Concept for a Technical Infrastructure for Management of Predictive Models in Industrial Applications

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Abstract. With the increasing number of created and deployed prediction models and the complexity of machine learning workflows we require so called model management systems to support data scientists in their tasks. In this work we describe our technological concept for such a model management system. This concept includes versioned storage of data, support for different machine learning algorithms, fine tuning of models, subsequent deployment of models and monitoring of model performance after deployment. We describe this concept with a close focus on model lifecycle requirements stemming from our industry application cases, but generalize key features that are relevant for all applications of machine learning.

Keywords: model management, machine learning workflow, model lifecycle, software architecture concept

1 Motivation

In recent years, applications of machine learning (ML) algorithms grew significantly, leading to an increasing number of created and deployed predictive models. The iterative and experimental nature of ML workflows further increases the number of models created for one particular ML use case. We require so called model management systems to support the full ML workflow and to cover the whole lifecycle of a predictive model. Such a model management system should improve collaboration between data scientist, ensure the replicability of ML pipelines and therefore increase trust in the created predictive models. To highlight the need for model management systems we follow a typical machine learning process and identify shortcomings or problems occurring in practice, that could be mitigated by a model management system.

 $^{^1}$ The final publication is available at https://link.springer.com/chapter/10.1007/978-3-030-45093-9_32

1.1 Model management in the machine learning workflow

A typical ML workflow, as described by the CRISP-DM data mining guide [1] and illustrated in Figure 1, is a highly iterative process. Business Understanding and Data Understanding is gained through assessment of the particular ML use case and the initial gathering and analysis of data. Meticulous Data Preparation, cleaning of data and feature engineering, is an important prerequisite for good modeling results, as selection and data transformation are critical for successful application of ML methods. In the subsequent Modeling task, different ML frameworks and algorithms are applied. Therein, it is necessary to test a variety of algorithm configurations. It is common that the data preparation step and modeling step are repeated and fiddled with, until satisfying results are achieved. Analysis of applied data preparation techniques and their affect on model quality can provide insights on the physical system and improve future modeling tasks in this domain. Similarly, comparison of all Evaluation results can provide additional insights about suitable algorithm configurations for similar ML problems.

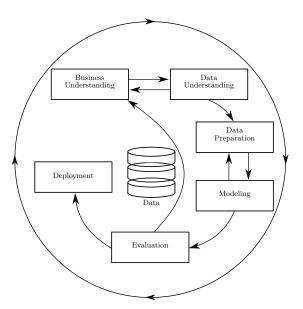


Fig. 1. Visualization of the typical machine learning workflow as described in the CRISP-DM 1.0 Step-by-step data mining guide [1]

Finally, when a suitable model is discovered, it is deployed to the target system. Typical ML workflows often end with this step. However, because of changes to the system's environment, i.e. concept drift, the model's predictive accuracy can deteriorate over time. Information about the several ML workflow steps that led to the deployed model might be forgotten, lost, or scattered around

different files or knowledge systems. Model management systems should aid by tracking the complete ML workflow and saving every intermediate artefact in order to ensure replicability.

1.2 Managing the model lifecycle - industrial applications

Predictive models are increasingly deployed to so-called edge computing devices, which are installed close to the physical systems, e.g. for controlling production machines in industry plants. In such scenarios, predictive models usually need to be tuned for each particular installation and environment, resulting in many different versions of one model. Additionally, models need to be updated or re-tuned to adapt to slowly changing systems or environmental conditions, i.e. concept drift. Once a tuned model is ready for deployment, the model needs to be validated to ensure the functional safety of the plant. The heterogenous landscape of ML frameworks, their different versions and software environments, further increases difficulty of deployment. We argue that model management system need to ML should borrow well established concepts from software development, i.e. continuous integration, continuous delivery, to cope with fast model iterations, and to cover the whole model lifecycle.

In a subsequent phase, the deployed model's prediction performance, during production use, needs to be monitored to detect concept drift or problems in the physical system. Continuous data feedback from the physical system back to the model management system provides additional data for training, and future model validation.

2 Related work

Kumar et al. [5] have fairly recently published a survey on research on data management for machine learning. Their survey covers different systems, techniques and open challenges in this areas. Each surveyed project is categorized into one of three data centric categorizations:

ML in Data Systems cover projects that combine ML frameworks with existing data systems. Projects like Vertica [7], Atlas [9] or Glade [2] integrate ML functionality into existing DBMS system by providing user-defined aggregates that allow the user to start ML algorithms in an SQL like syntax, and provide models as user-defined functions.

DB-Inspired ML Systems describe projects that apply DB proven concepts to ML workloads. Most projects apply these techniques in order to speedup or improve ML workloads. This includes techniques like asynchronous execution, query rewrites and operator selection based on data clusters, or application of indices or compression. ML.NET Machine Learning as described by Interlandi et al. [4] introduces the so called DataView abstraction which adapts the idea of views, row cursors or columnar processing to improve learning performance.

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ML Lifecycle Systems go beyond simply improving performance or quality of existing ML algorithms. These systems assist the data-scientist in different phases of the ML workflow. In their survey, Kumar et al. [5] further detail the area of ML Lifecycle Systems and introduce so called Model Selection and Management systems. These systems assist not one but many phases of the ML lifecycle.

One representative of *Model Selection and Management* systems is described by Vartak et al. [8]. Their so called ModelDB, is a model management system for the spark.ml and scikit-learn machine learning frameworks. ModelDB provides instrumented, wrapped APIs replacing the standard Python calls to spark.ml or scikit-learn. The wrapped method calls the ML framework functionality and sends parameters or metadata of the modelling process to the ModelDB-Server. This separation allows ModelDB to be ML framework agnostic, given that the ModelDB API is implemented. Their system provides a graphical user interface (GUI) that compares metrics of different model versions and visualizes the ML pipeline which lead to each model as a graph. However, ModelDB only stores the pipeline comprised of ML instructions that yielded the model. ModelDB does not store the model itself, training data, or metadata about the ML framework version. External changes to the data, for example, are not recognized by the system and could hamper replicability.

Another representative, ProvDB, as described by Miao et al. [6] uses a version control system (e.g. git) to store the data and script files and model files created during the ML lifecycle in a versioned manner. Therein, scripts can be used for either preprocessing or to call ML framework functionalities. Git itself only recognizes changes to the files and therefore treats changes to data, script or model files equally. In order to store semantic connections between e.g. data versions and their respective preprocessing scripts or the connection between data, the ML script and the resulting model, ProvDB uses a graph database (e.g. Neo4j) on top. Provenance of files and metadata about the ML workflow, stored in the graph database, can be recorded through the ProvDB command line or manually defined through the file importer tool or the ProvDB GUI. This design allows ProvDB to support data and model storage of any ML framework given that these artefacts can be stored as files and are committed to git. However, automatic parsing and logging of instructions to the ML framework only works in the ProvDB command line environment. Inside the ProvDB environment, calls to the ML framework and their parameters are first parsed and then forwarded which requires ML frameworks that provide a command line interface.

Similar to ProvDB we aim to store all artefacts created during the ML life-cycle and allow the definition of semantic connections between these artefacts. Our approach differs from ProvDB as we plan to use a relational database for the data persistence and aim to develop a tighter integration to the actual ML framework, comparable to the API approach of ModelDB. Moreover, we aim to support tuning, automated validation and deployment of ML models and provide functionality to monitor performance of deployed models.

In their conclusion Kumar et al. [5] identify the area of "Seamless Feature Engineering and Model Selection", systems that support end-to-end ML workflows, as important open areas in the field of data management for machine learning. They highlight the need for fully integrated systems that support the machine learning lifecycle, even if it only covers a single ML system/framework.

3 Design and architecture

In the following section we describe our concept of a model management system. This system is designed to be ML framework agnostic. Integration into the open source ML framework HeuristicLab¹, which is being developed and maintained by our research group, will serve as a prototypical template implementation. Figure 2 serves as illustration of the data-flows and individual components of the model management system described in the following sections. The described system can be used either locally by a single user or as a centralized instance to enables collaboration of different users. The model management system is described by the following key features:

- Centralized and versioned data storage for all artefacts of the ML framework.
- Definition of semantic connections between the different artefacts.
- Storage API for ML framework integration.
- Automatic evaluation of models on semantically connected snapshots.
- Bundling of models for deployment and subsequent monitoring.

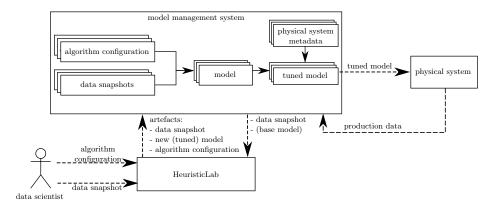


Fig. 2. Visualization of interaction between the envisioned model management system, a machine learning framework (e.g. HeuristicLab) and an external physical target system.

¹ https://dev.heuristiclab.com

3.1 Data management

The accuracy of prediction models, achievable by different ML algorithms, depends on the quality of the (training) data. Errors in data recording, or wrong assumptions made during business- and data-understanding phase affect data preparation and are therefore carried over to the modeling phase and will subsequently result in bad models. Though, bad models are not solely caused by poor data quality, as a model can become biased if certain information, contained in the dataset, was then not present in the training portion of the ML algorithm. These problems are especially hard to combat or debug if the connection between a specific model version and its training data was not properly documented or if the information is scattered around different knowledge bases and therefore hard to connect and retrieve. A model management system should therefore provide an integrated, versioned data-storage.

ML frameworks and supported preprocessing tools need to be able to query specific version of data, i.e. snapshots, from the database. Preprocessing tools also need to be able to store modified data as new snapshots. Additionally, data scientists should be able define semantical relations between snapshots. This connections can be used to mark compatible datasets that stem from similar physical systems or are a more recent data recording of the same system, as also discussed in Section 3.4. In such cases a model management system could automatically evaluate a model's prediction accuracy on compatible snapshots. The same semantic connections can be used to connect base datasets with the specific datasets from physical systems for model tuning. When a new, better model on the base dataset is created the model management system can automatically tune it to all connected specific datasets.

3.2 Model management

The section model management loosely encompasses all tasks and system components related to the ML model, this includes the ML training phase and the resulting predictive model, fine tuning the model to fit system specific data sets, evaluation of models (on training sets or physical system data) and the subsequent deployment of validated models.

Model creation or model training In order to conveniently support the ML workflow, a model management system should impose no usability overhead. In case of the *Modeling* phase this means that necessary instrumentation of ML framework methods, to capture ML artefacts, should not affect usage or require changes in existing pipelines/scripts. Therefore, method signatures of the ML framework must stay the same. Functionally, the model management system has to be able to capture all ML framework artefacts, configurations and metadata necessary to fully reproduce the training step. In our concept for a model management system we intend to provide an easy to use API for capturing artefacts that can be integrated by any ML framework. The resulting knowledge base of tried and tested ML algorithm parameters for a variety of

ML problems can serve as a suggestion for suitable configurations for future experiments, or meta-heuristic optimization for problem domains.

Model evaluation Besides ensuring replicability of the ML workflow, a model management system should also aid in the evaluation of models. In practice we require evaluation of a model's prediction accuracy not only on the test section of data, but also on "older" data snapshots, to evaluate whether a new model actually has achieved equal or better predictive quality than it's predecessor.

Similarly, functional safety of the prediction models in their production environments can be ensured by automated validation of models on past production data or on simulations of the physical system. This model evaluation process can be seen as the analogy of unit tests in the continuous development process. Facilitation of the semantic connections between datasets provides the necessary information these evaluation steps.

Model tuning Predictive models often need to be tuned in order to describe a specific target system. Model tuning refers to the task of using ML algorithms to adapt an existing predictive model, or model structure, to fit to a specific previously unknown environment. Model tuning can be used to fit an existing model to its changed environment after a concept drift was detected. Likewise, tuning can improve or speedup the ML workflow by using an existing, proven model as a starting point to describe another representative of a similar physical system. If a model type and ML framework support tuning, the model management system can trigger this tuning process and subsequent evaluation automatically. This process reassembles automated software build processes. If concept drift is detected or automated model tuning is enabled for a physical system, the model management system can take action autonomously.

3.3 Model deployment

The model management system should aid in the deployment of prediction models. This means providing the model bundled with all libraries necessary for execution of the model. The heterogenous landscape of ML frameworks and their different versions and software environments can cause compatibility issues on the target system. Crankshaw et al. [3] describe a system called Clipper, that solves this problem by deploying the model and its libraries bundled inside Docker images. This technique could also aid in distribution of the model, as the Docker ecosystem includes image management applications, that host image versions and provide deployment mechanisms. By applying this technique, the model management system can ensure executability and solve delivery of models to the target system.

3.4 Data feedback

Our concept for a model management system includes a data gathering component to capture feedback in the form of production data from the edge device.

Monitoring of the model's prediction accuracy during deployment and evaluation of the model on the production data enables the model management system to detect concept drift and to tune and subsequently re-deploy tuned models. The software necessary for monitoring and data gathering can be deployed to the edge device by addition to the bundle created during model deployment.

4 Summary

In this work we described our technological concept for a model management system. We describe the different features and components that are necessary to fully capture the machine learning lifecycle to ensure replicability of modeling results. Application of predictive models in industrial scenarios provides additional challenges regarding validation, monitoring, tuning and deployment of models that are addressed by the model management system. We argue that advances in model management are necessary to facilitate the transition of machine learning from an expert domain into a widely adopted technology.

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