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Chapter 5: Machine Learning Systems Design and Lifecycle Management

5.1. Introduction

Machine learning (ML) has gained global attention, transforming university curricula and leading to the creation of publications, conferences, services, and products spanning every aspect of industry and academia. From novel research contributions and dynamic visualizations to new-service developments and new-economy business models, ML appears to be penetrating almost every area of endeavor. Dubbed "AI" and "Big Data," the next wave of innovation promises to cause further disruption. Strategic alignment with stakeholder needs and expectations is crucial for success.

Complex ML applications rely on a combination of AI techniques augmented with effective data management, established in a computer engineering context by Peters et al. for AI-as-a-Service. Complex, general-purpose ML models (e.g., image classification and speech recognition) have demonstrated their advantages—including continuous improvement through learning from massive amounts of new data made available through service provision. Thus, they can be exploited as components of applications in any sector, creating an overlay market. These service-layer approaches implement components of the software development life cycle, specifically focused on capture and use of training data and model specification, training, validation, and test.

5.1.1. Scope and Objectives

While concepts and frameworks such as design thinking, user-centered design, and agile development have gained influence, they are sometimes misinterpreted as a prescriptive methodology to be applied at every stage of a project, leading to inconsistency and incomplete implementation with respect to both breadth and depth. To address these shortcomings, the ML Systems Design Lifecycle is a more specific design approach tailored to the unique role of ML systems in the AI landscape. Core ML systems differ

from conventional systems by exhibiting the need for a data pipeline architecture. By breaking this architecture into three categories, it is possible to further detail the principles, considerations, and recommendations that apply to each category: the data pipeline, the model development lifecycle, and the continuous integration strategy. These three categories cover all aspects of system design and operation that are influenced by factors such as stakeholder needs, products, and requirements. This structure can also act as an ML systems checklist to ensure completeness.

Machine Learning Systems Design is grounded in three aspects: Requirements and stakeholder alignment, System architecture, and Data management. Aligning the design of a ML system with business requirements and stakeholder needs is critical for its eventual success.

Fig 5.1: Machine Learning Systems Design and Lifecycle Management

5.1.2. Terminology and Core Concepts

Machine learning (ML) systems represent a specific class of intelligible systems driven by human-authored intellectual property embedded in ML models. These systems are typically created to support a particular set of stakeholder goals expressed as a narrowly defined ML problem. While the overall system design approach parallels that of other

systems, features and properties relevant to ML systems imposed by the unique characteristics of their ML core require consideration from multiple viewpoints. Since the intention is to create and deploy a solution that leverages the characteristics of ML to provide great value or reduce risk for stakeholders within a defined context, these considerations must also align with a requirements definition.

ML systems support the design and implementation of production-quality, operational, and intelligible ML solutions. Operations refers to maintaining the integrity of all components of an ML system throughout its operational life, in particular the continued alignment of the deployed models with the stated problem formulation expressed by the stakeholder community. The role of the data management viewpoint is to cover all aspects of establishing, controlling, and maintaining the quality and availability of the data used to build and serve models throughout the operational life of ML systems.

5.2. Requirements and Stakeholder Alignment

Achieving stakeholder alignment and formulating the problem correctly are key prerequisites for the successful development of machine learning (ML) systems. The requirements that drive the design and implementation of an ML system must be clearly articulated from the start, and the roles of the various parties involved in the system's lifecycle must be defined. The actual ML model is generally developed by a sub-team that includes at least one specialist in ML, and the successful delivery of a working ML model requires that stakeholders supporting the use case—including data providers, data quality experts, and application domain experts—not only provide input to the problem formulation and evaluation metrics but also participate actively in the model development itself. Interaction between the model development team and the deployment and operational sub-teams is also essential in order to address any challenges that arise during deployment and operationalization.

Cross-functional team members must collaborate on correctly formulating the business problem by thoroughly understanding its context and identifying the aspects of the problem and solution that match best with ML's unique capabilities. There are numerous reasons why a particular business problem might not be well suited for an ML-based solution, even though an ML application might represent the optimal solution or the least effort to value proposition. It is not uncommon for stakeholders to mistakenly believe that ML is the best match for their current problem, even when conventional rule-based approaches would be easier to calibrate, maintain, understand, and explain. Possible scenarios include simple segmentation of customers, requirements for low latency in delivering predictions or decisions, or problems with limited labelled data.

5.2.1. Problem Formulation

Machine Learning Systems Design and Lifecycle Management

Machine learning system design encompasses the entire lifecycle—from identifying the problem to deploying, operating, and maintaining an ML model for practical use. With the emergence of cloud services, pipelines for developing and maintaining ML models have become standard (continuous integration and deployment for machine learning). A critical aspect is understanding the various components beyond just the model, working with a larger team, and supporting people who lack a technical background. A holistic ML design needs to consider data quality, both in intake for training and in production, as well as the architectural design for serving.

Stakeholders and their influence on the ML lifecycle can vary significantly between models, and knowing who is involved and their role informs design decisions. When problems arise with an ML model, identifying the root cause can be challenging, especially in the absence of standard operational tools. Defining a problem clearly is a core part of designing an ML model. While phrasing an ML problem can be simple, problems can be misdiagnosed, which will affect the entire lifecycle. Thus, ensuring that stakeholders are aligned on what problem is being solved, the desired outcome, the risks, and how success is measured involves clearly articulating the design specification.

5.2.2. Stakeholder Roles and Responsibilities

Designing and deploying successful machine learning systems involves collaboration across various stakeholders, each with distinct responsibilities. Although a machine learning team working for a tech company may have different titles and responsibilities compared to a team working for an insurance firm, they nonetheless can be categorized into a set of common roles that are typically performed during the data pipeline, model development, and model serving lifecycle stages. The specific roles needed on the team depend on the type of problem being solved and the resources available to the organization. In multi-team projects, the set of roles may be distributed across several teams or consolidated within just a few teams. Regardless of the specific mapping of roles to individuals, it is critical that all stakeholders understand the roles with respect to the machine learning solution.

The data owner and data provider roles are often separated to ensure the quality of the data. Data originators may also be distinct from data owners. Domain experts are responsible for generating ground truth (i.e., labeled data that can be used for supervised learning models) and validating the quality of the machine learning model’s predictions. The responsibilities of the domain expert are often divided between multiple stakeholders: an individual who generates labeled data and a separate individual who

validates the model predictions. The modeler is responsible for generating, training, and evaluating the machine learning model. Depending on the organization and model type, the modeler may also be responsible for integrating the model into the production environment and monitoring the model's performance in production. A software engineer is often responsible for integrating the machine learning model into the production environment, developing the service API, and implementing the infrastructure needed to monitor the model's predictions.

5.3. System Architecture and Design Principles

Machine learning and artificial intelligence models support business decisions through application to concrete problems, the solutions to which deliver stakeholder benefits. The design and implementation of such systems require careful architecture and detailed development, aligned with the pertinent specifications and principles. Their modules include components for the data pipeline and model development, generally the most complex in the system.

Data pipelines comprise three functional layers: (1) data ingestion, integrating structured and unstructured sources; (2) data transformation, cleaning, labeling, and allocating the data; and (3) data serve, making the data contextually and temporally relevant for the ML models. Model development usually implements an iterative sequence of design, data preparation and testing, resulting in an ML model specification and artifacts, forming the basis for a model-serving capability.

Supporting these areas can be further supplemented, motivated by specific requirements or company capabilities, through the inclusion of experimental design, model validation, and continuous integration and deployment practices, extending the ideas and infrastructure from software engineering to ML applications. Wherever feasible, repositories of ML model share, reusability, and infrastructure-as-code logic serve to automate and streamline ML systems throughout their complete lifecycle, from concept through system retirement.

5.3.1. Data Pipeline Architecture

A critical and often underestimated aspect of ML systems is the data pipeline, which is progressively gaining attention. Its omission or incomplete specification in ML projects is primarily due to deep learning's data-hungry nature: in these settings, obtaining a large and qualitatively sufficient dataset overshadows the data pipeline as a risk factor. Nevertheless, as a data pipeline crosses lower punctures of the Axiomatic Machine, it adds new failure modes not present on the model development side. These failure modes

can affect prediction drift during operations and make model development impossible, e.g., if no validation set is available without data leakage. Sound data pipeline architecture and implementation ensure that the chances of these risks manifesting in production remain low.

A data pipeline for a ML system usually has a data sourcing module, which specifies where data comes from. The functional requirements for data sourcing — defined mainly by stakeholders in the business and operations roles — include data provenance, schema validation, data sampling backlog rotation, privacy constraints, and requirements for timely availability. Validation data can come from a separate source and undergo additional operations not applied to the rest of the training data before entering the model development cycle.

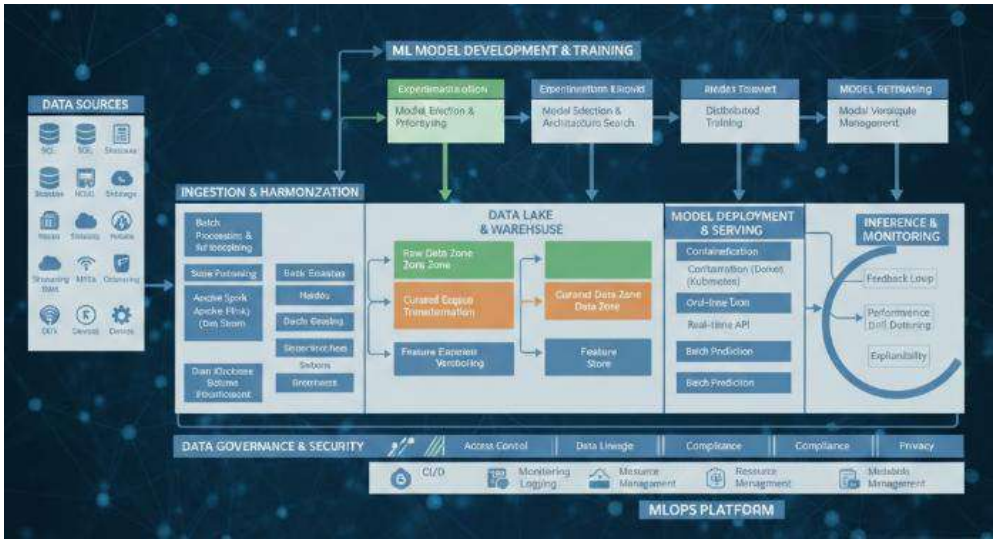

Fig 5.2: Data Pipeline Architecture of Machine Learning Systems

5.3.2. Model Development Lifecycle

The model development lifecycle considers all phases of how a model learns and serves its purpose in an ML pipeline. For the learning phase—from exploratory analysis to fitting, validation, and testing—special emphasis is placed on design reproducibility, easy error source identification, and understanding model generalization capacity. The deployment and serving phases, including APIs and resource stakeholders, are also covered.

The increasing demand for machine-learning-based services presents several challenges. Learning from data incurs significant costs that real-time ML algorithms must amortize through sustainable service levels. The quality of these services, both externally (e.g.,

throughput and response time) and internally (e.g., robustness, predictability, and security), is subject to natural variations that reflect those of the data. Service providers must ensure that these variations remain within acceptable limits while balancing ML service support with other services.

5.4. Data Management and Quality

Good-quality data is essential for successful machine learning systems. Yet, despite extensive work on modeling and algorithms, ensuring that appropriate data of sufficient quantity and quality is available for ML models is still often an afterthought. High-quality data underpins all aspects of ML model development, deployment, and maintenance phases, and a poor quality model in production is typically due to problems with the underlying data.

Data management comprises all aspects of data provenance, information and lineage capture, data cataloging, and data cleaning and labeling. It thus supports ML model lifecycle management. All data employed in the ML model lifecycle should be properly sourced, cleaned, labeled, and validated at the right quality and in the right quantity to enable system development and operations. Data sources need to be appropriate for testing, training, and evaluating the undertaking across different stakeholders' roles. Data provenance should be captured and securely stored over time and through various stages. Data cleaning and labeling require management and validation plans, together with processes and systems that guarantee adherence, recording, monitoring, and reporting.

5.4.1. Data Sourcing and Provenance

Machine learning is fundamentally dependent on data. In supervised and semi-supervised learning, the learning algorithm encounters a relatively large training data set, which is a part of the data set, and the availability of additional training data will not impact the performance. In unsupervised and reinforcement learning, however, the learning algorithm interacts with the environment as part of the learning process. In these types of ML, obtaining longer sequences of training data that account for all the areas of the space can lead to better models. Within these contexts, the sources of the model and training data have an impact on how the ML systems behave. Hence, the consideration of data does not stop at the selection and cleaning of the data but its origin and distribution is important. This is true both to understand possible bias in the current models and to create new supporting decisions.

The notions of data provenance and data sourcing are important in this regard. Data provenance considers where the data has come from as a track through the ML pipeline. Data sourcing, on the other hand, considers which data needs to be collected and how to collect it. Understanding the origin of the training and model data within the provenance aspects can highlight possible pitfalls. It is often considered as part of a quality assessment, since data can be biased and hence leads to an unreliable model.

5.4.2. Data Cleaning, Labeling, and Validation

Data cleaning, labeling and validation are key steps in the data management pipeline. Data cleaning prepares the raw dataset for training, testing, and validating machine learning models by removing noise and addressing data-quality-degradation factors such as missing values or outliers. The trained model assesses its environment and predicts its expected output using curated validation and test sets. The safety and quality of high-impact applications rely on humans to supervise and approve voluminous and automated labeling processes.

The achievability of a sufficiently large set of accurately labeled data is an essential factor in determining the best-suited deployment model for supervised learning. Sparse labeling with a heavy supervisory burden mirrors the costly and time-consuming processes of drug development. Automated labeling transitions these systems into application-oriented development, and emerging solutions such as game-theoretic designs for human-in-the-loop labeling programs promise to alleviate the continuous pressure to scale (for example, in moderating abuse on social-media platforms).

5.5. Model Development and Evaluation

Model development and evaluation for machine learning systems must accommodate the divergent objectives, responsibilities, and capabilities of the involved roles. The experimenter uses data to formulate and train an algorithm; the end user uses the algorithm to make predictions and inform decisions. Experimental design must focus on ensuring that deployments fulfill the needs and expectations of the end users and their stakeholders. Scalability and ease of deployment should therefore be guiding principles, and the system could be designed to reconnect the experimenters to the data after a model undergoes formal induction.

Experimental Reproducibility and Results Validity

Machine learning is an empirical discipline; results are tested by running algorithms, not by analytically demonstrating performance. As performance evaluation is an empirical process, careful planning and oversight can aid reproducibility and ultimately validation.

Model accuracy is a function of many choices that researchers make, and the model's ultimate utility depends on fulfilling the needs and expectations of diverse stakeholders. To gain confidence in a model's ability to fulfill those needs, its performance should first be assessed in a setting designed to minimize incidental support.

5.5.1. Experimental Design and Reproducibility

The multitude of factors contributing to the uncertainty of ML models impedes the reliable identification of effective models amongst the many considered. The ability to reproduce and explore the causes of both successes and failures is therefore essential; without reproducibility, models will likely be far more heavily influenced by noise or spurious correlations in the data than even standard statistical theory suggests.

As for classical ML models, the design of the experimental methodology can heavily influence findings. Determining the exact performance envelope of a model is generally intractable, but the completeness of the set of conditions tested and the variety and realism of the evaluation conditions have a significant impact on the conclusions drawn. In particular, a sparse evaluation of a single model's behaviour across input and ambient settings leads to the most serious concern, that it may perform well in an evaluation but simply overfit the evaluation set.

Fig 5.4: Experimental Design and Reproducibility

5.5.2. Evaluation Metrics and Validation Strategies

Formal evaluation of a machine learning system is especially complex due to the presence of learned components that introduce variability into the operation. Unlike traditional system components that can be evaluated in isolation without affecting other parts of the architecture, the core of a learning-based system can behave differently on similar input depending on where and when a sample was processed. As a consequence, the evaluation strategy must consider not only how to quantify the prediction performance and reliability of a machine learning model, but also how this model integrates with the rest of the system both during offline testing and while deployed in production. A thorough evaluation framework accounts for the uncertainties that arise through the representation learning process, and ensures that the system achieves its intended performance objectives and meets the expectations of its stakeholders.

Evaluation of any machine learning model must include a clear definition of the metrics used to quantify its performance, and a well-structured experimental design that addresses the specifics of the system being evaluated. Since most machine learning models can be understood as stochastic mapping processes, it is essential to employ validation strategies that appropriately account for the additional uncertainty introduced by learned representations. The training and validation splits of the underlying dataset should be resampled according to the natural variability present in the data-generating process, and the performance of the model should be described by the distribution of evaluations computed according to these resampled splits.

5.6. Deployment, Serving, and Operations

The deployment phase denotes the beginning of the operations phase and encompasses the serving architecture and runtime automation required to support the required model serving SLAs. These SLAs are defined by the users and recipients of the service from a business perspective. Providing an ML model in production is often viewed as a simple step in the ML lifecycle, but the realities are much more complex. The Cloud-Native paradigm of Software 2.0 allows ML models to be deployed using the same principles as traditional software releases, leveraging CI, CD, and DevOps principles for end-to-end automation Quality Control of the Machine Learning Pipeline integrates processes and tooling and crafts paradigms to address the data need in ML by recreating production-ready data pipelines in an agile DataOps fashion. Model monitoring is an essential component in CI/CD and mustn’t be considered a "nice to have" by product owners since tests in production would have the same validity as tests in a lab environment, i.e., due to the nature of Data Destructive Testing rather than Data Panel Testing. This realization and the embedding of runtime tests as part of the ML CI/CD

Lifecycle Engineering principles greatly facilitate the detection of the drift of models in production and ensure a seamless handover from model deployment to model serving.

Automating the operation of model serving in production is idiomatic for Systems for ML. From a more technical perspective, Several problems emerge in production since the serving of ML models is beyond their ML nature, i.e., addressing the problems associated with serving. Providing quality services at scale requires automating and addressing the concepts of quality and redundancy on demand while satisfying business SLA needs. Providing automation and redundancy for any Service as Code on demand at production scale reduces cloud cost. This gives the ML model serving systems the properties of any cloud service (Code for Service); Quality is achieved by providing the entire cosmic set of Unit Tests in production every second.

5.6.1. Continuous Integration and Deployment for ML

The process of integrating code changes into a shared repository and the automated deployment of applications are generally referred to as continuous integration (CI) and continuous deployment (CD). CI/CD for ML can be viewed as an extension of traditional software engineering practices to the ML domain. As in regular software CI/CD, the primary challenge here is automation, particularly the creation and validation of reproducible development environments and the automation of data and model pipelines.

Simply establishing CI/CD for ML systems along the lines of conventional engineering practices is insufficient. By virtue of the unique attributes of ML systems, there are additional challenges here that must be addressed. The key additional considerations when extending CI/CD practices to ML are proper data management, ML-specific environment constraints, and lifecycle management, particularly for models.

In the case of CI techniques, issues of data management arise when developing and validating these environments, including ensuring data availability (e.g., versioning) and integrity (e.g., corruptions) for test, training, and staging/prod sets. The original test sets must remain on the same underlying distribution as the training sets to ensure test validity. Staging priors must be immutable to prevent data leakage into live prod. Formal validation tests utilizing training/validation sets must be reproducible. These needs contradict the principle of “robots keep data clear” frequently cited for standard CI.

5.6.2. Model Serving Architectures

Providing an accurate answer to a given task does not guarantee that the answer is helpful, useful, or valuable for the end-user. In many application contexts, additional requirements apply.

i. User requirements: Contextual user guidance should be considered in addition to pure outcome accuracy. This may include the incorporation of stylistic preferences (e.g., balancing verbosity, conciseness, specificity; providing tones of formality, wit, sarcasm), granting freedom to ask for more than the original model scope, and inclusion of important policy-related information.

ii. Content requirements: In many value-added applications, the model result needs to meet additional, task-specific criteria. A task-specific evaluation must consider these extended requirements. In Machine Learning for the Natural Language Processing (ML/NLP) community, helper requirements are often – but are not necessarily – met by prompting additional helpers in parallel or sequentially.

ML/NLP systems frequently provide a narrow definition of a language model. In contrast, the concept of a language model encompasses any model that relates to natural language, irrespective of training paradigm or application objective. For example, LID models detect the language of a sample text, TS models assess the sentiment expressed, and PGT models indicate whether a human or a machine authored a textual passage.

Modern model serving architectures apply microservices principles: each model component is a stateless service that exposes an API endpoint over the web. Multiple models can be integrated into a single decision-making pipeline, composed as a directed acyclic graph. Asynchronous message-based communication may be employed, possibly combined with webhooks for series of tasks requiring different latencies. Multiple models, or multiple configurations of the same model, may be operated in parallel for many-to-one processes such as serving AD, LID, or NS capabilities.

5.7. Conclusion

Machine learning techniques can potentially improve future systems used for predicting the behavior of systems composed of individuals acting in their own best interests, including but not limited to Earth's climate system, economics, and wars. Towards this end, methods for designing and producing machine learning systems have been aligned with traditional approaches to designing and producing quality software systems. These methods, based on a review of machine learning operations lifecycle management, machine learning software engineering considerations, and considerations from software engineering research and practice, are organized into a framework representing the various stakeholder roles and responsibilities and key subprocesses of machine learning system design and production. Stakeholder roles and responsibilities include defining the problem and requirements, acquiring and preparing the data, constructing and evaluating model candidates, constructing the software system, deploying the system,

monitoring the system's performance, and maintaining and improving the system. Sourcing and also maintaining the system's input data are particularly critical elements.

These methods, however, do not directly address the design or assessment of the underlying machine learning model candidates beyond two considerations. First, a well-structured experimental design using representative data should produce reproducible model candidate performance results. Second, the appropriate evaluation metrics, validation datasets, validation methodologies, and validation sample sizes should be selected and applied. Work is needed to bring similar structure and quality to producing and selecting the machine learning model candidates that the remaining machine learning processes depend upon.

5.7.1. Future Directions

From a research perspective this discussion introduces an under-explored area of machine learning—namely, design and life cycle aspects. The success of a machine learning pipeline does not solely rely on the machine learning model selected. The entire pipeline and the flow of data through each stage are challenging and require careful design consideration. A badly designed machine learning pipeline can result in catastrophic failure, yet this is often not documented. Rather, only the success story is reported, with the lessons learned lost in the process.

A significant body of knowledge with a formal governance structure exists for established disciplines such as software engineering and database management, yet nothing comparable exists for designing, implementing, operating, and monitoring machine learning systems. The community is maturing, with established challenges in various applications illustrating the lessons learned. However, this body of knowledge is not yet well organised and formalised. Promising avenues for future research include a formal assessment of machine learning pipelines in the same way as a software project would be assessed for a particular domain or discipline, and an exploration of the supporting technologies such as a library of database abstractions for data retrieval that incorporates quality of service in addition to performance.

Machine learning is only part of the intelligence. The signals, voices, images, information and other data that are used are at least as important. The tools to gather, label, validate, clean, and construct them with meaning are essential building blocks of machine learning pipelines and will support the next generation of intelligent solutions. Although they are critical for machine learning, they are indeed domain- or application-independent. It is time for a software engineering approach to supporting and developing these techniques..

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