# The Machine Learning Bazaar: Harnessing the ML Ecosystem for Effective System Development

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Abstract—As machine learning is applied more and more widely, data scientists often struggle to find or create end-to-end machine learning systems for specific tasks. The proliferation of libraries and frameworks and the complexity of the tasks have led to the emergence of "pipeline jungles" - brittle, ad hoc ML systems. To address these problems, we introduce the Machine Learning Bazaar, a new approach to developing machine learning and AutoML software systems. First, we introduce ML primitives, a unified API and specification for data processing and ML components from different software libraries. Next, we compose primitives into usable ML programs, abstracting away glue code, data flow, and data storage. We further pair these programs with a hierarchy of search strategies — Bayesian optimization and bandit learning. Finally, we create and describe a general-purpose, multi-task, end-to-end AutoML system that provides solutions to a variety of ML problem types (classification, regression, anomaly detection, graph matching, etc.) and data modalities (image, text, graph, tabular, relational, etc.). We both evaluate our approach on a curated collection of 431 real-world ML tasks and search millions of pipelines, and also demonstrate real-world use cases and case studies.

Index Terms—machine learning, AutoML, software development, ML primitives

# I. INTRODUCTION

Many diverse fields have begun to incorporate large-scale data collection into their work. As a result, machine learning (ML), once limited to conventional commercial applications, is now being widely applied in physical and social sciences, in policy and government, and in a variety of industries. This diversification has led to difficulties in actually creating and deploying real-world solutions, as key functionality becomes fragmented across ML-specific or domain-specific software libraries created by independent communities. The pace of ML innovation also means that any one library is unlikely to support the latest techniques. In addition, the complex and difficult process of building problem-specific end-to-end solutions continues to be marked by challenges such as formulating achievable learning problems, managing and cleaning data, scaling tuning procedures, and deployment and serving.

In practice, data scientists or ML engineers often develop ad hoc programs for new problems, writing a significant amount of "glue code" to connect components from different software libraries, and spending significant time processing different forms of raw input and interfacing with external systems. These

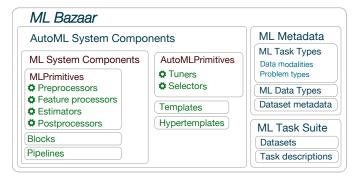


Fig. 1: The *ML Bazaar* universe. Components of machine learning software are carefully organized and designed to support effective development and deployment of end-to-end solutions for a variety of real-world tasks.

steps are tedious and error-prone and lead to the emergence of brittle "pipeline jungles" [1].

These points raise the question, "How can we make building machine learning solutions easier in practical settings?" This question applies to a spectrum of user populations, from a nuclear scientist performing a simple study to a data engineer creating an automated machine learning (AutoML) platform within a large enterprise.

A new comprehensive approach is needed to designing and developing software systems that solve machine learning tasks. Such an approach would address a wide variety of input data modalities, such as images, text, audio, signals, tabular data, relational data, time series, and graphs; it would support a wide variety of learning problem types, such as regression, classification, clustering, anomaly detection, community detection, graph matching, and collaborative filtering; it would cover the numerous intermediate stages involved in creating a solution for a ML task, such as data preprocessing, data munging, featurization, modeling, and evaluation; and it would support various levels of AutoML functionality to fine-tune solutions, such as hyperparameter tuning and model selection (Figure 2). Moreover, it would enable fast iteration on ideas, coherent APIs, and easy integration of new techniques and libraries. In sum, this ambitious goal would allow many or all end-to-end learning problems to be solved or built within a single framework.

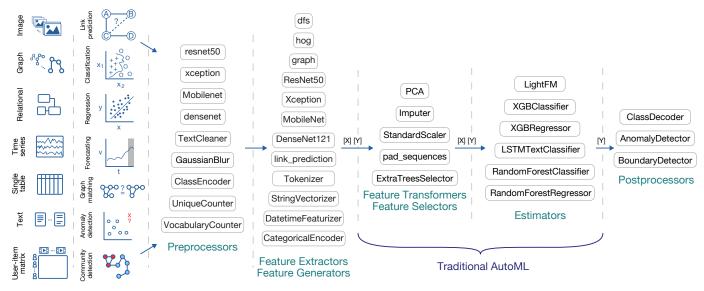


Fig. 2: Various ML task types that can be solved in *ML Bazaar* using composition of primitives (shown in the figure as boxes). Primitives are categorized into preprocessors, feature processors, estimators, and postprocessors and are drawn from many different ML libraries.

#### A. Introducing the Machine Learning Bazaar

In this paper, to address these challenges, we present the *Machine Learning Bazaar*, a multi-faceted approach to designing, organizing, and developing ML and AutoML software systems (Figure 1). We organize the ML ecosystem into a hierarchy of components, ranging from basic building blocks like individual classifiers to full-fledged AutoML systems. With our design, a user specifies an ML task (data modality, problem type, and the associated ML metadata), provides a raw dataset, and composes an end-to-end pipeline out of pre-existing annotated ML primitives. The resulting pipelines can be easily evaluated, tuned, and deployed across a variety of software and hardware settings. We also enable the rapid contribution, integration, and exchange of primitives from members of the community — promising components and pipelines can be thoroughly validated and evaluated across a variety of task types.

"Bazaar-style" software development is famously exemplified by the Linux community, "a great babbling bazaar of different agendas and approaches" [2]. Much like a bazaar, our approach is characterized by the availability of many compatible alternatives to achieve the same goal, a wide variety of libraries and custom solutions, broad coverage of ML task types, a space for contributors to bring primitives to support ML endeavors, and ready-to-use, pre-fit solutions for users who need to quickly complete a task.

Core components of *ML Bazaar* include a library of primitives (Section III-A), a runtime system for easily constructing pipelines (Section III-B), a hierarchy of AutoML search approaches (Section IV-B), and a full-fledged AutoML system developed using our own approaches (Section IV-C).

We have been successfully using *ML Bazaar* for a number of real-world use cases with industry collaborators, such as anomaly detection for satellite telemetry and failure prediction

in wind turbines (Section V-A). In addition, we have entered our *ML Bazaar* AutoML system in participation in the DARPA Data-Driven Discovery of Models (D3M) program [3]; ours is the first end-to-end, modular, publicly released system designed to meet the program's goal.

#### B. Contributions

Our contributions in this paper include:

A unified organization and API for ML and AutoML tasks: Our system enables users to specify a pipeline for any machine learning task, ranging from image classification to graph matching through a unified API.

The first general-purpose automated machine learning system: This is, to the best of our knowledge, the first publicly-available system with the ability to compose end-to-end solutions for a wide variety of ML task types defined over several different data types.

**Open source libraries**: Components of our system have been released as four modular libraries:

- MLPrimitives<sup>1</sup>: A specification for machine learning primitives (Section III-A) and an annotated collection from several libraries.
- MLBlocks<sup>2</sup>: A library for composing, training, and deploying end-to-end machine learning pipelines (Section III-B1).
- BTB<sup>3</sup>: An extensible library for developing AutoML systems (Section IV-B).

<sup>&</sup>lt;sup>1</sup>https://github.com/HDI-Project/MLPrimitives

<sup>&</sup>lt;sup>2</sup>https://github.com/HDI-Project/MLBlocks

<sup>&</sup>lt;sup>3</sup>https://github.com/HDI-Project/BTB

 piex<sup>4</sup>: A library for exploration and meta-analysis of machine learning task results.

**ML task suite**: We compile an extensive suite of machine learning datasets and tasks for experimentation, diagnostics, and more (Section III-C).

A comprehensive evaluation: We evaluated our AutoML system against our task suite (Section V), releasing a dataset of 3.9 million scored pipelines for community analysis.

# II. RELATED WORK

Researchers have developed numerous algorithmic and software innovations to make it possible to create ML and AutoML systems in the firstplace.

- a) ML libraries: Researchers today are fortunate to have access to high-quality libraries that have originated over a period of decades in separate academic communities. To support general ML applications, scikit-learn implements many different algorithms using a common API centered on the influential fit/predict paradigm [4]. For specialized analysis, libraries have been developed in separate academic communities, often with different and incompatible APIs [5]–[11]. In ML Bazaar, we connect and link components of these libraries, rather than creating any new functionality ourselves. Similarly, [12] standardizes interfaces and provides utilities for the R ecosystem, but without enabling more complex pipelines.
- b) AutoML libraries: In the AutoML setting, the best ML solution is sought for a particular problem without human involvement. Research in this area has often been limited to solving sub-problems of an end-to-end ML workflow, such as data cleaning [13], feature engineering [9], [14], or model selection and hyperparameter tuning [15]–[19]. Thus AutoML solutions are often not widely applicable or deployed in practice without human support. In contrast, ML Bazaar integrates many of these approaches and designs one coherent and configurable structure for joint tuning and selection of end-to-end pipelines.
- c) AutoML systems: These AutoML libraries, if deployed, are typically one component within a larger system that aims to manage several practical aspects such as parallel and distributed training, tuning, and model storage, and even serving, deployment, and graphical interfaces for model building. These include ATM [19], Vizier [20], and Rafiki [21], as well as commercial platforms like Google AutoML,<sup>5</sup> Amazon Forecast,<sup>6</sup> Azure Machine Learning Studio,<sup>7</sup> and DataRobot.<sup>8</sup> While these systems provide many benefits, they have several limitations. First, they each focus on a subset of ML use cases, such as vision, NLP, forecasting, or hyperparameter tuning, neglecting many of the other common practical uses of ML, which may require more careful data processing and pipeline composition. Second, these systems are designed as standalone applications and do not support community-driven integration

of new innovations. *ML Bazaar* provides a new approach to *developing* such ML and AutoML systems in the first place: it supports a wide variety of ML task types, and builds on top of a community-driven ecosystem of ML innovations. Indeed, it could serve as the backend for such ML services or platforms.

# III. THE MACHINE LEARNING BAZAAR

The *ML Bazaar* is a hierarchical organization and unified API of the ecosystem of machine learning software and algorithms. Within the *ML Bazaar*, we will find structured software components for every aspect of the practical machine learning process, from featurizers for relational datasets to signal processing transformers to neural networks to pretrained embeddings. From these components, or *primitives*, data scientists can easily and efficiently construct ML solutions for a variety of *ML task types*, and ultimately, automate much of the work of tuning these models (Section IV).

### A. ML Primitives

A *primitive* is the annotation of a reusable, self-contained, software component for machine learning. It is the most fundamental unit of machine learning computation in our system. It has a well-defined interface such that it receives input data in one of several formats or types, performs computations, and returns the data in another format or type, exposing a fit/produce interface.

As a result of this abstraction, widely varying machine learning functionality (from scikit-learn, XGBoost, networkX, LightFM, etc.) can be collected in a single curated repository, and each primitive can be re-used in chained computations (Section III-B) without callers writing any glue code.

Many primitives have no learning component and are trivial to specify, but are very important nonetheless. Useful primitives that fall into this category yet may be unfamiliar to many machine learning practitioners include the biomedical domain-specific functions in the MATLAB signal processing toolbox.

For each primitive, we annotate the conceptual types of declared inputs and outputs, providing a mapping between canonical types and synonyms used by specific libraries if necessary. This convenience will help dramatically decrease the amount of glue code users must write (Section III-B1).

The design of primitives is motivated by the following considerations:

- Lightweight wrappers: We aim to enable lightweight wrappers around the functionality of other existing libraries with mutually incompatible APIs to minimize redundancy and avoid the "yet-another-library" problem.
- *Evolving annotations*: We aim to naturally evolve primitive annotations, as primitives change due to hyperparameter settings, metadata tags, or improved implementations.
- Easy contribution: As new ML innovations and software emerge, we aim for contributors not even necessarily the original researchers to easily create and annotate new primitives, submit them for validation, and make them available to the community.

<sup>&</sup>lt;sup>4</sup>https://github.com/HDI-Project/piex

<sup>&</sup>lt;sup>5</sup>https://cloud.google.com/automl/

<sup>&</sup>lt;sup>6</sup>https://aws.amazon.com/blogs/aws/amazon-forecast-time-series-forecasting-made-easy/

<sup>&</sup>lt;sup>7</sup>https://azure.microsoft.com/en-us/services/machine-learning-studio/

<sup>8</sup>https://www.datarobot.com/

1) Implementation: Each primitive is annotated with metainformation about its inputs and outputs, with their ranges and data types, its hyperparameters, and other detailed metadata, such as the author, description, and documentation URL. The full annotation is provided in a self-contained JSON file with the following fields of note:

- primitive: The fully-qualified name of the underlying implementation as a Python object.
- fit, produce: The names and conceptual types of the primitive's inputs and outputs for the fit or produce phases. We call these recurring conceptual types *ML data types*, like a feature matrix X, a target vector y, or a space of class labels classes.
- hyperparameters: Details of all the hyperparameters of the primitive — their names, descriptions, data types, ranges, and whether they are fixed or tunable.

We have developed the open-source MLPrimitives library, which contains a curated set of high-quality, useful primitives, as well as formal specification of the primitive annotation format. Distributed as a widely-available Python package, end-users can pin versions of the package to access specific primitives, or update the package to gain access to the updated primitives. To support annotation of primitives from libraries that need significant adaptation to the fit/produce interface, MLPrimitives also provides a powerful set of adapter modules that assist in wrapping common patterns. Additionally, MLPrimitives enables easy contribution of new primitives in several ways by providing template and example primitive annotations and by providing procedures to validate proposed primitives against a formal JSON specification and a unit test suite.

# B. Building ML solutions

To solve practical machine learning problems, we must be able to instantiate and compose primitives into usable programs. These programs must be easy to specify with a natural interface, such that users can easily compose primitives without sacrificing flexibility. We aim to support both endusers trying to build an ML solution for their specific problem who may not be savvy about software engineering, as well as system developers wrapping individual ML solutions in AutoML components (Section IV) or otherwise. In addition, we provide an abstracted execution layer, such that learning, data flow, data storage, and deployment are handled automatically by various configurable and pluggable backends.

1) Blocks and Pipelines: While a primitive specifies an abstract unit of machine learning computation, to solve practical machine learning problems, we must be able to instantiate and compose these units into usable programs. We introduce ML blocks, software components that serve as the instantiations of primitives in a software program. Blocks load and interpret the underlying primitive annotation and provide a common interface to run a step in a larger machine learning system. Primitives are unique, but there may be multiple blocks representing one primitive in the same program.

Next, we introduce ML pipelines, which collect multiple blocks into a single computational graph. We define a pipeline as a directed acyclic multigraph  $L=\langle B,E,\lambda\rangle$ , where  $B=\{b_n\mid b_n\in A\}$  is a finite sequence of blocks, E are the directed edges between blocks representing data flow, and  $\lambda\in\Lambda$  is a hyperparameter vector. A valid pipeline— and its derivatives (Section IV-A) — must also satisfy acceptability constraints that require the inputs to each block to be satisfied by the outputs of another block connected by a directed edge.

We share the term "pipeline" with the ML/AutoML literature, which commonly refers to a chain of transformations of a feature matrix and target vector. However, we bring foundational data processing operations of raw inputs into this scope, like featurization of graphs, multi-table relational data, time series, text, and images, as well as simple data transforms, like encoding integer or string targets. This gives our pipelines a greatly expanded role, providing solutions to any ML task and spanning the entire machine learning process beginning with the raw dataset.

Large graph-structured workloads can be difficult to specify for end-users due to the complexity of the data structure. In ML Bazaar, we prioritize ease of specifying complex machine learning pipelines by providing a pipeline description interface (PDI) in which users specify only the topological ordering of all blocks in the pipeline without requiring any explicit dependency declarations. Full training-time (fit) and inference-time (predict) computational graphs can then be recovered from the PDI, without the user being required to write any "glue" code — the annotated ML data types of the blocks is usually sufficient to recover the graphs. The full graphs are then recovered by leveraging the observation that blocks that modify the same ML data type can be grouped into the same subpath. We add blocks to the graph in reverse order, iteratively adding edges when the block under consideration produces an output that is required by an existing block. This algorithm always recovers exactly one graph if a valid graph exists. In cases where multiple graphs have the same topological ordering, the user can additionally provide an input-output map to explicitly add edges and thereby select an alternate full graph. This process is demonstrated in Figure 3.

The resulting graphs describe abstract computational workloads, but we must be able to actually execute it for purposes of learning and inference. Many existing systems for scheduling and existing graph-structured workloads [22], [23] could be adapted to serve as backends to execute these machine learning workloads, which we compile to an intermediate representation. We implement one execution engine, MLBlocks, in which a collection of objects in a key-value store is iteratively transformed through sequential processing of blocks.

# C. ML task suite

As part of *ML Bazaar*, we release a comprehensive ML task suite for experimentation, evaluation, and diagnosis of

<sup>9</sup>We abuse "pipeline" to refer to a more complex, ML-specific computational graph which will not necessarily be a linear sequence of operations.

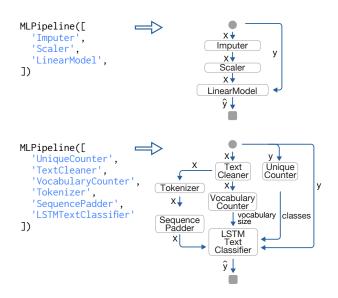


Fig. 3: Recovery of ML computational graphs from pipeline descriptions for a simple linear regression pipeline (top) and a more complex text classification pipeline (bottom). The ML data types that enable extraction of the graph, and stand for data flow, are labeled along edges.

primitives and pipelines. Our task suite consists of 431 real-world datasets spanning 14 ML tasks assembled from MIT Lincoln Laboratory, Kaggle, OpenML, Quandl, Crowdflower, and others, as well as annotated task descriptions, such as problem formulations and scoring metrics (Table I). We created train/test splits and organized the folder structure. Other than this, we do not do any preprocessing (sampling, outlier detection, imputation, featurization, scaling, or encoding), presenting data in its raw form as inputs to proposed end-to-end ML pipelines. Our holistic approach contrasts with other benchmarking approaches [20], [24], [25], which often target black-box optimization or estimation in isolation. We have organized and released these datasets and tasks for other researchers (Appendix B1).

ML experts developing new methods can use our ML task suite and integrate their proposed methods as replacement for a primitive or set of primitives. They can then evaluate the efficacy of the method across a realistic, general-purpose workload.

# IV. AUTOML SYSTEM DESIGN AND ARCHITECTURE

From the components of the *ML Bazaar*, data scientists can easily and effectively build machine learning pipelines with fixed hyperparameters for their specific problems. To improve the performance of these solutions, we first introduce *templates* and *hypertemplates*, which generalize pipelines by allowing a tunable hyperparameter configuration space to be specified. Next, we describe a set of *AutoML primitives* which facilitate hyperparameter tuning and model selection. Finally, we present the design and architecture of an AutoML system built on top of these innovations. Our system, which we have used to enter

Data ModalityProblem TypeTasksgraphcommunity detection graph matching link prediction vertex nomination2 9 1 2 2 2 2 3 4 4 1 2 3 4 4 4 5 4 5 5 6 1 2 3 4 4 4 5 4 5 4 5 5 6 6 7 7 8 9 9 1 1 1 2 2 3 4 4 4 5 5 5 6 1 1 2 3 4 4 5 4 5 5 5 6 1 7 8 9 9 1 1 1 2 2 3 4 4 4 5 4 5 4 5 4 5 5 5 6 7 8 9			
graph matching   9   link prediction   1   vertex nomination   1   limage   classification   5   regression   1   limage   classification   1   regression   1   limage   classification   234   collaborative filtering   1   regression   86   timeseries forecasting   35   lext   classification   17	Data Modality	Problem Type	Tasks
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timeseries forecasting 35 text classification 17	_	collaborative filtering	1
text classification 17		regression	86
		timeseries forecasting	35
timeseries classification 37	text	classification	17
	timeseries	classification	37

TABLE I: ML task types (data modality and problem type pairs) handled by the *ML Bazaar* AutoML system and the associated ML tasks counts in our evaluation corpus.

the DARPA D3M competition, automatically selects templates from available options and tunes the hyperparameters of those templates by evaluating millions of pipelines in a distributed setting.

#### A. Templates and Hypertemplates

Frequently, pipelines require hyperparameters to be specified at several places. Unless these values are fixed at annotationtime, hyperparameters must be exposed in a machine-friendly interface. This motivates generalizing pipelines through templates and hypertemplates and providing first-class tuning support.

We define a *template* as a directed acyclic multigraph  $T = \langle B, E, \Lambda \rangle$ , where B is a sequence of blocks, E are directed edges between blocks, and  $\Lambda$  is the hyperparameter configuration space for the underlying primitives. By providing values for the unset hyperparameters of a template, a concrete pipeline is created.

In some cases, certain values of hyperparameters can affect the domains of other hyperparameters. For example, the type of kernel for a support vector machine results in different kernel hyperparameters, and preprocessors used to adjust for class imbalance can affect the training procedure of a downstream classifier. We call these *conditional hyperparameters*, and accommodate them with hypertemplates. We define a *hypertemplate* as a directed acyclic multigraph  $H = \langle B, E, \bigcup_j \Lambda_j \rangle$ , where B is a sequence of blocks, E are directed edges between blocks, and  $\Lambda_j$  is the hyperparameter configuration space for template  $T_j$ . Note that a number of templates can be derived from one hypertemplate by fixing the conditional hyperparameters (Figure 4).

# B. AutoML Primitives

Just as primitives represent components of machine learning computation, AutoML primitives represent components of an AutoML system. We separate AutoML primitives into *tuners* and *selectors*. These underly our extensible AutoML

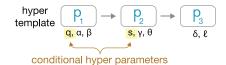


Fig. 4: A hypertemplate (top) has three primitives. The first primitive has a conditional hyperparameter q and the second has a conditional hyperparameter s. In this case, 4 templates, each with tunable hyperparameters, can be extracted from the hypertemplate by traversing the conditional hyperparameter tree.

library, BTB ("Bayesian Tuning and Bandits"), which facilitates easy integration of methodological developments by AutoML developers.

1) Tuners: Given a template, an AutoML system must find a specific pipeline with fully-specified hyperparameter values to minimize some cost. For template T with hyperparameter space  $\Lambda$ , and a function f that assigns a performance score to pipeline  $L_{\lambda}$  with hyperparameters  $\lambda \in \Lambda$ , we define the tuning problem as

$$\lambda^* = \operatorname*{arg\,max}_{\lambda \in \Lambda} f(L_{\lambda}). \tag{1}$$

Hyperparameter tuning is widely studied and its effective use is instrumental to maximizing the performance of machine learning solutions [15], [17], [26]. Since f is expensive to evaluate, as the model is trained several times to compute a desired metric via cross-validation, the number of evaluations should be minimized. Within ML Bazaar, we focus on Bayesian optimization, a black-box optimization technique in which expensive evaluations of f are minimized by forming and updating a meta-model for f. At each iteration, the next hyperparameter configuration to try is chosen according to an acquisition function.

Researchers have argued for different formulations of metamodels (often in terms of the different kernels of Gaussian Processes) and acquisition functions [15], [27], [28]. We structure these meta-models and acquisition functions as separate AutoML primitives that can be combined together to form a *tuner*. Tuners provide a record/propose interface in which evaluation results are recorded to the tuner and new hyperparameters are proposed. For example, the GCP-EI tuner uses the Gaussian Copula Process meta-model primitive and the Expected Improvement acquisition function primitive.

2) Selectors: For many ML task types, there may be multiple templates or hypertemplates available as possible solutions, each with their own tunable hyperparameters. The aim is to balance the exploration-exploitation tradeoff while selecting

promising templates to tune. For a set of templates  $\mathcal{T} = \{T_1, \dots, T_m\}$ , we define the selection problem as

$$T^* = \underset{T \in \mathcal{T}}{\arg \max} \ \mathbb{E}[\max_{\lambda_T \in \Lambda_T} f(L_{\lambda_T})]. \tag{2}$$

The selection problem is treated as a multi-armed bandit problem where for a selected template, the score achieved as a result of tuning can be assumed to come from an unknown underlying probability distribution. We structure selectors as AutoML primitives providing a compute\_rewards/select API, with different decision criteria acting on the history of pipeline scores. For example, the upper confidence bound method [29] is represented by the UCB1 selector, where scores achieved for each template are converted into rewards, given by

$$z_j = \frac{1}{n_j} \sum_i s_{ij} \tag{3}$$

where  $s_{ij}$  is the score achieved by template j at iteration i. The choice is then made using:

$$j^* = \arg\max_j z_j + \sqrt{\frac{2\log n}{n_j}},\tag{4}$$

where n is the total number of iterations and  $n_j$  is the number of times template j was chosen.

# C. Building an AutoML system

Whereas composition of high-quality primitives enables data scientists to build machine learning solutions (Section III), by combining AutoML primitives in a carefully designed and architected manner, we have built an end-to-end, general-purpose, distributed, multi-task, automated machine learning system. We have used this system to search millions of pipelines for a variety of tasks.

Our AutoML system is given a dataset D, a collection of primitives A, and an evaluation function f, which captures information about the problem type and scoring routine. First, it must assemble the primitives into a collection of candidate templates,  $\mathcal{T}$ . Next, it determines pipelines to evaluate and produces  $\{\langle L_{i,\lambda}, f(L_{i,\lambda})\rangle\}$ , where  $L_{i,\lambda}$  was generated from template i. Finally, it decides which of the evaluated pipelines best solves the problem and returns the trained pipeline,  $L^*$ .

The *ML Bazaar* AutoML system consists of several components: user interfaces for administration and configuration, loaders and configuration for ML tasks and primitives and other components, data stores for metadata and pipeline evaluation details, a pipeline execution engine, an AutoML coordinator, and distributed pipeline evaluation workers (Figure 5). In this section, we focus on key aspects of the design and architecture of our system. An overview of the system is shown in Figure 5.

Users with an ML task provide their dataset and its metadata, details about their learning problem, and access to available computational resources. They also can provide custom components, such as primitives or templates, from a personal- or organization-wide collection; these will be considered in the search process in addition to the default,

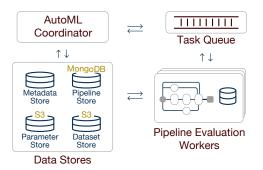


Fig. 5: System architecture of the ML Bazaar AutoML system

curated collection available in our open-source repositories. The AutoML coordinator is the master node that runs the main template selection and hyperparameter tuning loop. To begin, the coordinator determines the next ML task, and queries the database - which stores metadata about the ML tasks and records of all evaluated pipelines — for all associated pipelines. Using this, it asks the selector for the next template, and the associated tuner for the next pipeline, which it inserts to the database in a pending state and adds to a task queue. Pipeline evaluation workers wait on the task queue for new pipelines to evaluate. Once one is available, they get its full specification from the pipeline store and evaluate it using the configured pipeline execution engine, such as MLBlocks. The results are written to the relevant data stores and the coordinator is notified. The process concludes when all resources have been consumed.

While this is one example, AutoML system developers within an organization can support the efforts of their data scientists by configuring their system with custom backends or cloud-specific infrastructure on their cloud of choice. This development is aided by the organization we impose on system components.

#### V. EVALUATION

In this section, we evaluate *ML Bazaar* along several axes. We first describe the real-world use cases (both ML and AutoML) in which we have already deployed *ML Bazaar*. Next, we demonstrate the ability of the *ML Bazaar* AutoML system to automatically solve a wide variety of ML task types on a comprehensive evaluation corpus and assess the system's performance across a variety of metrics. Next, we leverage *ML Bazaar* to perform several case studies, in which we assess the value of specific ML and AutoML primitives.

# A. Use cases

*ML Bazaar* is currently used in four application domains. Below we highlight these domains and how it addresses their unique needs.

a) Anomaly detection for satellite telemetry: ML Bazaar is used by a communications satellite operator which provides video and data connectivity globally. This company wanted to monitor more than 10,000 telemetry signals from the satellites and identify anomalies, which might indicate a looming failure severely affecting the satellite's coverage. To enable

this, we added a new AnomalyDetector postprocessing primitive for time series. The primitive's input is a time series, and its output is a list of anomalies, identified by intervals  $\{[t_i,t_{i+1}]\}$ . We were then able to easily implement an end-to-end anomaly detection method [30] using pre-existing transformation primitives in ML Bazaar and through a new primitive for the specific LSTM architecture used in the paper. Much like the AutoML system presented in Section IV-C, a system created around ML Bazaar enables a database of pipelines, and anomalies detected by those pipelines are stored in a database.

b) Failure prediction in wind turbines: ML Bazaar is also used by a multinational energy utility to predict critical failures and stoppages in their wind turbines. Most prediction problems here pertain to time series classification. As a result, we were able to use time series from 140 turbines to develop multiple pipelines, tune them, and produce prediction results. A generic time series input representation allowed us to address two critical needs: (1) as more data sources became available, the pipelines could ingest this new data, without the need to change the software implementation; and (2) the input representation of the labels associated with each time series allowed the enduser to try many different problem formulations, predicting everything from stoppage and pitch failure to less common issues, such as gearbox failure.

c) Leaks and crack detection in water distribution systems: A global water technology provider uses *ML Bazaar* for a variety of machine learning needs, ranging from image classification for detecting leaks from images, to crack detection from time series data, to demand forecasting using water meter data. A system like *ML Bazaar* provides a unified framework for these disparate machine learning needs. The team also builds custom primitives internally and uses them directly with the MLBlocks backend.

d) DARPA D3M program: ML Bazaar is used to design an AutoML system and make submissions for DARPA's Data-Driven Discovery of Models (D3M) program [3]. With the help of the National Institute of Standards and Technology (NIST), DARPA runs the system on a number of datasets spanning several tasks. The system is run for an hour on each dataset. At the end of the run, the pipeline produced by the AutoML system is evaluated on the test data. For each dataset, a baseline solution is provided by MIT Lincoln Laboratory, and our system's solution is compared against it. We have submitted our system 3 times, adding new primitives each time. In Figure 6 we present results of our latest submission.

# B. Experimental setup

In our experiments, we use the *ML Bazaar* Task Suite (Section III-C) and the available templates and hypertemplates from our curated collection. We run the search process for all tasks in parallel on a heterogenous cluster of 400 AWS EC2 nodes, comprised of m4.xlarge (4 CPU, 16G RAM), m4.2xlarge (8 CPU, 32GB RAM), and m4.10xlarge (40 CPU, 160GB RAM) instances. In this multi-task architecture, pipelines for each task are independently tuned and scored

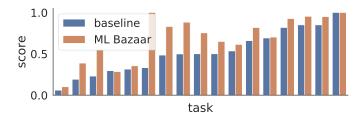


Fig. 6: Performance of *ML Bazaar* pipelines on DARPA D3M Challenge benchmark datasets. Our performance is compared to expert-generated baselines, for which *ML Bazaar* outperforms on 15/17 tasks. Performance metrics are all scaled to range on [0, 1].

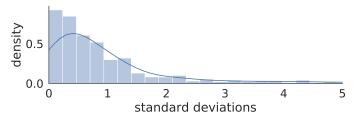


Fig. 7: Distribution of task performance improvement from *ML Bazaar* AutoML. Improvement for each task is measured as the score of the best pipeline less the score of the initial default pipeline, in standard deviations of all pipelines evaluated for that task.

via 5-fold cross-validation on separate machines over a 2-hour time limit, at a rate of 0.16 pipelines/node/second. Metadata and fine-grained details about every pipeline evaluated is stored in a MongoDB document store. Ultimately, the best pipeline for each task is selected by considering the cross-validation score on the training set, and is then re-scored on the held-out test set.

#### C. AutoML performance

We first compare the *ML Bazaar* system to strong human baselines from DARPA's D3M challenge. Experts at MIT Lincoln Laboratory manually designed and tuned pipelines and provided the best-performing pipeline's score on test data for 17 ML tasks. For these tasks, we run our system and select the pipeline that maximizes the cross-validation score, then compute scores on an unseen test set. The results are shown in Figure 6. We find that *ML Bazaar* substantially outperforms the baselines ( $\mu = 0.17$ ,  $\sigma = 0.18$ ), finding superior pipelines for 15/17 tasks.

Another important attribute of the system is the ability to improve pipelines for different tasks through search and tuning. We measure the improvement in the best pipeline per task in Figure 7. We find that the average task improves its best score by 0.96 standard deviations over the course of tuning, and that 29.3% of tasks improve by more than 1 standard deviation.

# D. Case study: evaluating new ML primitives

When new primitives are contributed by the ML community, they become candidates for inclusion in templates and

hypertemplates, either to replace similar blocks or to form the basis of new topologies. By running the end-to-end system on our evaluation corpus of datasets and tasks, we can assess the impact of the primitive *in general*, rather than on a small set of over-fit baselines.

In this first case study, we consider the hypothetical contribution of a new primitive that annotates the gradient boosting machine XGBoost (XGB) [10], [31]. This primitive replaces the default random forest (RF) estimator in any templates in which it appeared. To compare these two primitives, we ran two experiments, one in which XGB is used as the main estimator and one in which RF is used.

We evaluate 1.9 million pipelines in total. For each experiment, we determine the best scores produced per task. We find that the XGB pipelines significantly outperformed the RF pipelines, winning 64.5% of the comparisons. This confirms the experience of practitioners, who widely report that XGBoost is one of the most powerful ML methods for classification and regression.

# E. Case study: evaluating AutoML primitives

The design of the *ML Bazaar* AutoML system and our extensive evaluation corpus allows us easily swap in new AutoML primitives (Section IV-B) to see to what extent changes in components like tuners and selectors can improve performance in general settings.

In this case study, we revisit [15], a work which was partially responsible for bringing about the widespread use of Bayesian optimization for tuning ML models in practice. Their contributions include: (1) proposing the usage of the Matérn 5/2 kernel, (2) describing an integrated acquisition function that integrates over uncertainty in the GP hyperparameters, (3) incorporating a cost model into an expected improvement per second acquisition function, and (4) explicitly modeling pending parallel trials. How important was each of these contributions to the resulting tuner (or tuners)?

Using ML Bazaar, we show how a more thorough ablation study [32], not present in the original work, would be conducted to address these questions, by assessing the performance of our general-purpose AutoML system using different combinations of these 4 contributions. Here, we focus on the proposal of the Matérn 5/2 kernel for the tuner meta-model (Section IV-B1), given by

$$K_{\text{M52}}(\mathbf{x}, \mathbf{x}') = \theta_0 \left( 1 + \sqrt{5r^2(\mathbf{x}, \mathbf{x}')} + \frac{5}{3}r^2(\mathbf{x}, \mathbf{x}') \right)$$
$$\cdot \exp \left\{ -\sqrt{5r^2(\mathbf{x}, \mathbf{x}')} \right\},$$

where  $r^2(\mathbf{x}, \mathbf{x}') = \sum_{d=1}^D (x_d - x_d')^2/\theta_d^2$  and D is the dimensionality of the configuration space.

We run experiments using a baseline tuner with a squared exponential kernel (GP-SE-EI) and compare it with a tuner using the Matérn 5/2 kernel (GP-Matern52-EI). In both cases, the kernel hyperparameters are set by optimizing the marginal likelihood. This experiment allows us to isolate the

contributions of the proposed kernel in the context of general-purpose ML workloads.

We find that there is no significant improvement from using the Matérn 5/2 kernel over the SE kernel — in fact, the GP-SE-EI tuner outperforms, winning 60.1% of the comparisons. One possible explanation for this negative result is that the Matérn kernel is sensitive to hyperparameters which are set more effectively by optimization of the integrated acquisition function. This is supported by the over-performance of the tuner using the integrated acquisition function in the original work; however, the integrated acquisition function is not tested with the baseline SE kernel, and more study is needed.

#### VI. CONCLUSION

Throughout this paper, we have built up abstractions, APIs, and software components for data scientists and other practitioners to effectively develop machine learning software systems. Users of *ML Bazaar* can develop one-off pipelines, tuned templates, or full-fledged distributed AutoML systems. Researchers can contribute ML or AutoML primitives and make them easily accessible to a broad base for inclusion in end-to-end solutions.

We have applied this approach to three different real-world ML problems and entered our AutoML system in a modeling challenge. As we collect more and more scored pipelines, we expect opportunities will emerge for meta-learning and debugging on ML tasks and pipelines, as well as the ability to track progress and transfer knowledge within data science organizations.

In future work, we will focus on several complementary extensions. These include continuing to improve our AutoML system and making it more robust for everyday use by a diverse user base, as well as formalizing the AutoML benchmarking problem across pipelines and tasks to address the system comparison problem.

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#### REFERENCES

- D. Sculley, G. Holt, D. Golovin, E. Davydov, T. Phillips, D. Ebner, V. Chaudhary, M. Young, J.-F. Crespo, and D. Dennison, "Hidden technical debt in machine learning systems," in *Advances in neural* information processing systems, 2015, pp. 2503–2511.
- [2] E. Raymond, "The cathedral and the bazaar," Knowledge, Technology & Policy, vol. 12, no. 3, pp. 23–49, 1999.
- [3] R. Lippmann, W. Campbell, and J. Campbell, "An overview of the darpa data driven discovery of models (d3m) program," in NIPS 2016 Workshop on Artificial Intelligence for Data Science, 2016.

- [4] L. Buitinck, G. Louppe, M. Blondel, F. Pedregosa, A. Mueller, O. Grisel, V. Niculae, P. Prettenhofer, A. Gramfort, J. Grobler, R. Layton, J. VanderPlas, A. Joly, B. Holt, and G. Varoquaux, "API design for machine learning software: experiences from the scikit-learn project," in ECML PKDD Workshop: Languages for Data Mining and Machine Learning, 2013, pp. 108–122.
- [5] S. Bird, E. Klein, and E. Loper, Natural language processing with Python: analyzing text with the natural language toolkit. "O'Reilly Media, Inc.", 2009.
- [6] G. Bradski, "The OpenCV Library," Dr. Dobb's Journal of Software Tools, 2000.
- [7] A. A. Hagberg, D. A. Schult, and P. J. Swart, "Exploring network structure, dynamics, and function using networkx," in *Proceedings of the* 7th Python in Science Conference (SciPy2008), G. Varoquaux, T. Vaught, and J. Millman, Eds., pp. 11–15.
- [8] M. Kula, "Metadata embeddings for user and item cold-start recommendations," in *Proceedings of the 2nd Workshop on New Trends on Content-Based Recommender Systems*, vol. 1448, 2015, pp. 14–21.
- [9] J. M. Kanter, "Deep Feature Synthesis:Towards Automating Data Science Endeavors," in 2015 IEEE International Conference on Data Science and Advanced Analytics (DSAA), 2015, pp. 1–10.
- [10] T. Chen and C. Guestrin, "XGBoost: A scalable tree boosting system," in *Proceedings of the 22nd ACM SIGKDD International Conference on Knowledge Discovery and Data Mining*, ser. KDD '16. New York, NY, USA: ACM, 2016, pp. 785–794.
- [11] A. Paszke, S. Gross, S. Chintala, G. Chanan, E. Yang, Z. DeVito, Z. Lin, A. Desmaison, L. Antiga, and A. Lerer, "Automatic differentiation in pytorch," 2017.
- [12] M. Kuhn, "Building Predictive Models in R Using the caret Package," Journal of Statistical Software November, vol. 28, no. 5, pp. 159–160, 2008.
- [13] D. Deng, R. Castro, F. Ziawasch, A. Sibo, A. Elmagarmid, I. F. Ilyas, S. Madden, M. Ouzzani, and N. Tang, "The Data Civilizer System," 8th Biennial Conference on Innovative Data Systems Research (CIDR 17), 2017
- [14] U. Khurana, D. Turaga, H. Samulowitz, and S. Parthasrathy, "Cognito: Automated feature engineering for supervised learning," in *Data Mining Workshops (ICDMW)*, 2016 IEEE 16th International Conference on. IEEE, 2016, pp. 1304–1307.
- [15] J. Snoek, H. Larochelle, and R. P. Adams, "Practical bayesian optimization of machine learning algorithms," in *Advances in neural information processing systems*, 2012, pp. 2951–2959.
- [16] C. Thornton, F. Hutter, H. H. Hoos, and K. Leyton-Brown, "Auto-weka: combined selection and hyperparameter optimization of classification algorithms," in KDD, 2013.
- [17] M. Feurer, A. Klein, K. Eggensperger, J. Springenberg, M. Blum, and F. Hutter, "Efficient and robust automated machine learning," in *Advances in Neural Information Processing Systems*, 2015, pp. 2962–2970.
- [18] R. S. Olson, N. Bartley, R. J. Urbanowicz, and J. H. Moore, "Evaluation of a tree-based pipeline optimization tool for automating data science," in GECCO, 2016.
- [19] T. Swearingen, W. Drevo, B. Cyphers, A. Cuesta-Infante, A. Ross, and K. Veeramachaneni, "Atm: A distributed, collaborative, scalable system for automated machine learning," in *IEEE International Conference on Big Data*, 2017.
- [20] D. Golovin, B. Solnik, S. Moitra, G. Kochanski, J. Karro, and D. Sculley, "Google Vizier: A Service for Black-Box Optimization," in *Proceedings* of the 23rd ACM SIGKDD International Conference on Knowledge Discovery and Data Mining, 2017.
- [21] W. Wang, J. Gao, M. Zhang, S. Wang, G. Chen, T. K. Ng, B. C. Ooi, J. Shao, and M. Reyad, "Rafiki: machine learning as an analytics service system," *Proceedings of the VLDB Endowment*, vol. 12, no. 2, pp. 128– 140, 2018.
- [22] M. Rocklin, "Dask: Parallel computation with blocked algorithms and task scheduling," in *Proceedings of the 14th Python in Science Conference*, K. Huff and J. Bergstra, Eds., 2015, pp. 130 – 136.
- [23] M. Zaharia, R. S. Xin, P. Wendell, T. Das, M. Armbrust, A. Dave, X. Meng, J. Rosen, S. Venkataraman, M. J. Franklin, A. Ghodsi, J. Gonzalez, S. Shenker, and I. Stoica, "Apache spark: A unified engine for big data processing," *Commun. ACM*, vol. 59, no. 11, pp. 56–65, Oct. 2016.
- [24] B. Bischl, G. Casalicchio, M. Feurer, F. Hutter, M. Lang, R. G. Mantovani, J. N. van Rijn, and J. Vanschoren, "Openml benchmarking suites and the openml100," arXiv preprint arXiv:1708.03731, 2017.

- [25] I. Guyon, K. Bennett, G. Cawley, H. J. Escalante, S. Escalera, T. K. Ho, N. Macià, B. Ray, M. Saeed, A. Statnikov, and E. Viegas, "Design of the 2015 ChaLearn AutoML challenge," *Proceedings of the International Joint Conference on Neural Networks*, vol. 2015-September, 2015.
- [26] J. S. Bergstra, R. Bardenet, Y. Bengio, and B. Kégl, "Algorithms for hyper-parameter optimization," in *Advances in neural information processing systems*, 2011, pp. 2546–2554.
- [27] C. Oh, E. Gavves, and M. Welling, "Bock: Bayesian optimization with cylindrical kernels," *arXiv preprint arXiv:1806.01619*, 2018.
- [28] H. Wang, B. van Stein, M. Emmerich, and T. Back, "A new acquisition function for bayesian optimization based on the moment-generating
- function," in 2017 IEEE International Conference on Systems, Man, and Cybernetics (SMC). IEEE, 2017, pp. 507–512.
- [29] P. Auer, N. Cesa-Bianchi, and P. Fischer, "Finite-time analysis of the multiarmed bandit problem," *Machine learning*, vol. 47, no. 2-3, pp. 235–256, 2002.
- [30] K. Hundman, V. Constantinou, C. Laporte, I. Colwell, and T. Soderstrom, "Detecting spacecraft anomalies using lstms and nonparametric dynamic thresholding," arXiv preprint arXiv:1802.04431, 2018.
- [31] L. Breiman, "Arcing the edge," Statistics, vol. 4, pp. 1–14, 1997.
- [32] Z. C. Lipton and J. Steinhardt, "Troubling trends in machine learning scholarship," arXiv preprint arXiv:1807.03341, 2018.

#### **APPENDIX**

#### A. Replicating ML Bazaar evaluation

In Section V, we analyzed a corpus of 3.9 million pipelines that solve 431 datasets and ML tasks. We include exact replication files here:

```
https://github.com/micahjsmith/ml-bazaar-2019
```

Instructions are provided in the repository; all figures and analyses can be reproduced using the make command, which builds a Docker image, installs software dependencies, and runs analysis files.

#### B. Using piex

The datasets and tasks we used in our experiments can be accessed using the piex pipeline explorer and analysis Python package that we have released as part of our research. The same package enables user to explore experimental results, pipelines and templates. Detailed instructions on usage of piex are available here:

```
https://github.com/HDI-Project/piex
```

In this section, we will highlight several key commands of the piex package to enable the exploration and analysis of our exact datasets, tasks, and test results.

```
1 >>> from piex.explorer import S3PipelineExplorer
2 >>> ex = S3PipelineExplorer('ml-pipelines-2018')
```

1) Datasets and tasks: The list of all datasets that we have used in Task Suite can be obtained as follows:

```
1 >>> datasets = ex.get_datasets()
```

The result of the command above is a DataFrame with four columns: dataset, data\_modality, task\_type, task\_subtype. One can select the datasets by running the command:

2) Tests and Results: Throughout our description we refer to a search process as a test. A test is defined as a search process for a given ML task (dataset, problem definition) and template. This consists of proposing and scoring pipelines generated from the template using our AutoML library, BTB, before identifying the best-performing pipeline.

The list of tests that have been executed can be obtained as follows:

```
1 >>> tests = ex.get_tests()
```

This method returns a DataFrame that contains a row for each test that has been run. There are several fields recorded for each test and we present a snapshot in Table II.

In total we have run 2152 tests across 431 datasets.

a) Getting results for a test: Results for a single test—an end-to-end AutoML run for 2 hours for a ML task can be extracted as follows:

A number of metrics are collected for each test and a subset of them are described in Table III. With these, one can calculate the improvement in cv-score or the score as a function of time and/or tuning iterations.

b) Getting the best pipeline or template: Information about the best pipeline for a dataset can be obtained using the get\_best\_pipeline method. This method returns information about the pipeline that obtained the best cross validation score during the tuning, as well as the template that was used to build it.

```
1 >>> ex.get_best_pipeline('185_baseball')
```

It returns among other information the *id* of the best pipeline, the score, and the template *id* associated with it.

```
88dcfe93-2d4a-41d4-889b-90377153cf76
dataset
                     185_baseball_dataset_TRAIN
metric
                                         f1Macro
name
            single_table/classification/default
rank
                                        0.307683
                                        0.692317
score
template
                       5bceaa5d49e71569e8bf7f81
test id
                            20181129084807729996
                        2018-11-29 09:26:39.757
pipeline
            single_table/classification/default
data_modality
                                    single table
task_type
                                  classification
Name: 2187854, dtype: object
```

Similarly, one can also obtain the name of the best template for a dataset.

3) Scoring a pipeline: This command runs a cross validation test and generates a cv-score for the dataset using the pipeline.

Column	Description
budget	time or number of iterations provided as a budget for the test
checkpoints	points in time when the best pipeline so far is evaluated on validation set
commit	commit tag of the repository used for running the tests
dataset	name of the dataset
insert_ts template status test_id update_ts data_modality task_type task_subtype metric	timestamp when the first pipeline was fit for the task template used for the test status of whether test finished unique identifier for the test the last time a pipeline was fit data modality of the dataset problem type of the test (note differing terminology) problem subtype of the test metric used to evaluate the pipeline
test_features	number of features in the validation set
test_samples	number of samples in the validation set
train_features	number of features in the training set
train_samples	number of samples in the training set

TABLE II: Test metadata, available through the piex library.

Column	Description
test_id	unique identifier for the test
template	the template used in the test
score	score achieved on the validation set
cv_score	cross validation score achieved on the training set
elapsed	time elapsed since the beginning of the test
iterations	number of tuning iterations executed

TABLE III: Test results, available through the piex library.