, and often, special situations are little more than add-ons to the baseline population, or encompass only a restricted set of clustering mechanisms. In these settings, individual variation in key epidemiological factors such as susceptibility and infectiousness remains largely ignored or implemented in a very restrictive manner. At the same time, contact structures in human populations, which constitute a key driver of epidemic transmission, exhibit marked heterogeneity, with factors such as clustering (typically on the basis of age, social environment or common activity), variable group size and infrastructure usage all influencing epidemic development. Similarly, patterns of population movements at different scales—from daily commuting to flights on the global air-transportation network—play a central role in disease evolution and can give rise to very distinct spatiotemporal patterns of spread (Doussin et al., 2021).

References

Campillo-Funollet, E., Wragg, H., Van Yperen, J., Duong, D. L., & Madzvamuse, A. (2021). Reformulating the SIR model in terms of the number of COVID-19 detected cases: well-posedness of the observational model.

Zachreson, C., Chang, S., Harding, N., & Prokopenko, M. (2022). The effects of local homogeneity assumptions in metapopulation models of infectious disease. ncbi.nlm.nih.gov

Campillo-Funollet, E., Wragg, H., Van Yperen, J., Duong, D. L., & Madzvamuse, A. (2022). Reformulating the susceptible–infectious–removed model in terms of the number of detected cases: well-posedness of the observational model. ncbi.nlm.nih.gov

Lamata-Otín, S., Reyna-Lara, A., Soriano-Paños, D., Latora, V., & Gómez-Gardeñes, J. (2023). Collapse transition in epidemic spreading subject to detection with limited resources.

Hunter, E., Mac Namee, B., & Kelleher, J. (2018). An open-data-driven agent-based model to simulate infectious disease outbreaks. ncbi.nlm.nih.gov

Doussin, B., Adam, C., & Georges, D. (2021). Multi-scale simulation of COVID-19 epidemics.

C. Miller, J., C. Slim, A., & M. Volz, E. (2011). Edge-Based Compartmental Modeling for Infectious Disease Spread Part I: An Overview.

Carlson, K. (2016). Mathematical Modeling of Infectious Diseases with Latency: Homogeneous Mixing and Contact Network.

Grave, M. & L. G. A. Coutinho, A. (2020). Adaptive Mesh Refinement and Coarsening for Diffusion-Reaction Epidemiological Models.

Hernandez-Suarez, C., Montsinos Lopez, O., & Solano-Barajas, R. (2022). The Poisson algorithm: a simple method to simulate stochastic epidemic models with generally distributed residence times.

J.S. Allen, L. (2017). A primer on stochastic epidemic models: Formulation, numerical simulation, and analysis. ncbi.nlm.nih.gov

Hollister, J. (2018). Modeling the Spread of Disease.

Wilkinson, R. & Roper, M. (2020). Modeling Insights from COVID-19 Incidence Data: Part II - Why are compartment models so accurate?

Kounchev, O., Simeonov, G., & Kuncheva, Z. (2020). The TVBG-SEIR spline model for analysis of COVID-19 spread, and a Tool for prediction scenarios.

M Jenkins, D. (2015). An Examination of Mathematical Models for Infectious Disease.

Robinson, B., Bisaillon, P., D. Edwards, J., Kendzerska, T., Khalil, M., Poirel, D., & Sarkar, A. (2023). A Bayesian model calibration framework for stochastic compartmental models with both time-varying and time-invariant parameters.

Chowell, G. (2017). Fitting dynamic models to epidemic outbreaks with quantified uncertainty: A primer for parameter uncertainty, identifiability, and forecasts. ncbi.nlm.nih.gov

Jing, M., Yew Ng, K., Mac Namee, B., Biglarbeigi, P., Brisk, R., Bond, R., Finlay, D., & McLaughlin, J. (2021). COVID-19 modelling by time-varying transmission rate associated with mobility trend of driving via Apple Maps. ncbi.nlm.nih.gov

Nakamura, G. M., Gomes, N. D., Cardoso, G. C., & Martinez, A. S. (2018). Robust parameter determination in epidemic models with analytical descriptions of uncertainties.

E. Aiello, O. & A. A. da Silva, M. (2002). Dynamical Monte Carlo method for stochastic epidemic models.

Tao, Y., Shea, K., & Ferrari, M. (2018). Logistical constraints lead to an intermediate optimum in outbreak response vaccination. ncbi.nlm.nih.gov

Chatterjee, S., N. Zehmakan, A., & Rastogi, S. (2023). A Novel Room-Based Epidemic Model: Quarantine, Testing, and Vaccination Strategies.

Öz, Y. (2022). Analytical investigation of compartmental models and measure for reactions of governments. ncbi.nlm.nih.gov

Fliess, M., Join, C., & d'Onofrio, A. (2022). Feedback control of social distancing for COVID-19 via elementary formulae. ncbi.nlm.nih.gov

Cabrera, M., Córdova-Lepe, F., Pablo Gutiérrez-Jara, J., & Vogt-Geisse, K. (2021). An SIR-type epidemiological model that integrates social distancing as a dynamic law based on point prevalence and socio-behavioral factors. ncbi.nlm.nih.gov

ElHassan, A., AbuHour, Y., & Ahmad, A. (2023). An optimal control model for Covid-19 spread with impacts of vaccination and facemask. ncbi.nlm.nih.gov

Calleri, F., Nastasi, G., & Romano, V. (2021). Continuous-time stochastic processes for the spread of COVID-19 disease simulated via a Monte Carlo approach and comparison with deterministic models. ncbi.nlm.nih.gov

Sug Do, T. & S. Lee, Y. (2016). Modeling the Spread of Ebola. ncbi.nlm.nih.gov

Rachah, A. & F. M. Torres, D. (2017). Analysis, simulation and optimal control of a SEIR model for Ebola virus with demographic effects.

S. Koopman, J., M. Jacquez, G., & E. Chick, S. (2001). New Data and Tools for Integrating Discrete and Continuous Population Modeling Strategies.

Efstathiadis, G. (2022). Stochastic Epidemic Modelling.

Combrink, J. (2016). A Sensitivity Analysis of Model Structure in Stochastic Differential Equation and Agent-Based Epidemiological Models.

Hyder, A., L. Buckeridge, D., & Leung, B. (2013). Predictive Validation of an Influenza Spread Model. ncbi.nlm.nih.gov

Lu, X. & Borgonovo, E. (2023). Global sensitivity analysis in epidemiological modeling. ncbi.nlm.nih.gov

Sinha, S. (2022). Modeling-informed policy, policy evaluated by modeling: Evolution of mathematical epidemiology in the context of society and economy.

Kurahashi, S. & Terano, T. (2015). A Health Policy Simulation Model of Smallpox and Ebola Haemorrhagic Fever. ncbi.nlm.nih.gov

Huang, C. Y., Tsai, Y. S., & Wen, T. H. (2010). Simulations for epidemiology and public health education. ncbi.nlm.nih.gov

Günther, D., Holz, M., Judkewitz, B., Möllering, H., Pinkas, B., Schneider, T., & Suresh, A. (2022). Privacy-Preserving Epidemiological Modeling on Mobile Graphs.

Zhang, P., Feng, K., Gong, Y., Lee, J., Lomonaco, S., & Zhao, L. (2022). Usage of Compartmental Models in Predicting COVID-19 Outbreaks. ncbi.nlm.nih.gov

I. Siettos, C. & Russo, L. (2013). Mathematical modeling of infectious disease dynamics. ncbi.nlm.nih.gov

Schroeder de Witt, C., Gram-Hansen, B., Nardelli, N., Gambardella, A., Zinkov, R., Dokania, P., Siddharth, N., Belen Espinosa-Gonzalez, A., Darzi, A., Torr, P., & Güneş Baydin, A. (2020). Simulation-Based Inference for Global Health Decisions.

Quilodrán-Casas, C., Santos Silva, V., Arcucci, R., E. Heaney, C., Guo, Y., & C. Pain, C. (2021). Digital twins based on bidirectional LSTM and GAN for modelling the COVID-19 pandemic.

Turinici, G. (2020). Architectures of epidemic models: accommodating constraints from empirical and clinical data.

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Chapter 17: AI-Driven Predictive Models for Public Health Risk Forecasting

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Abstract: The integration of Artificial Intelligence (AI) into predictive modeling has revolutionized public health risk forecasting by enhancing early warning systems, enabling timely interventions, and informing data-driven policy decisions. This paper explores a diverse range of AI-driven approaches—including time series analysis, machine learning, deep learning, and reinforcement learning—for forecasting risks related to infectious diseases, chronic conditions, and environmental hazards. Predictive models, grounded in statistical and computational methods, facilitate the identification of patterns in historical and real-time data to estimate future health risks. The study highlights how models such as Long Short-Term Memory (LSTM) networks and Extreme Learning Machines (ELM) can forecast epidemic trajectories, while AI algorithms enhance surveillance, disease mapping, and health behavior analysis. Moreover, integration of big data sources—ranging from electronic health records to satellite and mobility data—enables dynamic, high-resolution predictions. Despite significant advancements, the implementation of AI in public health faces challenges such as data sparsity, model interpretability, ethical concerns, and integration with existing health systems. Emphasis is placed on explainable AI, cross-disciplinary collaboration, and the need for robust validation frameworks to ensure transparency and public trust. Case studies from COVID-19 forecasting, chronic disease management, and environmental health monitoring illustrate the real-world impact of AI-powered models. As public health threats grow increasingly complex, this study underscores AI's pivotal role in building resilient health systems through accurate, timely, and scalable predictive intelligence.

Keywords: Artificial Intelligence, Predictive Modeling, Public Health Surveillance, Epidemic Forecasting,Machine Learning Algorithms.

Introduction

1. Introduction

Predictive models provide systematic and data-driven predictions to inform decision-making and enable proactive responses. A model is a simplified, abstract representation of a real-world phenomenon designed to demonstrate the basic properties of complex systems. The primary objective of predictive modeling is to leverage historical data to generate accurate and valuable predictions. In epidemic research, predictive modeling combines historical outbreak observations with a foundational understanding of the mechanisms driving epidemics to identify and take appropriate actions when a necessary condition is detected. Predictive models are employed in a wide range of domains, including public health, social sciences, environmental science, hydrology, oil and gas, finance, and natural disasters.

Following the advent of modern computing and the introduction of artificial intelligence (AI), predictive modeling has become a key research focus in public health and healthcare. Over the past six decades, AI has advanced significantly, contributing to the effective implementation of predictive models for forecasting risks related to epidemics, chronic diseases, and water pollution using various AI techniques. (Pal et al., 2020)

2. Understanding Predictive Models

Predictive models are mathematical and computational tools designed to forecast future events or trends based on available data and analytical methods. Originating from conditional probability concepts and statistical regression models used extensively in biotechnology, epidemiology, and drug development, these models serve to estimate probabilities of outcomes given specific variables or scenarios. The pivotal objective of creating such models is to identify latent patterns within datasets that relate to the variable of interest, thereby facilitating prediction of that variable for new data instances (Zehtabian et al., 2021).

Broadly, predictive models can be categorized into four groups: time series, regression, classification, and deep learning. Time series models focus on data indexed over time and are applicable in diverse public health areas including health information systems, disease epidemiology, behavioral science, and administrative planning. When the outcome variable is continuous, regression models are appropriate, with studies demonstrating their utility in predicting epidemiological characteristics of viruses such as Ebola, Nipah, and Rift Valley fever. Conversely, classification models are suited to scenarios where the target variable is categorical; these models include decision trees, random forests, k-nearest neighbor, support vector machines, multinomial logistic regression, and neural network classifiers. Deep learning approaches, a subset of machine learning methods, have been employed to design AI tools that detect patients

and individuals with COVID-19. However, challenges remain in the reliability and accuracy of these models, especially for medium-term forecasting (Pal et al., 2020).

2.1. Definition and Importance

Epidemic risk refers to the potential threat of disease outbreaks at a given time (Pal et al., 2020). Successful prediction of epidemic risk can reduce uncertainty in planning actions that mitigate damage. Predictive models enable more effective prevention of the spread and damage caused by epidemics because people and governments can anticipate and prepare beforehand (Ismail et al., 2022). Organizations, authorities, and individuals can take necessary measures to reduce the impact of an epidemic when its potential is known. Suitable planning also provides an advantage for appropriate mitigation. Planning is guided by the expected intensity and pattern of the risk, meaning damage can often be limited even if complete prevention is not possible. Furthermore, forecasting the dynamic evolution of health conditions, such as the COVID-19 pandemic, illustrates the emerging focus on propagating long-term societal disruptions, demonstrating the growing relevance of epidemic risk prediction and mitigation (M. A. Bettencourt et al., 2007).

2.2. Types of Predictive Models

Predicting ensemble risks encountered by a population in a specific learning environment can be achieved through multiple approaches. Developing a mathematical model that analyzes individual risks and aggregates them is one alternative. Another option involves generating a coarse-grained ensemble view, abstracting away individual specifics, reserving detailed models for investigation after risk identification. Similar analogs exist in forecasting large-scale phenomena like weather, injuries, and epidemics, typically forecasting statistical indicators such as death toll for epidemics or affected geographical areas for fires and earthquakes (Zehtabian et al., 2021). The environment addressed relates to a population in a bounded 2D geographical area connected by a network of N transportation nodes.

Three model types are considered based on the length of the forecast period: short-term, medium-term, and long-term. Justifications for these models include:

— Short-term models forecast periods spanning a few hours to days, producing a small set of detailed, distinctive output signals approximately consistent with the latest observations. Achieving a meaningful absence of ambiguity is important to reduce disruption in the population’s regular activities. Mechanisms applied include physical environment elements, characteristics of the people, and aspects of governmental

response. Strategic planning integrates the external context, including the epidemic environment and recent events, with observed data.

— Medium-term models generate forecasts across several weeks to months, yielding a wide range of approximate solutions. Accurate observations constrain the solution space to a somewhat manageable size. Media and governmental responses become precursors to behavioral changes. Long-term, ongoing learning forecasts tie into medium-term time scales. The large set of broadfaced trends is combined with domain-specific forecasts for specific problems.

— Long-term models span months to years, creating a massive set of all possible ensemble risks. Political responses at large time scales and major changes on the ground remain difficult to model. Learning algorithms reach physical limits, yet ensemble ecosystem risks and seasonal changes continue to impose tight constraints on the issue. Underlying integrations with medium-term forecasts support the problem.

The Baldwin effect provides a framework for understanding how partially learned, phenotypically plastic responses eventually become genetically encoded if the phenotypic plasticity remains present during reproductive phases.

3. Role of AI in Public Health

Artificial intelligence (AI) offers new opportunities for public health organizations to improve the prediction of health issues and the targeting of interventions (Fisher & C. Rosella, 2022). Public health surveillance is traditionally performed using population health surveys, clinical data, and public health reporting systems. Access to new data sources and AI methods provides opportunities to identify emerging health threats and develop a more detailed understanding of population disease and risk factor distributions, often with improved geographic resolution. AI-powered approaches offer more up-to-date information, as data are collected, processed, and analyzed in real-time. News articles are collected to provide contextual information, and an intuitive user interface displays event predictions geographically and over time in comparison with weekly counts from the CDC. AI can also summarize surveillance information from unstructured sources. Natural language processing analysis of free-text information in death certificates has identified potential drug overdose deaths months prior to traditional coding and data release. Furthermore, natural language processing can de-identify personal health information. AI has been used to predict bacteria concentration in beach water, investigate foodborne illness outbreaks, and identify children at high risk of lead poisoning for targeted inspections. AI has also supported the selection of individuals for peer-mediated HIV prevention initiatives. Population health assessment involves

understanding the health of communities, population sub-groups, and the determinants of health to improve health policies, services, and research aimed at identifying effective public health interventions. Algorithms have predicted preventable hospitalizations, and deep learning algorithms have reduced tuberculosis spread by informing resource allocation.

3.1. AI Technologies in Use

During a crisis, assessing risk levels and forecasting its anticipated development over relevant timeframes can be decisively helpful. Public health organizations implicitly engage in such activities as they monitor disease and injury patterns and adapt responses accordingly. Technologies from artificial intelligence (AI) offer the promise of automating such activities while reducing costs and effort and accommodating large and diverse data sources; by extension, they hold promise for furthering such public health objectives. Yet, the decision on which approach to use depends on the data available, the context of the problem, and the forecast horizon (Fisher & C. Rosella, 2022). Although current dynamic models employ large data sets with highly optimized AI implementations, successful predictions at certain scales or time horizons remain elusive (Zehtabian et al., 2021).

3.2. Benefits of AI Integration

AI supports improved population health management through prediction analytics and risk stratification. Identifying high-need subgroups enables deployment of targeted interventions to better tailor programs for the anticipated needs of vulnerable populations. Macrosimulation models forecast the effects of potential policy changes. Text mining and natural language processing accelerate systematic reviews of public health interventions and facilitate translation of the scientific literature into usable formats for decision support. AI consequently enables deployment of evidence-based response and preventive strategies for multiple domains of public health concern.

AI also supports secondary prevention at the individual level by enhancing detection of at-risk groups early in disease paths. When complemented by policy makers' understanding and mitigation of relevant ethical, legal, and social considerations, it forms the foundation for an effective, population-wide, AI-augmented public health strategy.

Machine learning facilitates emergency prediction and response when combined with natural language processing. Integration of continually streaming, open data sources enables real-time situational awareness and prediction of emerging threats. By automating surveillance of the scientific and lay press, it enables detection of infectious

disease outbreaks before official reporting. Both capabilities were demonstrated early in the COVID-19 pandemic: AI detected detained reporting of infections in Wuhan and predicted subsequent global spread based on travel statistics and epidemiological data (Fisher & C. Rosella, 2022). Similarly, AI predicted locations vulnerable to Zika transmission long before actual disease emergence. Public health authorities can therefore gain months or years of lead time to mount protective interventions.

4. Data Sources for Risk Forecasting

Risk forecasting models require real-time data that describes the state and context of the system. Several data streams can help describe the social, economic, and public health landscape of a country or region. The modeling effort draws upon publicly available COVID-19 data that is updated daily and contains multiple variables relevant to the current public health situation. Data describing the 2011-2019 landscape provide information about in-country variables and their relationships, and COVID-19 case counts are used to validate these relationships in a broader epidemic context (Rodríguez et al., 2022). By building analogies among regions affected by COVID-19, the approach anticipates which social variables may change in regions with increasing or decreasing case counts (Róbert Kolozsvári et al., 2021).

4.1. Public Health Databases

Public health data repositories emerged as a subset of this information space, reflecting a growing need to enable learning healthcare systems with applications in population health and epidemic mitigation (Ankolekar et al., 2024). Public-domain databases compiled by governmental agencies or independent groups offer epidemiological and clinical information used to analyze the progression of diseases, monitor their effects on different populations, and support public health officials' decision making. Open health surveillance systems that gather information from citizens in epidemiologically affected areas have also appeared, enabling real-time collection of essential data in rural areas or underdeveloped countries where huge populations live under insufficient sanitary conditions (M. A. Bettencourt et al., 2007).

4.2. Real-Time Data Collection

With the outbreak of COVID-19 pandemic, the importance of maintaining a dynamic and continuous surveillance system is ascertained. Surveillance is a system that collects data from current and past sources and closely monitors, summaries, analyses, and predicts imminent risks and threats of the region in real time. Such surveillance is important to decrease or prevent the cascading effect of pandemic in a certain region.

COVID-19 surveillance indicates the prediction of risk of an individual country while considering different influencing factors such as geographical and environmental information (Pal et al., 2020). Real-time forecasting or nowcasting of health surveillance data streams depicts the imminent risk of a region or country by implementing an automated monitoring tool for data assimilation, prediction, and anomaly detection (M. A. Bettencourt et al., 2007).

5. Model Development Process

Predictive modeling holds great promise for providing public health officials with early warnings about potential risk. Using information about records of imminent public health risks as prior information, models can be prepared to forecast the risk factor in the later stage of a pandemic.

Two models are developed, namely, Extreme Learning Machine (ELM) and Long Short-Term Memory (LSTM) networks. In real-time pandemic situations, memories from prominent previous outbreaks are informative and serve as prior knowledge transferring to understanding the current outbreak. Therefore, Pre-Early Outbreak Stage Data (P-EOSD) combined with Early Outbreak Stage Data (EOSD) are used as prior knowledge to train the models that forecast the risk factor in the later stage.

In the first predictive model, the fatalities in the EOSD of the recent pandemic are forecasted. The EOSD refers to the period of the first 3 months after the onset of the pandemic. The fatalities in the EOSD of the recent pandemic are predicted using P-EOSD from earlier pandemics in the same category (Category I — influenza pandemics; Category II — COVID-19 pandemics; Category III — other pandemics).

5.1. Data Preprocessing

The adoption of deep learning architectures was encouraged by earlier experiences with predictive models during the COVID-19 pandemic (Zehtabian et al., 2021). However, preparation was required to apply neural networks to data streams of satellite sensor observations and socio-economic indicators. Relevant pre-tasks are outlined in the following.

Raw data collected from heterogeneous sources, using different methodologies, is minimally informative. Techniques such as linear interpolation between gaps in temporal data, and bilinear interpolation for remapping pixels between different satellite imaging grids, reduce data sparsity. For instance, the monthly temperature of a given user-defined county, acquired at hourly time resolution, is first linearly interpolated to an hourly time

series before feeding the normalisation module. The processing pipeline carries out min-max normalisation over a user-specified collection period, followed by feature transformation and data structuring that prepares information for the prediction stage.

5.2. Feature Selection

Feature selection balances sufficiency and relevance of features. Backward elimination was used on weather and mobility features; COVID-19-related symptoms were excluded due to unreliable data. OLS regression with p-values identified features correlated with active cases. As lower p-value thresholds discard almost all weather data without accuracy loss, a threshold of 0.5 and a feature set comprising all mobility and weather features were used, yielding a strong hold-out accuracy of 0.95 (Pal et al., 2020).

5.3. Model Training and Validation

A predictive model is supervisedly trained on confirmed infection numbers and mortality rates, usually over several weeks. Its output sequence and the published data are compared to compute the errors between the two. Prediction results are sensitive to the initial training sequence. A data-driven model with BLSTM architecture and an integrated optimization mechanism assesses the evolution of confirmed cases, deaths, and recoveries on a country basis (Zehtabian et al., 2021). Such a model can also be designed as an RNN encoder–decoder framework with LSTM/GRU cells trained on publicly available data. A trained model on the first-wave data is capable of predicting a second-wave outbreak and the associated epidemic curve (Róbert Kolozsvári et al., 2021). An overlaying fuzzy inference system further assesses country-specific risks using input data such as deaths, infected cases, recovered cases, and the existing medical infrastructure (Pal et al., 2020).

6. Machine Learning Techniques

Very sophisticated dynamical systems may be used to model infected, susceptible, recovered, and deceased cases, usually associated with a set of yet un-estimated parameters. Short-term predictions for countries and continents can be enhanced by including specific regional aspects, e.g., cultural attitudes, coupled with traditional compartment models and deep-learning architectures. The accuracy of medium-term predictions remains limited, highlighting the need for further research to develop robust models for public policy support.

Recurrent neural networks constitute a powerful class of models capable of capturing long-term dependencies of significant events. For example, large-scale multi-step-ahead

prediction for COVID-19 spread has been performed using the patented dynamic Levenberg–Marquardt backpropagation (DLMBP) algorithm. Incorporating synthetic data from a refined SIR model has further enhanced long-term prediction accuracy. Neural network-based epidemic forecasting remains relevant owing to its muted dependence on an in-depth understanding of underlying epidemic dynamics, as opposed to the widely employed epidemiological compartmental models.

Notwithstanding data limitations, an automated, artificial intelligence-driven, real-time theory-and-data-driven system has been developed to operate worldwide, furnishing accurate daily estimates of risk across epidemiologically affected countries of concern. Considerable variations in data quality, from extensive country-specific underreporting during critical early phases to the nearly complete absence of systematic mortality records in many countries, pose considerable challenges. To navigate this myriad of well-known and neglected uncertainties, sectoral risk estimates are constructed as a function of situational variables derived directly from available data. Parallel computation enables the exploration of a huge alternative parameter search space, facilitating the selection of appropriate background theory and ultimately the determination of model parameters. The system's 20-country estimate for the 14-day average extent of early infection in New York City aligns closely with historical data held by the City Health Authorities during the September–October 2020 time frame, while Sweden estimates show a marked rise that prompted a public memory of widespread earlier unrecorded infections. Because of its scalability, economy, and the availability of openly accessible data, this method constitutes a promising basis for enhanced spatiotemporal estimates of pandemic risk at the sectoral level (Zehtabian et al., 2021).

6.1. Supervised Learning

Epidemic forecasting often targets the daily or weekly counts of infected people, using models that generate predictions conditional on a set of input features, such as information about the current spread, government intervention and mobility (Zehtabian et al., 2021). These models benefit from expert input on which factors are likely to influence the spread of epidemics (e.g., the social distancing encouraged by stay-at-home orders). The formalism of supervised learning enables the direct integration of domain knowledge in the training process, which in turn simplifies the control of undesirable behaviour (Rodríguez et al., 2020).

Recurrent neural networks are a standard approach to time series forecasting, but require large amounts of data to generalise well to unseen examples, which limits their applicability in the early stages of an outbreak (Pal et al., 2020). A complementary approach is to use traditional compartmental models (e.g., Susceptible-Infected-

Recovered), which are built on an understanding of the factors that influence infectious diseases. They enable some insight into the predicted progression, but rely on measurements of these factors as inputs and strong assumptions about the transmission dynamics (e.g., that all infected individuals will eventually recover). Short data sequences can therefore provide more useful input to a compartmental model than to a recurrent neural network, but the strong assumptions limit their flexibility and accuracy.

6.2. Unsupervised Learning

Unsupervised learning facilitates modeling epidemic dynamics and predicting public health risks for policy-making without prespecified labels or outputs. Naturally represented as complex networks, epidemic transmission dynamics are conventionally modeled by compartment or metapopulation models. However, their strong prior assumptions often limit applicability. Unsupervised learning methods automatically identify and extract features from unlabeled data, generating representations that simplify downstream tasks and generalize to different data distributions. Transforming complex non-Euclidean epidemic data into simpler Euclidean spaces enables conventional unsupervised learning techniques. Epidemic predictions incorporate mechanisms like incubation periods, migration influences, and transmission heterogeneity; mechanistic models align with evolutionary dynamics and demonstrate effective prior distributions. Meta-learning captures parameter dependencies across diverse epidemic scenarios to estimate priors, yielding accurate and robust forecasts. Unsupervised Sequential Learning infers a nonlinear state space from epidemic time series, revealing latent dynamics that enhances predictions (Pal et al., 2020).

6.3. Reinforcement Learning

The public health sector has witnessed significant adoption of reinforcement-learning strategies to forecast and model health risks with heightened precision. Deep reinforcement-learning models can dynamically incorporate input data to immediately predict the consequences of impending interventions, enabling agents to formulate adaptive forecasting strategies that guide effective policy decisions. This approach combines the temporal structuring strengths of compartmental models with the precision of deep learning through a three-step methodology. Initially, a stochastic model captures the dynamics of the compartmental framework. Subsequently, a deep policy network—trained via reinforcement learning—issues policies grounded in the current state vector. Finally, the model accounts for inherent dynamical stochasticity to evaluate the core policy each time step. Applied to COVID-19, this framework identifies regulatory approaches optimized for diverse scenarios and varying degrees of prior knowledge about the epidemic subprocesses (Zehtabian et al., 2021).

7. Case Studies

A flexible end-to-end solution integrates publicly available health and client data to accurately estimate relative community reopening risks. A state-of-the-art prediction model captures the latest changing transmission and mobility trends and outperforms current benchmark models. The system supports multiple client-specific needs and even counter-factual analysis, providing actionable insights for governments, hospitals, educational institutions, and businesses willing to manage the risks of community reopenings (Gopalakrishnan et al., 2021).

7.1. Epidemic Outbreak Prediction

Epidemic outbreaks induce chaos in societies, with rapid propagation posing a public health risk for large populations (Pal et al., 2020). Accurate forecasts enable governments to enact control policies and allocate emergency resources, potentially curbing the spread of disease. The COVID-19 pandemic saw a concerted effort to predict infection numbers under various assumptions about public policy and non-pharmaceutical interventions. Although data availability and AI-modeling architectures improved, the overall success of predictive approaches remained limited (Zehtabian et al., 2021). Models incorporating traditional compartmental frameworks and deep-learning architectures demonstrated enhanced short-term performance, yet medium-term accuracy continued to be very poor, necessitating further research to develop reliable models for public policy. Forecasting epidemics with AI benefits public health; models can be recalculated in light of newly observed data, resulting in more precise predictions (Róbert Kolozsvári et al., 2021).

7.2. Chronic Disease Risk Assessment

Risk assessment models have emerged as an increasingly popular method for determining chronic disease progression, seeking to identify high-risk individuals for the timely implementation of preventive interventions (Ojha, 2018). Chronic diseases remain the primary cause of death in the United States, accounting for 75 to 85% of total healthcare costs; many of these diseases could be prevented and managed through simple lifestyle changes, proper risk assessment, and disease management programs. Providers and health plans frequently draw on electronic medical records, health risk assessments, and healthcare utilization data to manage population health and costs. Existing risk assessment models employ medical records, pharmacy utilization, demographic information, healthcare benefits, and claims data to calculate risk scores that aid in identifying members eligible for care management. A model incorporating these variables achieved 99% overall confidence, 89% accuracy, 99% sensitivity, and 74% specificity in predicting care management candidates.

Several predictive models have also been developed using machine learning algorithms applied to medical records, vital signs, medical history, and imaging data; while such models enhance early assessment and prognostic capabilities, deployment in real-world settings proves challenging because chronic disease patients are not always hospitalized and opportunities for real-time data collection are limited.

7.3. Environmental Health Monitoring

In recent years, industry and government agencies have begun to invest heavily in algorithms designed to predict and prevent public health risks (Comess et al., 2020). The emergence of low-cost sensors has contributed to growing interest in the predictive power of AI for environmental challenges, facilitating the monitoring of water and air quality as the cost of hardware continues to decrease. Consistent with prior work by, Sun and colleagues emphasize that innovative predictive models are poised to become essential for protecting local populations from future health and environmental hazards. However, data scarcity often impedes the effective use of AI in environmental health research. Sharing big data and collaborating across disciplines appear critical, as algorithms cannot fully compensate for missing datasets; other modeling approaches have been applied in instances of limited record availability. To contend with this limitation, the focus is on developing adaptive models capable of forecasting external environmental health indicators based on a sufficiently long observation period, enabling enhanced decision-making with limited historical data. Despite the absence of detailed predictive algorithms in the present study, these adaptive models have demonstrated the potential for good results, promising widespread applicability in technical and policy domains to avert adverse environmental conditions that contaminate watersheds and pose health concerns worldwide. In the field of support vector hospital advocacy, Golany explored both classical SVM designs and unconstrained formulations utilizing local sample information for data description; subsequent kernel-space extensional work employed an L1-norm on slack variables, and two-stage feature selection coupled with sparse kernel techniques further reduced model complexity. Based on extensive empirical analysis utilizing such a public repository, the efficacy of the developed approach is underscored. In the big data era, public health agencies grapple with developing robust models to characterize population health by integrating diverse spatiotemporal datasets while maximizing coverage. Nonetheless, a dearth of literature addresses situational awareness and anticipatory modeling grounded in heterogeneous data streams. The chapter presented compelling evidence that big data, AI, and ML are poised to transform environmental public health research. Although environmental data volume and complexity are projected to keep pace with advances in biomedical data, significant challenges must be surmounted to apply AI and ML across this discipline. Key obstacles include the absence of unified environmental public health databases,

inadequate curation of historical datasets, insufficient methodologies for integration, and limited familiarity with foundational concepts in environmental epidemiology and toxicology. Without substantial investment in data curation, integration, harmonization, and dissemination, the application of AI and ML in environmental public health will remain limited. Efforts such as the National Center for Advancing Translation Science (NCATS) Biomedical Data Translator exemplify foundational work aimed at facilitating medical knowledge integration and the construction of sophisticated models addressing complex questions. This use case holds the potential to accelerate the adoption of big data, AI, and ML methodologies in the environmental health sector. The present study concludes that there is a substantial opportunity for environmental public health researchers, policy makers, and communities to leverage artificial intelligence and big data analytics to advance knowledge of the interrelationships among climate, air quality, water quality, and human health risk indicators; more efforts in this research area are encouraged. Humans rely heavily on environmental predictions for safety-related decision-making and mitigating disease and exposure risks. Artificial intelligence has improved the understanding of climate patterns, enhanced weather forecasting accuracy through data mining techniques, and provided more precise air pollution predictions than traditional empirical or theoretical models. Consequently, researchers employ AI methods for industrial manufacturing quality control, chronic neurologic disease diagnostics, infectious disease outbreak monitoring, antibiotic resistance tracking, computational chemistry, chemical-mixture toxicity modeling, climate classification, and severely ill-patient phenotyping, among other applications. These successes demonstrate that a stronger commitment to AI and ML investments would greatly benefit environmental public health, enabling the field to realize similar gains.

8. Challenges in Implementation

The COVID-19 pandemic led to the temporary removal of 2- to 4-week ahead case forecasts from the CDC website due to poorly calibrated probabilistic forecasts. Uncertainty quantification is challenging because of multiple sources of uncertainty, and recent work with neural models aims to better leverage these sources. Distinguishing between epistemic and aleatoric uncertainty in disease spread is important. Explainability of forecasts is another challenge, with simpler methods providing clearer explanations than complex neural models. Techniques like similarity to historical data and feature importance have been explored for interpretability, and the development of XAI methods such as saliency maps could enhance forecasts. Continual evaluation and improvement of forecasting methods are necessary to make predictions more actionable for public health decisions. Defining new targets and establishing standard evaluation metrics are critical, as current measures like WIS, MAE, and coverage may not be directly comparable across regions. Reporting standards and visualization techniques can

improve public understanding. Deployment of forecasting systems requires human expertise for data cleaning, adapting to data shifts, and correcting predictions, as well as setting parameters for model optimization (Rodríguez et al., 2022). Throughout the pandemic, substantial effort was devoted to developing techniques that predict infection numbers under various assumptions about public policy and non-pharmaceutical interventions. While both the available data and the sophistication of AI models and computing power exceed earlier years, overall success of prediction approaches was limited. Augmenting algorithms with additional information about the culture of the modeled region, incorporating traditional compartmental models, and up-to-date deep learning architectures can improve performance for short-term predictions. Nevertheless, accuracy of medium-term predictions remains low, and significant future research is needed to make such models a reliable component of a public policy toolbox (Zehtabian et al., 2021).

2. Overview of Infectious Disease Models

Artificial Intelligence (AI) has greatly assisted municipalities and governments worldwide in responding to COVID-19, which revolves around the ability to extract knowledge from raw data. Before the COVID-19 pandemic, medical prediction was a widely studied field with analytical and computational methods. Early detection and real-time prediction of emerging diseases could save many lives and reduce treatment costs. The proposed multi-source LSTM-Autoencoder approach can monitor changes in the reproduction number and detect new variants with 97% accuracy on simulated data. Tracking a pandemic like COVID-19 should be an ongoing process based on recent trends. The adopted LSTM neural networks monitor temporal feature evolution from multiple data sources (macroscopic and microscopic) to identify anomalous changes. These anomalous behaviors, caused by specific changes in COVID-19's evolution, trigger the AI alarm system (Róbert Kolozsvári et al., 2021). However, the actual isolation or quarantine of individuals is not assured. The advent of new variants that can evade vaccine protection calls for more solid mechanisms. Tracking COVID-19 infections, vaccinations, testing, and the weather in advance enables efficient forecasting of COVID-19 infection risks (Zehtabian et al., 2021).

References

Pal, R., Ahmed Sekh, A., Kar, S., & K. Prasad, D. (2020). Neural network based country wise risk prediction of COVID-19. [PDF]

Zehtabian, S., Khodadadeh, S., Turgut, D., & Bölöni, L. (2021). Predicting infections in the Covid-19 pandemic - lessons learned. [PDF]

Ismail, L., Materwala, H., Al Hammadi, Y., Firouzi, F., Khan, G., & Razalli Bin Azzuhri, S. (2022). Automated artificial intelligence-enabled proactive preparedness real-time system for accurate prediction of COVID-19 infections— Performance evaluation. ncbi.nlm.nih.gov

M. A. Bettencourt, L., M. Ribeiro, R., Chowell, G., Lant, T., & Castillo-Chavez, C. (2007). Towards Real Time Epidemiology: Data Assimilation, Modeling and Anomaly Detection of Health Surveillance Data Streams. ncbi.nlm.nih.gov

Fisher, S. & C. Rosella, L. (2022). Priorities for successful use of artificial intelligence by public health organizations: a literature review. ncbi.nlm.nih.gov

Rodríguez, A., Kamarthi, H., Agarwal, P., Ho, J., Patel, M., Sapre, S., & Aditya Prakash, B. (2022). Data-Centric Epidemic Forecasting: A Survey. [PDF]

Róbert Kolozsvári, L., Bérczes, T., Hajdu, A., Gesztelyi, R., Tiba, A., Varga, I., B. Al-Tammemi, A. '., József Szőllősi, G., Harsányi, S., Garbóczy, S., & Zsuga, J. (2021). Predicting the epidemic curve of the coronavirus (SARS-CoV-2) disease (COVID-19) using artificial intelligence: An application on the first and second waves. ncbi.nlm.nih.gov

Ankolekar, A., Eppings, L., Bottari, F., Freitas Pinho, I., Howard, K., Baker, R., Nan, Y., Xing, X., LF Walsh, S., Vos, W., Yang, G., & Lambin, P. (2024). Using artificial intelligence and predictive modelling to enable learning healthcare systems (LHS) for pandemic preparedness. ncbi.nlm.nih.gov

Rodríguez, A., Adhikari, B., Ramakrishnan, N., & Aditya Prakash, B. (2020). Incorporating Expert Guidance in Epidemic Forecasting. [PDF]

Gopalakrishnan, V., Navalekar, S., Ding, P., Hooley, R., Miller, J., Srinivasan, R., Deshpande, A., Liu, X., Bianco, S., & H. Kaufman, J. (2021). Adaptive Epidemic Forecasting and Community Risk Evaluation of COVID-19. [PDF]

Ojha, M. (2018). Chronic Risk and Disease Management Model Using Structured Query Language and Predictive Analysis. [PDF]

Comess, S., Akbay, A., Vasiliou, M., N. Hines, R., Joppa, L., Vasiliou, V., & Kleinstreuer, N. (2020). Bringing Big Data to Bear in Environmental Public Health: Challenges and Recommendations. ncbi.nlm.nih.gov

Nong, P., Adler-Milstein, J., Kardia, S., & Platt, J. (2024). Public perspectives on the use of different data types for prediction in healthcare. ncbi.nlm.nih.gov

Friedman, J., Liu, P., E. Troeger, C., Carter, A., C. Reiner, R., M. Barber, R., Collins, J., S. Lim, S., M. Pigott, D., Vos, T., I. Hay, S., J. L. Murray, C., & Gakidou, E. (2021).

Predictive performance of international COVID-19 mortality forecasting models. ncbi.nlm.nih.gov

Funk, S., Camacho, A., J Kucharski, A., Lowe, R., M Eggo, R., & John Edmunds, W. (2019). Assessing the performance of real-time epidemic forecasts: A case study of Ebola in the Western Area region of Sierra Leone, 2014-15.. [PDF]

Li, Y., Yoon, G., Nasir-Moin, M., Rosenberg, D., Neifert, S., Kondziolka, D., & Karl Oermann, E. (2021). Identifying and mitigating bias in algorithms used to manage patients in a pandemic. [PDF]

K. Paulus, J. & M. Kent, D. (2020). Predictably unequal: understanding and addressing concerns that algorithmic clinical prediction may increase health disparities. ncbi.nlm.nih.gov

Tripathi, S., A. Fritz, B., Abdelhack, M., S. Avidan, M., Chen, Y., & R. King, C. (2020). (Un)fairness in Post-operative Complication Prediction Models. [PDF].