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Taming the Diversity of Computational Notebooks

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ABSTRACT

In many applications of Computational Science and especially Data Science, notebooks are the cornerstone of knowledge and experiment sharing. Their diversity is multiple (problem addressed, input data, algorithm used, overall quality) and is not made explicit at all. As they are heavily reused through a clone-and-own approach, the tailoring process from an existing notebook to a specific problem is cumbersome, error-prone, and particularly uncertain. In this paper, we propose a tooling approach that captures the different dimensions of variability in computational notebooks. It allows one to seek an existing notebook that suits her requirements, or to generate most parts of a new one.

CCS CONCEPTS

• **Software and its engineering** → **Software product lines**; • **Computing methodologies** → *Machine learning*.

KEYWORDS

computational science, software variability, clone-and-own

1 INTRODUCTION

The development of Machine Learning (ML) brings multiple new challenges to the scientific community, including the discovery, reuse, and production of ML models [26, 41]. Designing a new ML model to solve an industrial ML task involves a series of iterations. These iterations consist in collecting data and business requirements from the domain expert, analyzing the data, transforming them accordingly to the domain expert's insights, then evaluating different workflow configurations [4, 40]. Besides code-sharing platforms such as GitHub or GitLab, many supporting environments aim to rationalize the ML life cycle, particularly by promoting the sharing of ML models. Thus, widely used platforms such as OpenML [37] or ModelDB [25] allow the specific sharing and discovery of ML models by scientists. Notebook sharing, more specifically, is widely supported by popular platforms such as Kaggle¹ (over 400K notebooks today), Google Colab², Jupyter Notebook, JupyterLab³, or Baidu AI Studio⁴.

¹<https://kaggle.com/>

²<https://colab.research.google.com/>

³<https://jupyter.org/>

⁴<https://aistudio.baidu.com/aistudio/index>

Building effective data science systems is a challenging sociotechnical endeavor that involves both technical and human work [28]. Designing a universal solution that can work for any Machine Learning (ML) problem specification is not possible due to the high combinatorial diversity of both data [7] and business requirements [15]. Additionally, the pool of available ML solutions is continuously growing, making it increasingly difficult for data scientists to navigate this "wilderness" of possibilities [12, 41]. Consequently, a data scientist may, for the same problem, try several preprocessing libraries, several types of models (e.g., decision trees and neural networks), and even multiple frameworks for the same type of model (e.g., TensorFlow and PyTorch) [41]. A recent study [22] highlights the importance of code reuse in notebook production, with 18% of participants' time spent searching for code samples online. Duplication and reuse of code rely on tutorials or APIs and various sources because solutions are problem sensitive, and the field is evolving rapidly.

To the best of our knowledge, search options to retrieve notebooks are mostly based on a textual search (on domain keywords, benchmarks/competitions, machine learning artifacts, language, author, or dataset), possibly using ontologies as in the case of ModelDB [25]. Such search options could lead to various types of errors. For example, in the case of searching notebooks by keywords, this can result in an overwhelming number of notebooks, some of which are not even related to the field, without the problem being addressed. The key issue is then to reduce the solution space to the suitable solutions only. In this context AutoML-like approaches and recommender systems will learn from the past runs to find one *best* solution only according to the datasets, while this solution may not fit the current requirements [15]. Instead, we believe that a data science tool support could provide guidance in finding an appropriate set of solutions taking into account both datasets and requirements. It should provide a comprehensive view of the data science landscape, including the solutions already developed and their applicability to different problem specifications. Consequently, it should help them identify the effective solution set for their problems.

Facing the issues of clone-and-own in computational notebook usage (*cf.* section 2) this paper describes emerging ideas along with a possible tooling approach for resolving them. It captures the different dimensions of variability in computational notebooks and distinguishes two layers (*cf.* section 3). The upper layer focuses

We rely on simplified examples of feature models in the domain of anomaly detection in time series to illustrate our points (cf. Figure 4). Some constraints connecting these spaces are illustrated in Figure 4e, with the corresponding arrows in Figure 2 denoted by circled numbers.

3.2.1 Initial data. InitialData submodel characterizes the space of initial datasets. The data scientist configures this submodel through semi-automatic data analysis and manual selection of properties that depend on expert knowledge, such as the nature of missing values.

Figure 4a illustrates this submodel emphasizing the availability of data labels or annotations, the data type (which could comprise image data such as sound spectrograms) and the normalization status of the data prior to analysis.

3.2.2 Business requirements. BusinessRequirements submodel captures requirements, such as limited memory usage to comply with hardware constraints. The data scientist configures this submodel through a manual selection of requirements. While the initial data space does not impose restrictions on other feature models, specificities regarding the initial data, such as sampling rates, can be included as part of the business requirements. This dependency is illustrated by arrow 1 in Figure 2.

Figure 4b illustrates this submodel highlighting three significant considerations. Firstly, the deployment platform during production should be taken into account, especially if it involves microcontrollers for embedded models. Secondly, an understanding of potential deviations between anomalies observed in the production environment and those represented in the training data is crucial. Lastly, experts' interest in the types of anomalies, such as outliers or single point amongst others should not be overlooked.

3.2.3 ML artifacts & states. MLArtifacts submodel organizes the algorithmic hierarchy and specifies the types of workflows used during the learning and deployment phases (e.g., active learning workflow). On its side, the States submodel represents the different stages that the data passes through, with preconditions and the impact of ML artifacts expressed through constraints relative to each state. For example, an algorithm may require the data to be in a scaled state without necessarily needing that state to be the initial one. The MLArtifacts submodel is manually configured by the data scientist based on their specific problem and preferences. In contrast, the States submodel is only configured through the propagation of information about the data and ML artifact choices.

The separation of concerns in the ML artifacts model and Business Requirements model (arrow 4 in Figure 2) facilitates this management of evolution. Additionally, the state of the data depends not only on its initial state (arrow 2) but also on its transformations and processing throughout the ML pipeline (arrow 3). The intermediate States model plays a critical role in managing this variability and ensuring the overall effectiveness of the ML solution.

Figure 4c illustrates the MLArtifacts submodel, while Figure 4d illustrates the States submodel. MLArtifacts submodel comprises three primary types of solution components. Preprocessing elements such as mathematical transformations of time series, from time domain to frequency. Next, the algorithm components consist of features such as neural networks, support vector machines, and tree-based models. Finally, the postprocessing component exclusively includes

the Quantizing algorithm, which serves to reduce the model size and facilitates embedding in microcontrollers.

3.3 Variability of realized products and assets

We use the vocabulary of Idowu et al. in [17] to present the assets that enable us to find notebooks or generate a primitive version of a new one⁵. We structure the application space into two main areas: firstly, the code source and job assets, which represent possible products (notebooks), and secondly, the already realized products that we organize into variability subspaces ExperimentProducts and NotebookProducts for easy retrieval and potential cloning.

3.3.1 Code source and job assets. Code Source and Job Assets are the core of the generation (see Figure 1). They are mapped to the MLArtifacts submodel, in order to maintain a mapping between model and implementation. These assets do not contain the datasets as they are not used in the generation process. Technical details on generation are given in section 3.5.

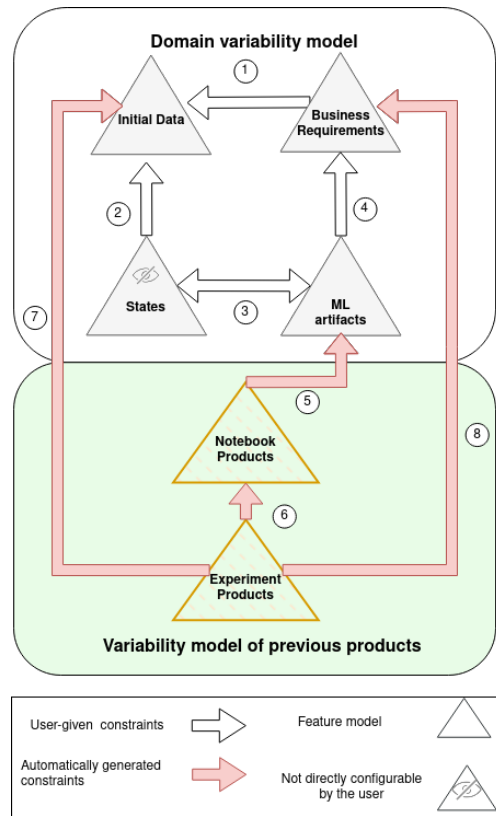


Figure 2: Feature model spaces

⁵Some of the assets we use, such as the authors of the notebooks and the source scientific articles, are not presented even if they help with the selection of notebooks. They are, however, not decisive to establish a matching between the specification of a problem and the past ML artifacts, which is the focus of this paper.

3.3.2 Experiments. An experiment artifact refers to a specific configuration that defines the problem to be solved and the notebook that implements the solution. Our platform automatically extracts a representation of these artifacts and adds it to the variability submodel `ExperimentProducts`. Further details on this aspect will be given in section 3.4. This model enables us to capture and organize the products produced by data scientists and facilitates the search for past experiments. The `ExperimentProducts` variability submodel is available from the configuration phase and allows for quick identification of experiments addressing similar problems.

3.3.3 Notebooks. Data scientists can save updated notebooks along with the experiments they are associated with. We capture a simplified representation of each notebook in the `NotebookProducts` variability submodel, which consists mainly of constraints (cf. section 3.4). This submodel is accessible from the configuration phase onwards. It enables rapid identification of notebooks that could be cloned, or accelerates the configuration process by selecting the most appropriate notebook for the problem at hand and by automatically selecting ML artifacts. The constraints depicted by arrows 5, 6, 7, and 8 support the identification of past products and ML artifacts based on Domain variability model configuration.

All constraints that drive this interplay between the four FMs capturing domain variability are provided by data scientists (indicated by white arrows in Figure 2)⁶ All other constraints, from the two FMs capturing previous products' variability, are automatically generated (indicated by arrows 5, 6, 7, and 8 in Figure 2).

3.4 Formal definition of the interactions

We provide here a formal explanation of how interactions with the realized product variability model are defined.

Domain variability model. Configurations are our primary tool for determining *experiment* context. Let $\llbracket FM_D \rrbracket$ be the set of valid configurations of the domain variability model FM_D . In line with the domain modeling, a configuration c is composed of three subsets: $c \in \llbracket FM \rrbracket$, $c = \text{initData}(c) \cup \text{busReq}(c) \cup \text{mlArt}(c) \cup \text{states}(c)$.

Partial configurations to specify ML problems. As we work on *experiments* whose context is difficult to define and the SPL evolves, some features about the initial data or business requirements can be neither selected nor deselected, they are simply "unknown." A set of features s in a configuration can then be defined as three subsets $s = \text{selected}(s) \cup \text{deselected}(s) \cup \text{undefined}(s)$. The intersection is empty between these three subsets.

Experiments. An *experiment* e is defined by a name n_e , the reference to a notebook nb_e and a valid configuration c_e , we note $e = (n_e, nb_e, c_e)$ where $c_e \in \llbracket FM_D \rrbracket$. The subsets $\text{initData}(c_e)$ and $\text{busReq}(c_e)$ may have a non-empty subset of undefined features. In contrast, $\text{mlArt}(c) \cup \text{states}(c)$ is complete; all the features are selected or deselected.

Variability model of realized products. The domain of realized products is defined by a set of experiments, E . The constraint system uses the experiment's name and the notebook's name to select or

⁶Some of these constraints have been learned through the study of past experiments, but always in interaction with the data scientist, while others related to states correspond to the application of patterns upon the data scientist's request.

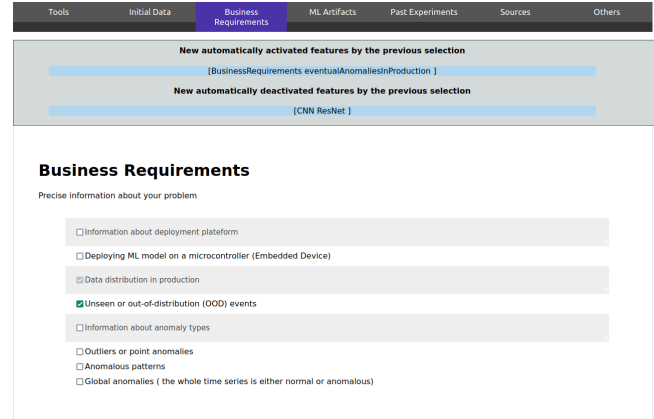


Figure 3: Tool UI for Business Requirements configuration

deselect them, depending on the other features that characterize the problem to be solved. The defined interactions are as follows.

$$\forall e_i \in E, e_i = (n_{e_i}, nb_{e_i}, c_{e_i}),$$

$$\text{(arrow 6) } n_{e_i} \Rightarrow nb_{e_i},$$

$$\text{(arrow 5) } nb_{e_i} \Rightarrow \Lambda \text{ selected}(\text{mlArt}(c_{e_i})),$$

$$\text{(arrow 7) } n_{e_i} \Rightarrow \Lambda \text{ selected}(\text{initData}(c_{e_i})) \cup \text{deselected}(\text{initData}(c_{e_i})),$$

$$\text{(arrow 8) } n_{e_i} \Rightarrow \Lambda \text{ selected}(\text{busReq}(c_{e_i})) \cup \text{deselected}(\text{busReq}(c_{e_i})).$$

The constraint corresponding to arrow 5 deselects a notebook when an artifact used by the notebook can no longer be selected and, therefore, the experimentation associated with it (arrow 6). By restricting this constraint to the selected elements, it is possible to keep a notebook as an aid to clone even though it lacks components. The constraint (arrow 6) separates the deselection of the experimentation relative to the notebook from the deselection of the notebook. The two last constraints establish the correspondence between the experiment, the specification of the business requirements, and the initial data. Adding experimentation builds all the above constraints automatically.

3.5 Tooling overview

Figure 3 depicts the tool interface developed based on Elias Kuiters' feature-configurator⁷. Data scientists use the *Initial Data*, *Business Requirements*, and *ML Artifacts* tabs to configure their experiments. Visualization, including questions, is achieved by associating features with questions through a CSV file. The tool provides access to past experiments and notebooks through the *Past Experiments* tab. The generation step is accessible through the *Tools* Tab. Technically, the generation of a totally new notebook is handled as such: Once the user requests from the tool to generate the notebook, the *generator* is only given the `MLArtifacts` part of the configuration. It then uses the mapping of the concerned submodel to Job Assets to find the requested product implementations. Those implementations are then copied into a data structure that represents the notebook cells. This data structure is provided by Jupyter Python library designed to programmatically generate Jupyter Notebook. It must be noted that the choice of algorithms and ML workflows is considered part of the configuration, allowing data scientists to select established

⁷<https://github.com/ekuiters/feature-configurator>

algorithms [18]. This configuration at a level usually considered as low [10] then automatically drives the configuration of business requirements.

4 ILLUSTRATION

To evaluate our approach, we discuss two illustrative scenarios, each one corresponding to a real-world case that has been simplified to clarify the propagation principles. Still, they enable us to demonstrate the capabilities of our approach. A reproduction package of our tool covering the two scenarios is available as a Zenodo artifact [9].

As explained in section 3.2 and illustrated in Figure 4c, the solution space comprises three primary types of solution components (preprocessing elements, algorithm components, and postprocessing components). As depicted in Figure 4d, the state space structure is similar to the one of the initial data space. However, it captures the current state of the data, which differs from the former in terms of data properties that may change over time. For instance, converting data from time series to a collection of spectrograms alters the data type to images, thereby enabling the utilization of solution components that may have been restricted before.

We then limit the space of realized products to two experiments with their associated notebooks. XP1 is an experiment conducted on non-labeled and non-normalized time series data of motor vibrations to detect acquisition errors in the data, specifically the occurrence of single-point anomalies. The associated notebook includes a normalization algorithm (e.g., `MinMaxScaler`) and an LSTM-type neural network. However, due to the non-quantizable nature of LSTM, this experiment cannot be embedded.

XP2, which refers to NB2, pertains to an experiment conducted on partially labeled and non-normalized time series data of sounds to detect identifiable malfunction anomalies in motor sounds with abnormal patterns (e.g., `patternAnomaly`). The notebook associated with this experiment employs a spectrogram calculation to transform data into the time-frequency domain, enabling better detection of anomalies via (e.g., `SFFT_createSpectrograms`), normalization via `MinMaxScaler`, and a CNN-type neural network. This model was not embedded in a microcontroller.

4.1 Scenario 1: Retrieve and clone notebook

Objectives. With this scenario, we want to illustrate how our approach differentiates itself from current practices. To determine whether a solution to a similar problem already exists, the user relies on her expert’s insight. Once the constraints are applied, suitable solutions are proposed, enabling the user to choose an experiment or ML components.

Unfolding the scenario: Lea, a data scientist, is tasked with solving an anomaly detection problem on a dataset of motor vibrations. She must produce a solution that raises alarms when abnormal patterns indicate a defect in the motor bearing:

Lea first configures the `InitialData` FM (cf. Figure 4a), specifying the data type is `TimeSeries`, `PartiallyLabelled`, and not `NormalizedData`. *The given specification is sufficient to exclude Experiment XP1, which dealt with motor vibration but was performed on unlabeled data. However, this finding does not contradict the associated notebook, which employs an algorithm capable of handling*

partially labeled data. The constraints represented by arrow 8 in Figure 2 were applied. Lea selects in the BusinessRequirements FM (cf. Figure 4b) `NovelAnomaliesEmergeInProd` and identifies the anomalies to be detected as `patternAnomaly`. Based on the current state of the configuration, CNN and Resnet algorithms cannot be selected anymore, as they are not suitable for handling new anomalies in production (according to arrow 4 in Figure 2, i.e., constraints 6 and 7 in Figure 4e). At this stage, several experiments are compatible with the current configuration. Lea then clones the experiment XP2 to work with it. As a result, she has been able to retrieve several past experiments and notebooks by giving the system her configuration. Thanks to the constraints model she has been able to clone one that matches her problem.

4.2 Scenario 2: Generate a new notebook

Objectives. With this scenario, we want to illustrate the correctness of the generative process, from the proposed code artifacts to the generated notebook. In the case where none of the experiments nor notebooks are reusable, we want to validate that our approach leverages constraint system propagation to reduce the number of unsuitable component compositions.

Unfolding the scenario. Lea is tasked with solving another anomaly detection problem. This time she has to use a collection of inline process control measurements from various sensors during the processing of silicon wafers for semiconductor fabrication. She must build a solution that raises the alarm for faulty wafers.

Lea informs the data properties as being `TimeSeries` and `FullyLabelled`. She also deselects `NormalizedData` as the data are not normalized. *No experiments are compatible with her data configuration.* As Lea knows that no new anomalies will arise during the production use, she then deselects `NovelAnomaliesEmergeInProd` in the business requirements. Following a discussion with the expert, she is able to determine that the series is irregular. Thus she checks `globalAnomaly`. *The two still available notebooks do not fully meet the new requirements. The tool suggests available algorithms that Lea can select.* To compare the two models, Lea generates two notebooks that share a `MinMax` scaling preprocessing, one notebook featuring a CNN classifier and the other featuring a Resnet classifier. *She chose to conduct a generative process by picking machine learning components. Only configuration-suitable features were provided to her. In order to test several classifiers, Lea had to generate as many notebooks.*

5 CONCLUSION

In this work, we proposed a first tooling approach to tackle the problem of diversity in computational notebooks. To help data scientists tailor a notebook to their own problem, our approach uses several variability models coupled with a constraint system. This allows the user to get feedback according to the data and business requirements of the new problem. The presented scenarios demonstrated that the user can retrieve past experiments based on problem configuration, or can totally tailor a new one. These scenarios acknowledge the potential of the proposed solution. Furthermore, an ongoing case study with an industrial partner will assess the usefulness of the configuration process, and gives us

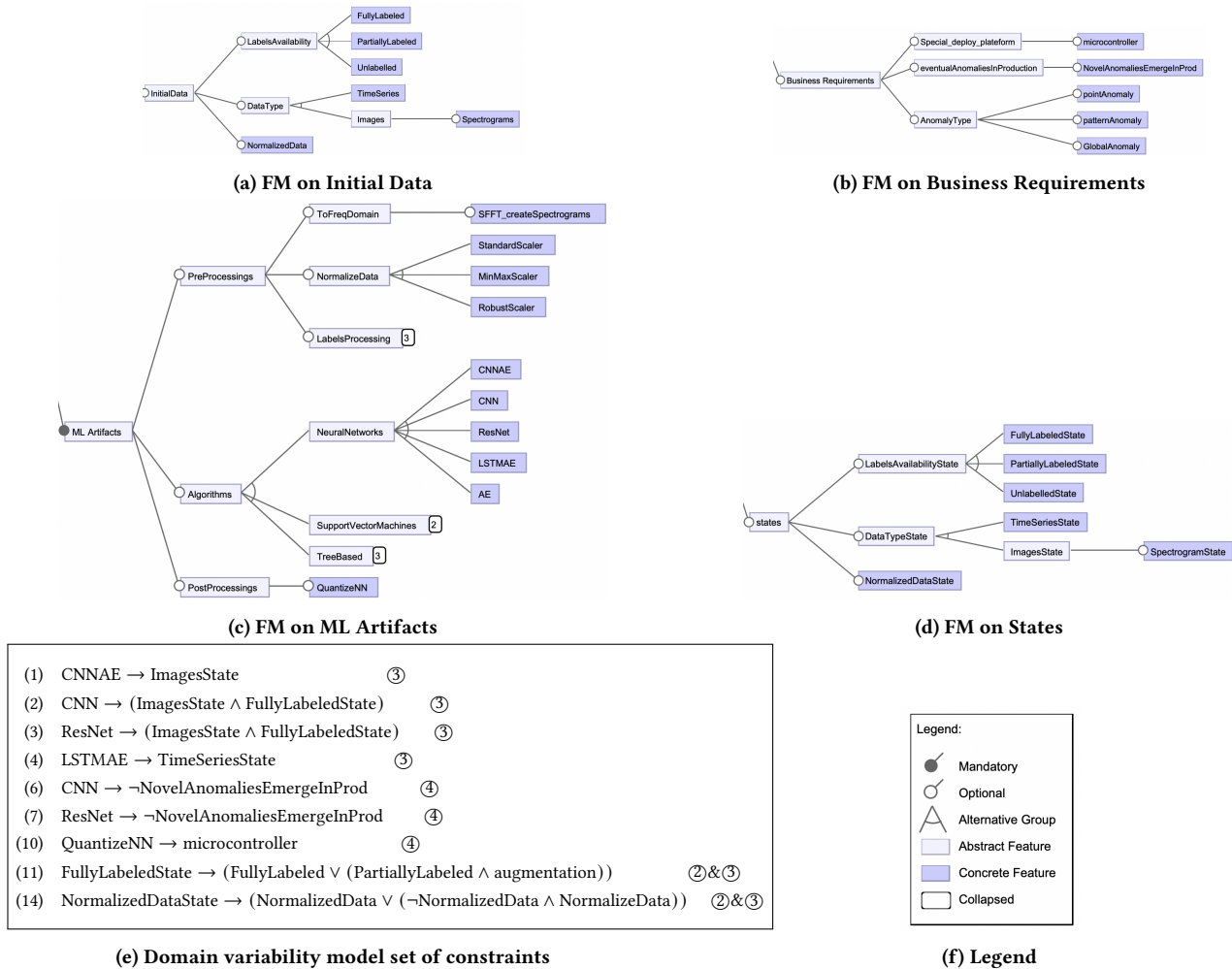


Figure 4: Features and constraints

confidence that our findings will be soon applicable to various machine learning subdomains, considering a much broader domain modeling.

We are pursuing two different complementary validation approaches to strengthen our results. First, we plan to enhance the knowledge base through an empirical study by analyzing popular notebook repositories to characterize similarities at various levels and across different spaces, extracting the necessary information for managing the SPL [19, 27]. To validate the approach's effectiveness in reducing the solution space, we are conducting comparisons with autoML-like approaches and compared the results of novice data scientists using the approach to solve given exercises in an academic setting.

In the longer term, we aim to evolve the SPL by involving data scientists in the enrichment process. This includes using automated reasoning techniques based on past configurations [5, 14, 24, 35] and exploring model evolution [2, 6, 13, 16, 36]. Additionally, we plan to support multiple implementations within ML components using the Multi-Level Feature Trees approach [10, 31]. Improving

feature visualization during configuration [8] is also a key aspect. We expect these future results to advance SPL management and enhance configuration processes in machine learning.

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