Collaborative, open, and automated data science

by

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Submitted to the Department of
Electrical Engineering and Computer Science
in partial fulfillment of the requirements for the degree of

Doctor of Philosophy in Computer Science

at the

MASSACHUSETTS INSTITUTE OF TECHNOLOGY

September 2021

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Abstract

Data science and machine learning have already revolutionized many industries and organizations and are increasingly being used in an open-source setting to address important societal problems. However, there remain many challenges to developing predictive machine learning models in practice, such as the complexity of the steps in the modern data science development process, the involvement of many different people with varying skills and roles, and the necessity of, yet difficulty in, collaborating across steps and people. In this thesis, I describe progress in two directions in supporting the development of predictive models.

First, I propose to focus the effort of data scientists and support structured collaboration on the most challenging steps in a data science project. In *Ballet*, we create a new approach to collaborative data science development, based on adapting and extending the open-source software development model for the collaborative development of feature engineering pipelines, and is the first collaborative feature engineering framework. Using Ballet as a probe, we conduct a detailed case study analysis of an open-source personal income prediction project in order to better understand data science collaborations.

Second, I propose to supplement human collaborators with advanced automated machine learning within end-to-end data science and machine learning pipelines. In the *Machine Learning Bazaar*, we create a flexible and powerful framework for developing machine learning and automated machine learning systems. In our approach, experts annotate and curate components from different machine learning libraries, which can be seamlessly composed into end-to-end pipelines using a unified interface. We build into these pipelines support for automated model selection and hyperparameter tuning. We use these components to create an open-source, general-purpose, automated machine learning system, and describe several other applications.

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On the Internet, nobody knows you're a dog.

Peter Steiner

Acknowledgements

To my adviser, Kalyan Veeramachaneni, thank you for being a mentor, a teacher, a collaborator, and a friend. I think it's fair to say that we took a chance on each other and that it has turned out pretty well so far. You have shown me that there is more to research than academia.

To my thesis readers, Saman Amarasinghe and Rob Miller, thank you for your support in my thesis formulation and defense and for your helpful feedback.

To my co-authors and other collaborators during my Ph.D. research, I am grateful and proud to have worked with every single one of you: Carles Sala, ChengXiang Zhai, Dongyu Liu, Huamin Qu, Jack Feser, Jürgen Cito, José Cambronero, Kelvin Lu, Lei Xu, Max Kanter, Md. Mahadi Hasan, Plamen Kolev, Qianwen Wang, Qiaomu Shen, Roy Wedge, Sam Madden, Santu Karmaker, Yao Ming, and Zhihua Jin. Without you, this research would not be possible. In particular, to Carles Sala, thanks for your close collaboration on so many projects and for our strong-headed disagreements that have made me a better designer and developer.

To my fellow Ph.D. students, postdocs, and other researchers in the Data to AI Lab at MIT over the years, thank you for feedback and discussion on research ideas and software, keeping me company in 32-D712, and tolerating my wisecracks in our group meetings: Alicia Sun, Lei Xu, Ola Zytek, Dongyu Liu, Iván Ramírez Díaz, Santu Karmaker, and many others.

To all those who have collaborated with me in one way or another on the Ballet project, especially those who have contributed to the *predict-house-prices*, *predict-census-income*, and *predict-life-outcomes* projects, I thank you for your time and effort in moving forward the vision of collaborative and open data science.

To the staff at MIT, thanks for all you do to support other students and me: Michaela Henry, Arash Akhgari, Brian Jones, Leslie Kolodziejski, Janet Fischer, Gracie Jin Gao, and Cara Giaimo.

To (most) anonymous reviewers of my research papers, thank you for engaging honestly with my work and providing helpful feedback, whether positive or negative.

As maligned as it, I believe in the power of high-quality peer review. My research has significantly improved as a result of peer review over the course of my Ph.D. program.

To academic mentors past, thank you for your wisdom and your investment in me: Seyhan Erden, Marco Del Negro, Marc Giannoni, Mike Woodbury, Gregory Wornell.

To teachers and instructors in computer science and mathematics over the years who have filled me with wonder, amazement, and passion for these beautiful subjects: Adam Cannon, Jae Woo Lee, Rachel Ollivier, Hubertus Franke, Benjamin Goldberg, Leslie Pack Kaelbling, Michael Sipser, Rob Miller, Casey Rodriguez, Max Goldman.

To the Muddy Charles and everyone in the community, thank you for keeping me sane. The three best things about going to MIT are the Charles River, the Stata Center, and the Muddy. To Mike Grenier, for showing a greater love for *science* than anyone I know.

To friends at MIT, thank you for talking shop, letting loose, inspiring me with the amazing things you do, always showing humility, being surprisingly normal, helping me survive this experience in one piece, and touching my time at MIT in one way or another: Maz Abulnaga, Caris Moses, José Cambronero, Flora Meng, Will Stephenson, Anish Agarwal, Jason Altschuler, Amanda Beck, Sam DeLaughter, Josh Saul, Anne Tresansky, Tarfah Alrashed, Willie Boag, Leilani Gilpin.

To all my friends, thank you for your friendship, support, and love: you know who you are.

To my family, thank you for your love and support. You keep me grounded and inspire me with your commitment to education and intellectual inquiry.

To Mamba, who can't read this but has shown me great wonder and joy, especially during the most trying days.

To my wife Alex, you have been with me through this entire journey, from filling out graduate school applications on Mulberry Street, to riding intercity buses around the Northeast, to going on adventures with our friends and family all over the world, to trying to stay sane in our living room during a pandemic, to planning our wedding (twice!) in the breaks from research. Thank you for your support, your patience, and your belief in me. I love you always.

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Chapter 1

Introduction

Data science and machine learning have become vital decision-making tools in enterprises across many fields. In recent years, a subfield of data science called predictive machine learning modeling has seen especially widespread usage. Companies use predictive modeling to automatically monitor computer logs and digital sensors to detect anomalies or identify cyberattacks. Social media platforms use predictive modeling to rank the items that appear in the feeds of their users in an attempt to serve more engaging and interesting content. Physicians use predictive modeling to more effectively detect signs of cancer in medical imaging. Banks use predictive modeling to identify and reject fraudulent financial transactions. And cities and real estate companies use predictive modeling to estimate the assessed values of homes from property records, to forecast government revenues, and to identify trends.

As predictive modeling has matured and expectations for it have grown, researchers have studied the processes through which data science projects are created, developed, evaluated, and maintained, whether by large organizations, open data communities, scientific researchers, or individual practitioners. There are three main challenges in the development of predictive models.

First, the modern data science development process is complex and highly iterative, with multiple stages and steps (Figure 1.1). These stages can be summarized as preparation, modeling, and deployment. In the *preparation* stage, data scientists prepare raw data for modeling by formulating a prediction task, acquiring data resources,

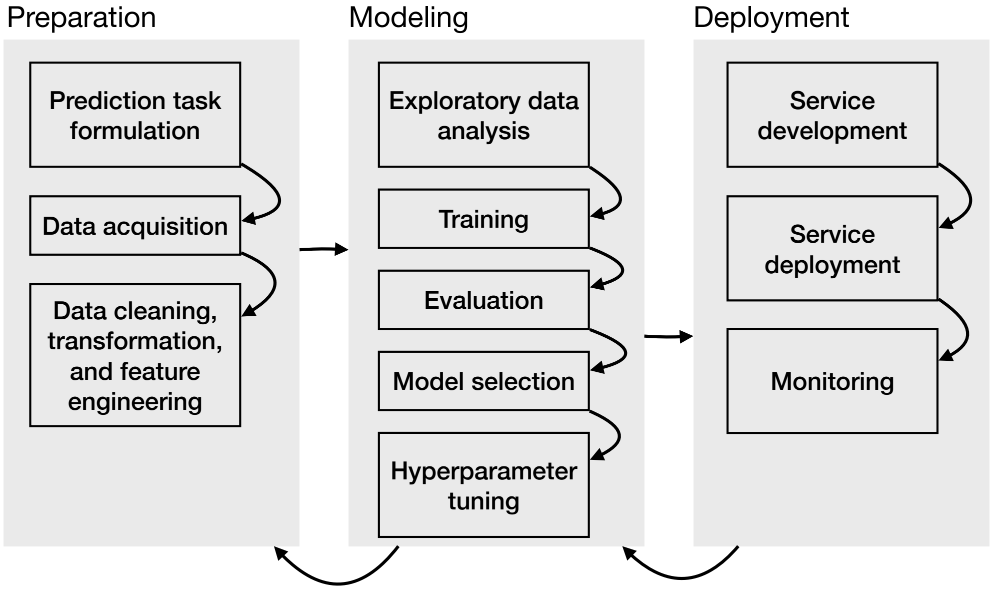


Figure 1.1: Typical stages and steps of a data science process for predictive machine learning modeling.

cleaning and transforming raw data, and engineering features. In the *modeling* stage, data scientists explore patterns and relationships in the feature values and prediction targets, train and evaluate machine learning models, select from among alternative models, and tune hyperparameters. In the *deployment* stage, data scientists expose the model as a service, assess performance metrics such as latency and accuracy, and monitor it for drift.

During any of these stages, data scientists may need to backtrack and revisit prior steps. For example, if a model does not achieve a desired level of performance during a training and evaluation step, the data scientist may return to an earlier step and acquire more labeled examples, integrate new data sources, or engineer additional features in order to improve the downstream predictive performance. In addition, each of these individual steps can be arbitrarily complex — for instance, exposing a model as a service can require intensive engineering work.

Second, data science projects generally involve people with varying skill sets and roles, or *personas*. A *domain expert* is a persona with a deep understanding of many aspects of a problem domain or application, such as business and organizational pro-

Persona	Description
Domain expert	Has a deep understanding of many aspects of a problem domain or application, such as business and organizational processes, underlying science and technology, and the provenance of and relationships between data sources
Software developer	Designs and implements software systems or applications and has mastery of team-based development processes
Statistical and machine learning modeler	Uses statistics, machine learning, and mathematics to understand and model relationships between different quantities of interest

Table 1.1: Description of personas involved in predictive modeling projects. These stylized personas are expressed to varying degrees in any given individual.

cesses, underlying science and technology, and the provenance of and relationships between data sources. A *software developer* is a persona who designs and implements software systems or applications and has mastery of team-based software development processes. A *statistical and machine learning modeler* is a persona who uses statistics, machine learning, and mathematics to understand and model the relationships between different quantities of interest. These personas are usually expressed to varying degrees by people with different backgrounds, roles, and job titles (Table 1.1).

Multiple personas may be expressed within an individual. For example, according to the "data science Venn diagram" (Figure 1.2), the ideal data scientist expresses all three of these personas and more. In this understanding, the ideal data scientist is an expert in statistics and math, software development, and the problem domain. But in reality, very few people develop expertise in all three of these disparate areas.[1]

Third, individual steps in the data science process may require a complicated interplay of contributions from these three different personas. Domain experts and data scientists must collaborate in order to properly scope a data science project in terms of inputs, outputs, and requirements, and to obtain insight into the important factors that might lead to successful predictive models. Data scientists must also

[1] In this thesis, we will consider a data scientist to be anyone who contributes to a data science project, while being mindful that this individual may have different skill sets, and will be more specific as needed.

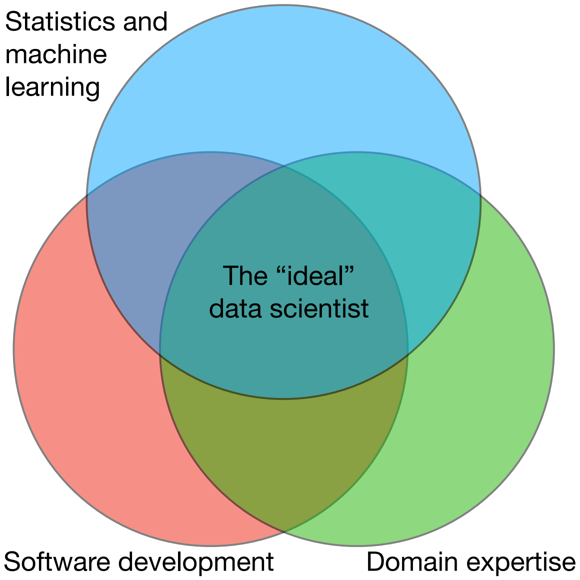


Figure 1.2: The "data science Venn diagram" (adapted from Conway 2013). The "ideal" data scientist is an expert in statistics and machine learning, software development, and the problem domain.

collaborate with each other so that each can contribute knowledge, insight, and intuition. The need for collaboration among different personas during a project can cause friction due to differing technical skills, as well as struggles to integrate conflicting code contributions.

We can see how these three challenges play out by going through just one part of the process — feature engineering. In the feature engineering step, data scientists write code to transform raw variables into feature values, which can then be used as input for a machine learning model. Features form the cornerstone of many data science tasks, including not only predictive modeling, but also causal modeling through propensity score analysis, clustering, business intelligence, and exploratory data analysis. Each feature should yield a useful measure of a data instance such that a model can use it to predict the desired target. For problems involving text, image, audio, and video processing, modern deep neural networks are now able to automatically learn feature representations from unstructured data. However, for other data modalities such as relational and tabular data, handcrafted features by experts are necessary to achieve the best performance.

Suppose that a data scientist is trying to create a model to predict the selling price of a house. Many features of this house may be easy to define and calculate, such as its age or living area. Others may be more difficult, such as its most recent assessed value as compared to other houses in the vicinity. Still others may be even more complex, such as the walking distance from the house to the nearest grocery store or yoga studio, or the average amount of direct sunlight the house receives given its orientation and latitude. Domain expertise is required to best identify these creative features, which can be highly predictive. Just as a realtor or property assessor is able to estimate the value of a house from an inspection, so too does knowledge of real estate and property assessment allow someone to identify those measurable attributes of a house that impact its selling price.

But while some steps in predictive modeling, such as feature engineering, still require collaboration, other steps are reaching full automation and require little to no human involvement. For example, due to advances in hyperparameter tuning algorithms, an automated search over a predefined configuration space can find the best-performing hyperparameters for a given machine learning algorithm more efficiently than a data scientist.

These dynamics are complicated even further in the emerging practice of open data science, where predictive models are developed in an open-source setting by citizen scientists, volunteers, and machine learning enthusiasts. These models are meant to help with important societal problems by performing tasks such as predicting traffic crashes, predicting adverse interactions between police and citizens, analyzing breakdown and pollution of water wells, and recommending responses to legal questions for *pro bono* organizations. Open data science projects are usually very transparent, with practitioners making source code and data artifacts publicly available and soliciting community input on project directions. Contributors may use their own computational resources and/or take advantage of limited shared community resources to run test suites, build documentation sites, and host chat rooms. In these *low-resource* settings, collaboration and automation cannot rely on commercial development platforms and cloud infrastructure.

Though these challenges remain pressing, we can take inspiration from related fields, like software engineering, that have surmounted similar ones. Software engineering is a mature field with time-tested processes for team-based development. For example, the Linux operating system kernel came from humble origins in the early 1990s to become one of the most complex pieces of software ever developed. Using (and often pioneering) open-source software development processes, the project has received and integrated code contributions from over 20,000 developers, numbering over one million commits and over 28 million lines of code, and now runs on billions of devices (Stewart et al., 2020).

What would it look like to overcome similar challenges in predictive modeling? Scores of data scientists with different levels of domain expertise, software development skills, and statistical and machine learning modeling prowess could work together on a single, impactful predictive model. Domain experts could easily express their ideas and have them incorporated into the project, even if they have a limited ability to write production-grade code. Data scientists could contribute code to a shared repository while remaining confident that their code will work well with that of their collaborators. Software developers could easily build in the latest advances in data science automation and focus their engineering efforts where they are most needed. And large collaborations in the open data science setting could lead to useful predictive models for civic technology, public policy, and scientific research.

In this thesis, I describe progress toward this vision in two areas. First, I propose ways to focus the efforts of data scientists and support structured collaboration for the most challenging steps in a data science project such as feature engineering. Second, I propose supplementing human collaborators with advanced automated machine learning within end-to-end data science and machine learning pipelines. Taken together, these approaches allow data scientists to collaborate more effectively, fall back on collaborators or automated agents where they lack skills, and build highly performing predictive models for the most challenging problems facing our society and organizations.

1.1 Summary of contributions

This thesis makes the following contributions in collaborative, open, and automated data science and machine learning.

1.1.1 Adapting the open-source development model

First, in *Ballet*, we show that we can support collaboration in data science development by adapting and extending the open-source software development model.

The open-source software development model has led to successful, large-scale collaborations in building software libraries, software systems, chess engines, and scientific analyses, with individual projects involving hundreds or even thousands of unique code contributors. Extensive research into open-source software development has revealed successful models for large-scale collaboration, such as the pull request model exemplified by the social coding platform GitHub.

We show that we can successfully adapt and extend this model to support collaboration on important data science steps by introducing a new development process and ML programming model. Our approach decomposes steps in the data science process into modular data science "patches" that can be intelligently combined, representing objects like "feature definition," "labeling function," or "slice function." Prospective collaborators each write patches and submit them to a shared repository. Our framework provides a powerful embedded language that constrains the space of new patches, as well as the underlying functionality to support interactive development, automatically test and merge high-quality contributions, and compose accepted contributions into a single product. While data science and predictive modeling have many steps, we focus on feature engineering on tabular data as an important step that could benefit from a more collaborative approach.

We instantiate these ideas in Ballet, a lightweight software framework for collaborative data science that supports collaborative feature engineering on tabular data.

Ballet is the first collaborative feature engineering framework and represents an exciting new direction for data science collaboration.

We present Ballet in Chapter 3.

1.1.2 Understanding collaborative data science in context

Second, we seek to better understand the opportunities and challenges present in large open data science collaborations.

Research into data science collaborations has mostly focused on projects done by small teams. Little attention has been given to larger collaborations, partly because of a lack of real-world examples to study.

Leveraging Ballet as a probe, we create and conduct an analysis of *predict-census-income*, a collaborative effort to predict personal income through engineering features from raw individual survey responses to the U.S. Census American Community Survey (ACS). We use a mixed-method software engineering case study approach to study the experiences of 27 developers collaborating on this task, focusing on understanding the experience and performance of participants from varying backgrounds, the characteristics of collaboratively built feature engineering code, and the performance of the resulting model compared to alternative approaches. The resulting project is one of the largest ML modeling collaborations on GitHub, and outperforms both state-of-the-art tabular AutoML systems and independent data science experts. We find that both beginners and experts (in terms of their background in software development, ML modeling, and the problem domain) can successfully contribute to such projects and that domain expertise in collaborators is critical. We also identify themes of goal clarity, learning by example, distribution of work, and developer-friendly workflows as important touchpoints for future design and research in this area.

We present our analysis of the *predict-census-income* case study in Chapter 4.

1.1.3 Supporting data scientists with automation

Third, we complement collaborative work on data science steps like feature engineering with a full-fledged framework for ML pipelines and automated machine learning (AutoML).

As data scientists focus their efforts on certain steps, we want to ensure that other steps in the process are not ignored, but rather automated using the best available tools. We introduce the *Machine Learning Bazaar* (ML Bazaar), a framework for constructing tunable, end-to-end ML pipelines.[2] While AutoML is increasingly being used in large data-native organizations, and is offered as a service by several cloud providers, there was no existing open-source AutoML system flexible enough to be incorporated into end-to-end ML pipelines to meet these needs.

ML Bazaar differentiates itself from other AutoML frameworks in several ways. First, we introduce new *abstractions*, such as ML primitives — human-driven annotations of components from independent ML software libraries that can be seamlessly composed within a single program. Second, we emphasize *curation* as a key principle. We empower ML experts to identify the best-performing ML primitives and pipelines from their experience and recommend only these curated components to users. Third, we design for *composability* of the libraries that comprise ML Bazaar. Fourth, we enable *automation* over all components in the framework, such that primitives and pipelines can expose their hyperparameter configuration spaces to be searched. As a result, our underlying libraries can be used in different combinations, such as for a black-box AutoML system, an anomaly detection system for satellite telemetry data, or several other applications that we highlight. The combination of Ballet and ML Bazaar comprises an important step toward end-to-end ML in a collaborative and open-source setting.

The Machine Learning Bazaar is presented in Chapter 6.

1.1.4 Putting the pieces together

Fourth, we combine the elements of this thesis and deploy them in a collaborative project to predict life outcomes.

Social scientists are increasingly using predictive ML modeling tools to gain insights into problems in their field, although the practice and methods of machine learning are not widely understood within many social science research communities.

[2] `https://mlbazaar.github.io`

One recent attempt to bridge this gap was the Fragile Families Challenge (FFC, Salganik et al., 2020), which aimed to prompt the development of predictive models for life outcomes from data collected as part a longitudinal study on a set of disadvantaged children and their families. Unfortunately, after a massive effort to design the challenge and develop predictive models, FFC organizers concluded that "even the best predictions were not very accurate" and that "the best submissions [...] were only somewhat better than the results from a simple benchmark model" (Salganik et al., 2020).

Can collaborative data science offer something that was not achieved by a competitive approach? We use both Ballet and ML Bazaar on this challenging prediction problem, performing collaborative feature engineering within a larger ML pipeline that is automatically tuned. We compare our approach to the results of the FFC challenge, and offer a discussion of the future of collaboration on prediction problems in the social sciences.

Our exploration of the Fragile Families Challenge using the tools introduced in this thesis is presented in Chapter 8.

1.2 Statement of prior publication

Chapters 3 to 5 are adapted from and extend the previously published works, *Enabling Collaborative Data Science Development with the Ballet Framework* (Smith et al., 2021a), which will appear at the ACM Conference on Computer-Supported Cooperative Work and Social Computing (CSCW), and *Meeting in the Notebook: A Notebook-Based Environment for Micro-Submissions in Data Science Collaborations* (Smith et al., 2021b).

Chapters 6 and 7 are adapted from and extend the previously published work, *The Machine Learning Bazaar: Harnessing the ML Ecosystem for Effective System Development* (Smith et al., 2020), which appeared at the ACM International Conference on Management of Data (SIGMOD).

All co-authors have given permission for these works to be adapted and reproduced in this thesis. I am grateful for their collaboration on these shared ideas and projects, and this research would not have been possible without them. In particular, Carles Sala is the lead developer and designer of several software libraries and systems described in Chapter 6, including MLBlocks and AutoBazaar, and has been a wonderful collaborator throughout the ML Bazaar project.

1.3 Thesis summary

In the rest of this thesis, I describe these four aspects of my research. This research lays building blocks for an emerging type of collaborative data analysis and machine learning, which can allow us to more effectively use these powerful tools to address the most important problems facing our society. While the road to fully collaborative, open, and automated data science is long, I believe that much progress will continue to be made.

Chapter 2

Background

2.1 Data science and feature engineering

The increasing availability of data and computational resources has led many organizations to turn to data science, or a data-driven approach to decision-making under uncertainty. Consequently, researchers have studied data science work practices on several levels, and the data science workflow is now understood as a complex, iterative process that includes many stages and steps. The stages can be summarized as Preparation, Modeling, and Deployment (Muller et al., 2019; Wang et al., 2019b; Santu et al., 2021) and encompass smaller steps such as task formulation, prediction engineering, data cleaning and labeling, exploratory data analysis, feature engineering, model development, monitoring, and analyzing bias. Within the larger set of data science workers involved in this process, we use *data scientists* to refer to those who contribute to a data science project.

Within this broad setting, the step of feature engineering holds special importance in some applications. Feature engineering is the process through which data scientists write code to transform raw variables into feature values, which can then be used as input for a machine learning model. (This process, also called feature creation, development, or extraction, is sometimes grouped with data cleaning and data preparation steps, as in Muller et al. 2019.) Features form the cornerstone of many data science tasks, including not only predictive ML modeling, in which a learning algorithm finds predictive relationships between feature values and an outcome of interest, but also causal modeling through propensity score analysis, clustering, business intelligence, and exploratory data analysis. Practitioners and researchers have widely acknowledged the importance of engineering good features for modeling success, particularly in predictive modeling (Domingos, 2012; Anderson et al., 2013; Veeramachaneni et al., 2014).

Before we continue discussing feature engineering, we introduce some terminology that we will use throughout this thesis. A *feature function* is a transformation applied to raw variables that extracts *feature values*, or measurable characteristics and properties of each observation. A *feature definition* is source code written by a data scientist to create a feature function.[1] If many feature functions are created, they can be collected into a single *feature engineering pipeline* that executes the computational graph made up of all of the feature functions and concatenates the result into a *feature matrix*.

In an additional step in ML systems, feature engineering is increasingly augmented by applications like feature stores and feature management platforms to help with critical functionality like feature serving, curation, and discovery (Hermann and Del Balso, 2017; Wooders et al., 2021).

Though there have been attempts to automate the feature engineering process in certain domains, including relational databases and time series analysis (Kanter and Veeramachaneni, 2015; Khurana et al., 2016; Christ et al., 2018; Katz et al., 2016), it is widely accepted that in many areas that involve large and complex datasets, like health and business analytics, human insight and intuition are necessary for success in feature engineering (Domingos, 2012; Smith et al., 2017; Wagstaff, 2012; Veeramachaneni et al., 2014; Bailis, 2020).

Human expertise is invaluable for understanding the complexity of a dataset, theorizing about different relationships, patterns, and representations in the data, and implementing these ideas in code in the context of the machine learning problem.

[1] Any of these terms may be referred to as "features" in other settings, but we make a distinction between the source code, the transformation applied, and the resulting values. In cases where this distinction is not important, we may also use "feature."

Muller et al. (2019) observe that “feature extraction requires an interaction of domain knowledge with practices of design-of-data.” As more people become involved in this process, there is a greater chance that impactful “handcrafted” feature ideas will be expressed; automation can be a valuable supplement to manual development.

Indeed, in prior work that led to the ideas presented in this thesis, we explored the potential of FeatureHub, a cloud-hosted feature engineering platform (Smith et al., 2017; Smith, 2018). In this conception, data scientists log into a cloud platform and submit source code directly to a machine learning backend server. Features in FeatureHub are simple Python functions that map a collection of data frames to a vector of feature values, but have no learning or supervised components and do not expose any metadata. The feature source code is stored in a database and is compiled during an automated machine learning process. In experiments with freelance data scientists, an automated model built using all features submitted to the database outperformed individual models built using only features from one data scientist at a time. However, it underperformed models created by data scientists on a machine learning competition platform.

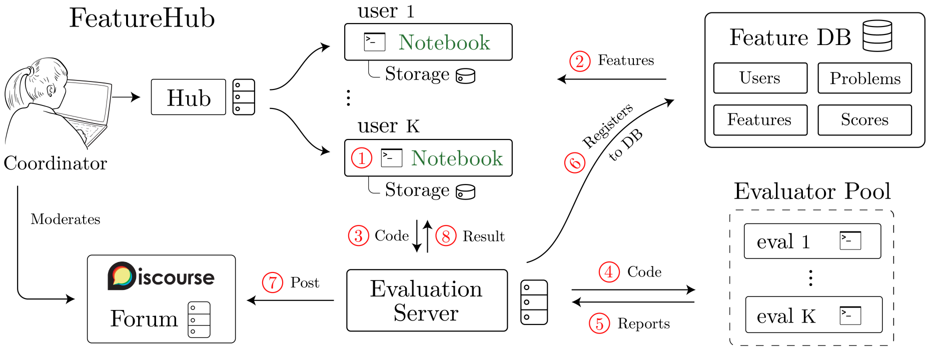


Figure 2.1: Architecture of the FeatureHub platform from our prior work, comprising the JupyterHub-based computing platform, Discourse-based discussion platform, backend feature database and automated machine learning evaluation server (from Smith et al., 2017).

FeatureHub was a complicated system with many moving parts (Figure 2.1). Building it posed significant engineering challenges, and it competed with highly-resourced data science platform companies. We also identified challenges relating to financial costs, environment flexibility, trust and security, transparency, and freedom

(Smith, 2018, Section 6). As a way forward, we proposed a turn toward "platformless collaboration," with the goal of finding free and open-source replacements for the functionality that a hosted data science platform usually provides.

In this thesis, we address and move well beyond the issues raised in our prior work. We also build on understanding of the importance of human interaction within the feature engineering process by creating a workflow that supports collaboration in feature engineering as a component of a larger data science project. Ballet takes a lightweight and decentralized approach suitable for the open-source setting, an integrated development environment, and a focus on modularity and supporting collaborative workflows.

2.2 Collaborative and open data work

Just as we explore how multiple human perspectives enhance feature engineering, there has been much interest within the human-computer interaction (HCI) and computer-supported cooperative work (CSCW) communities in achieving a broader understanding of collaboration in data work. For example, within a wider typology of *collaboratories* (collaborative organizational entities), Bos et al. (2007) study both community data systems and open community contribution systems, such as the Protein Databank and Open Mind Initiative. Zhang et al. (2020) show that data science workers in a large company are highly collaborative in small teams, using a plethora of tools for communication, code management, and more. Teams include workers in many roles such as researchers, engineers, domain experts, managers, and communicators (Muller et al., 2019), and include both experts and non-experts in technical practices (Middleton et al., 2020). In an experiment with the prototype machine learning platform described above, Smith et al. (2017) show that 32 data scientists made contributions to a shared feature engineering project and that a model using all of their contributions outperformed a model from the best individual performer. Functionalities including a feature discovery method and a discussion forum helped data scientists learn how to use the platform and avoid duplicating work.

Contrary to popular understandings of collaboration as relying on direct communication, *stigmergy* is the phenomenon of collaboration by indirect communication mediated by modifications of the environment (Marsh and Onof, 2008). Stigmergic collaboration is a feasible collaborative mode for data science teams, allowing them to coordinate around a shared work product such as a data science pipeline. Crowston et al. (2019) introduce these ideas in the context of the MIDST project. They first introduce a conceptual framework for stigmergic collaboration in a data science project built around the concepts of visibility, combinability, and genre. They then create an experimental web-based data science application that allows data scientist to compose a data flow graph based on different "nodes" like executable scripts, data files, and visualizations. The tool was evaluated on teams of 3–6 data science students and was shown to be "usable and seemingly useful" and facilitated stigmergic coordination. Like MIDST, in Ballet we are inspired by open-source software development practices and the desire to improve development workflows for data science pipelines. We expand on this body of work by extending the study of collaborative data work to predictive modeling and feature engineering, and by using the feature engineering pipeline as a shared work product to coordinate collaborators at a larger scale than previously observed. Instead of communicating directly, data scientists can collaborate indirectly by browsing, reading, and extending existing feature engineering code structured within a shared repository.

One finding in common in previous studies is that data science teams are usually small, with six or fewer members (Zhang et al., 2020). There are a variety of explanations for this phenomenon in the literature. Technical and non-technical team members may speak "different languages" (Hou and Wang, 2017). Different team members may lack common ground while observing project progress and may use different performance metrics (Mao et al., 2019). Individuals may be highly specialized, and the lack of a true "hub" role on teams (Zhang et al., 2020) along with the use of synchronous communication forms like telephone calls and in-person discussion (Choi and Tausczik, 2017) make communication challenges likely as teams grow larger. In the context of open-source development, predictive modeling projects

Software engineering		ML modeling	
torvalds/linux	20,000+	tesseract-ocr/tesseract	130
DefinitelyTyped/DefinitelyTyped	12,600+	CMU-PCL/openpose	79
Homebrew/homebrew-cask	6,500+	deepfakes/faceswap	71
ansible/ansible	5,100+	JaidedAI/EasyOCR	62
rails/rails	4,300+	ageitgey/face_recognition	43
gatsbyjs/gatsby	3,600+	*predict-census-income* (Chapter 4)	27
helm/charts	3,400+	microsoft/CameraTraps	21
rust-lang/rust	3,000+	Data4Democracy/drug-spending	21

Table 2.1: The number of unique contributors to large open-source collaborations in either software engineering or predictive machine learning modeling. ML modeling projects that are developed in open-source have orders of magnitude fewer contributors.[2]

generally have orders of magnitude fewer collaborators than other types of software projects (Table 2.1).

One possible implication of this finding is that, in the absence of other tools and processes, human factors of communication, coordination, and observability make it challenging for teams to work well at scale. Difficulties with validation and curation of feature contributions presented challenges for Smith et al. (2017), which points to the limitations of existing feature evaluation algorithms. Thus, algorithmic challenges may complement human factors as obstacles to scaling data science teams. However, additional research is needed into the question of why data science collaborations are not larger. We provide a starting point through a case study analysis in this work.

Moving from understanding to implementation, other approaches to collaboration in data science work include crowdsourcing, synchronous editing, and competition. Unskilled crowd workers can be harnessed for feature engineering tasks within the Flock platform, such as by labeling data to provide the basis for further manual feature engineering (Cheng and Bernstein, 2015). Synchronous editing interfaces, like those of Google Colab and others for computational notebooks (Garg et al., 2018; Kluyver et al., 2016; Wang et al., 2019a), facilitate multiple users to edit a machine learning model specification, typically targeting pair programming or other

[2] Details and methodology are available at Smith et al. (2021a, Appendix A) or `https://github.com/micahjsmith/ballet-cscw-2021`.

very small groups. In our work, we explore *different-time, different-place* collaboration (Shneiderman et al., 2016) in an attempt to move beyond the limitations of small group work. A form of collaboration is also achieved in data science competitions like the KDD Cup, Kaggle, and the Netflix Challenge (Bennett and Lanning, 2007) and using networked science hubs like OpenML (Vanschoren et al., 2013). While these have led to state-of-the-art modeling performance, there is no natural way for competitors to systematically integrate source code components into a single shared product. In addition, individual teams formed in competitions hosted on Kaggle are small, with the mean team having 2.6 members and 90% of teams having four or fewer members, similar to other types of data science teams as discussed above.[3]

Closely related is *open data analysis* or *open data science*, in which publicly available datasets are used by “civic hackers” and other technologists to address civic problems, such as visualizations of lobbyist activity and estimates of child labor usage in product manufacturing (Choi and Tausczik, 2017). Existing open data analysis projects involve a small number of collaborators (median of three) and make use of synchronous communication (Choi and Tausczik, 2017). A common setting for open data work is hackathons, during which volunteers collaborate with non-profit organizations to analyze their internal and open data. Hou and Wang (2017) find that civic data hackathons create actionable outputs and improve organizations’ data literacy, relying on “client teams” to prepare data for analysis during the events and to broker relationships between participants. Looking more broadly at collaborative data work in open science, interdisciplinary collaborations in data science and biomedical science are studied in Mao et al. (2019), who find that readiness of a team to collaborate is influenced by its organizational structures, such as dependence on different forms of expertise and the introduction of an intermediate broker role. In our work, we are motivated by the potential of open data analysis, but focus more narrowly on data science and feature engineering.

[3] Author’s calculation from Meta Kaggle of all teams with more than one member.

2.3 Open-source development

In the early 1990s, a programmer named Linus Torvalds started working on a new implementation of a UNIX-like operating system kernel. The development of the new kernel came as a shock to seasoned companies. A loose group of developers from around the world were sharing their source code and sending patches over email. The project, which became known as the Linux kernel, quickly took off. It was only later in the decade that Eric S. Raymond popularized the term "open-source software" to define what this process looked like for Linux and similar efforts.

In just thirty years, the open-source phenomenon has had a dramatic impact on the computing and internet revolutions. By 2020, countless open-source projects were hosted on popular platforms like GitHub, GitLab, SourceForge, and Bitbucket, with over 200 million repositories on GitHub alone (GitHub). The largest technology companies share the source code of ambitious projects that cost millions of engineer dollars to create and, in turn, receive contributions from growing communities of users. Linux runs on billions of devices. Open-source has enabled thousands or tens of thousands of unique contributors from around the world to come together to create popular and high-performance web frameworks, deep learning libraries, database systems, chess engines, electronics platforms, and more. The open-source paradigm has also come to be applied to other artifacts beyond software applications and libraries, including online courses, books, and resource lists.

The *open-source model* for developing software has been adopted and advanced by many individuals and through many projects (Raymond, 1999). In the open-source model, projects are developed publicly and source code and other materials are freely available on the internet; the more widely available the source code, the more likely it is that a contributor will find a defect or implement new functionality ("with enough eyes, all bugs are shallow"). With freely available source code, open-source projects may attract thousands of contributors: developers who fix bugs, contribute new functionality, write documentation and test cases, and more. With more contributors comes the prospect of conflicting patches, leading to the problem of *integration*. In order to support open-source developers, companies and organizations have made a variety of lightweight infrastructure and developer tooling freely available for this community, such as build server minutes and code analysis tools.

Closely associated with the open-source model is the *open-source software development process*, exemplified by the *pull-based development model* (or *pull request model*), a form of distributed development in which changes are pulled from other repositories and merged locally. As implemented on the social code platform GitHub, developers fork a repository to obtain their own copy and make changes independently; proposed changes — pull requests (PRs) — are subject to discussions and code reviews in context and are analyzed by a variety of automated tools. The pull request model has been successful in easing the challenges of integration at scale and facilitating massive software collaborations.

As of 2013, 14% of active repositories on GitHub used pull requests. An equal proportion used shared repositories without pull requests, while the remainder were single-developer projects (Gousios et al., 2014). Pull request authors use contextual discussions to cover low-level issues but supplement this with other channels for higher-level discussions (Gousios et al., 2016). Pull request integrators play a critical role in this process but can have difficulty prioritizing contributions at high volume (Gousios et al., 2015). Additional tooling has continued to grow in popularity partly based on these observations. Recent research has visited the use of modern development tools like continuous integration (Vasilescu et al., 2015; Zhao et al., 2017; Vasilescu et al., 2014), continuous delivery (Schermann et al., 2016), and crowdsourcing (Latoza and Hoek, 2016). In this work, we specifically situate data science development within the open-source development process and explore what changes and enhancements are required for this development model to meet the needs of data scientists during a collaboration.

2.4 Testing for machine learning

As part of our framework, we discuss the use of testing in continuous integration to validate contributions to data science pipelines. Other research has also explored the use of continuous integration in machine learning. Renggli et al. (2019) investigate practical and statistical considerations arising from testing conditions on overall model accuracy in a continuous integration setting. Specific models and algorithms can be tested (Grosse and Duvenaud, 2014) and input data can be validated directly (Hynes et al., 2017; Breck et al., 2019). Testing can also be tied to reproducibility in ML research (Ross and Forde, 2018). We build on this work by designing and implementing the first system and algorithms that conduct ML testing at the level of individual feature definitions.

Feature engineering is just one of many steps involved in data science. Other research has looked at the entire endeavor from a distance, considering the end-to-end process of delivering a predictive model from some initial specification. Automated machine learning (AutoML) systems like AutoBazaar, AutoGluon, and commercial offerings from cloud vendors (Smith et al., 2020; Erickson et al., 2020) can automatically create predictive models for a variety of ML tasks. A survey of techniques used in AutoML, such as hyperparameter tuning, model selection, and neural architecture search, can be found in Yao et al. (2019). On the other hand, researchers and practitioners are increasingly realizing that AutoML does not solve all problems and that human factors such as design, monitoring, and configuration are still required (Cambronero et al., 2020; Xin et al., 2021; Wang et al., 2019c, 2021). In our experiments, we use an AutoML system to evaluate the performance of different feature sets without otherwise incorporating these powerful techniques into our framework.

2.5 Machine learning systems

Researchers have developed numerous algorithmic and software innovations to make ML and AutoML systems possible in the first place.

ML libraries High-quality ML libraries have been built over a period of decades. For general ML applications, scikit-learn implements many different algorithms using a common API centered on the influential `fit`/`predict` paradigm (Buitinck et al., 2013). Libraries more suitable for specialized analysis have been developed in various academic communities, often with different and incompatible APIs (Bradski, 2000; Hagberg et al., 2008; Kula, 2015; Kanter and Veeramachaneni, 2015; Bird et al., 2009; Abadi et al., 2015). In *ML Bazaar*, we connect and link components of these libraries, supplementing with our own functionalities only where needed.

ML systems Prior work has provided several approaches that make it easier to develop ML systems. For example, caret (Kuhn, 2008) standardizes interfaces and provides utilities for the R ecosystem, but without enabling more complex pipelines. Recent systems have attempted to provide graphical interfaces, including Gong et al. (2019) and Azure Machine Learning Studio. The development of ML systems is closely tied to the execution environments needed to train, deploy, and update the resulting models. In SystemML (Boehm et al., 2016) and Weld (Palkar et al., 2018), implementations of specific ML algorithms are optimized for specific runtimes. Velox (Crankshaw et al., 2015) is an analytics stack component that efficiently serves predictions and manages model updates.

AutoML libraries AutoML research has often been limited to solving the individual sub-problems that make up an end-to-end ML workflow, such as data cleaning (Deng et al., 2017), feature engineering (Kanter and Veeramachaneni, 2015; Khurana et al., 2016), hyperparameter tuning (Snoek et al., 2012; Gomes et al., 2012; Thornton et al., 2013; Feurer et al., 2015; Olson et al., 2016; Jamieson and Talwalkar, 2016; Li et al., 2017; Baudart et al., 2020), or algorithm selection (van Rijn et al., 2015; Baudart et al., 2020). AutoML solutions are often not widely applicable or deployed in practice without human support. In contrast, *ML Bazaar* integrates many of these existing approaches and designs one coherent and configurable structure for joint tuning and selection of end-to-end pipelines.

AutoML systems AutoML libraries typically make up 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 (Swearingen et al., 2017), Vizier (Golovin et al., 2017), and Rafiki (Wang et al., 2018), as well as commercial platforms like Google AutoML, DataRobot, and Azure Machine Learning Studio. While these systems provide many benefits, they have several limitations. First, they each focus on a specific subset of ML use cases, such as computer vision, NLP, forecasting, or hyperparameter tuning. Second, these systems are designed as proprietary applications and do not support community-driven integration of new innovations. *ML Bazaar* provides a new approach to *developing* such 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.

The DARPA D3M program (Lippmann et al., 2016), which we participated in, supports the development of automated systems for model discovery that can be used by non-experts. Several differing approaches are being developed for this purpose. For example, Alpine Meadow (Shang et al., 2019) focuses on efficient search for producing interpretable ML pipelines with low latencies for interactive usage. It combines existing techniques from query optimization, Bayesian optimization, and multi-armed bandits to efficiently search for pipelines. AlphaD3M (Drori et al., 2018) formulates a pipeline synthesis problem and uses reinforcement learning to construct pipelines. In contrast, *ML Bazaar* is a framework for developing ML or AutoML systems in the first place. While we present our open-source AutoBazaar system, it is not the primary focus of our work and represents a single point in the overall design space of AutoML systems using our framework libraries. Indeed, one could use specific AutoML approaches like the ones described by Alpine Meadow or AlphaD3M for pipeline search within our own framework.

Santu et al. (2021) present a recent survey of AutoML, summarizing seven levels of automation that can be provided by AutoML systems and contextualizing existing work within the framework. ML Bazaar is categorized as a system with "Level 4" automation in that it automates machine learning, alternative models exploration, testing, validation, and some feature engineering, but does not provide automated prediction engineering, task formulation, or result summary and recommendation.

2.6 Prediction policy problems

The predominant quantitative methodology in the social sciences is that of causal inference. Social scientists and policy makers use the tools of causal inference to identify factors that influence outcomes of interest or to explore counterfactual scenarios. What is the effect of an increase in the minimum wage on employment levels? Would increasing the amount of food assistance to needy families lead to less truancy in school? These are questions typically answered using the tools of causal inference such as randomized controlled trials or regression analysis.

While causal inference allows us to clearly answer many relevant socio-political questions, it can be a challenge to a conduct an analysis rigorously. Models must be well-specified, all confounding variables must be accounted for, assumptions must be made and validated about the distribution of variables and errors, and statistical tests must be chosen appropriately for the setting. These methodological challenges and many others have led to researchers to explore alternative paradigms (Breiman, 2001).

Another increasingly popular approach is to use the toolkit of predictive machine learning to gain insight into societal problems. With this approach, researchers identify an outcome of interest and attempt to build a predictive model, often using machine learning, to predict this outcome using all available information. Prediction can be used as an actual policy tool (i.e., while implementing a policy intervention, such as targeting or prioritizing the provision of social services) and as an alternative method for better understanding different phenomena. The primary validation method is to estimate generalization performance by evaluating out-of-sample predictive accuracy, rather than by assessing goodness of fit or parsimony. Problems that can be addressed using these tools are known as *prediction policy problems* (Kleinberg et al., 2015).

There are many recent examples of prediction policy problems:

- Sadilek et al. (2018) developed a predictive model, "FINDER" to identify sources of foodborne illness outbreaks and thereby prioritize restaurant health inspections. Using anonymized cell phone location data and internet search histories, they can classify whether and where a person experienced foodborne illness.

- Data scientists at Chicago's Department of Innovation and Technology similarly built a predictive model to determine which restaurants were at highest risk of being in violation of health codes, and thereby prioritize health inspector visits to these sites (Spector, 2016). The source code for the model was released and it was later adopted by Montgomery County, Maryland.

- Chouldechova et al. (2018) developed a predictive risk modeling tool to be used in child welfare screening, which they evaluated in Allegheny County, PA. The tool supplements case workers in determining risks involved in referrals to child protection agencies. Investigation is prioritized for children identified as highest risk.

- Kleinberg et al. (2015) also report on a case study predicting which hip replacement surgeries for Medicare beneficiaries are most likely to prove "futile," in that they do not improve patients' quality of life relative to their remaining months or years, yet still cost the health care system. Those with lower mortality risk, rather than higher, would benefit most from such procedures.

For every report of machine learning successfully being used in a policy prediction problem, there are two showing the biases or ethical challenges of such practices. For example, using machine learning in recidivism risk prediction is a contentious issue, with competing claims that either using or not using recidivism prediction models leads to more racial bias. Law enforcement organizations like police departments use systems for "predictive policing" that aim to identify "hot spots" of crime, but may actually result in over-policing of predominantly communities of color without a public safety benefit. A common thread in these more controversial uses of machine learning for public policy is that algorithmic systems may be used to “launder” human biases — for instance, that they seem to prioritize public resources in a race-neutral way, but actually perpetuate discrimination. In addition, not every policy problem can be a prediction policy problem — for example, we may be (rightly) uncomfortable using the output of a model to deny someone welfare payments because of a predicted risk of some negative behavior that has not yet occurred (Kleinberg et al., 2016).

2.7 The Fragile Families Challenge

Part of the challenge here is that it is difficult for practitioners, researchers, and policymakers to think sufficiently rigorously about ML methodology. The practice and methods of machine learning are not widely understood by experts within many social science research communities. One recent attempt to connect the social science community to these new tools was the Fragile Families Challenge (FFC, Salganik et al., 2020). Here we give some detailed background on the challenge in order to contextualize our later discussions of collaborative data science development (Chapters 3 and 8).

The Fragile Families Challenge spurred the development of models meant to predict life outcomes from data collected as part of the Fragile Families and Child Wellbeing Study (Reichman et al., 2001), which includes detailed longitudinal records on a set of disadvantaged children and their families. Organizers released anonymized and merged data on a set of 4,242 families, with data collected from the birth of the child until age nine. Participants in the challenge were then tasked with predicting six life outcomes of the child or family when the child reached age 15: child grade point average, child grit, household eviction, household material hardship, primary caregiver layoff, and primary caregiver participation in job training. Submissions were evaluated with respect to the mean squared error on a held-out test set. The FFC was run over a four month period in 2017 and received 160 submissions from 437 entrants, who comprised social scientists, machine learning practitioners, students, and others.

Organizers cited three reasons for approaching a social science problem through a machine learning challenge. First, they noted the increased use of machine learning in prediction policy problems, as we have reviewed above. Second, in the context of social science research into life outcomes, measuring the predictability itself of life outcomes gives a measure of "social rigidity," or the degree to which life outcomes are dictated by one's circumstances at birth. Third, the sustained effort involved in a machine learning challenge could lead to developments in theory, methods, and data collection, such as has been observed in the Netflix Prize (Bennett and Lanning, 2007) and elsewhere.

In addition to ML performance, organizers sought out solutions that could be documented, published, and reproduced. Teams were invited to publish descriptions of their solutions in a special issue of the journal *Socius* (Salganik et al., 2019), with an assessment of computational reproducibility as part of the peer review process (Liu and Salganik, 2019). Organizers found that reproducibility was difficult to achieve, as only 7/12 accepted manuscripts were able to be reproduced even after an extensive revision process.

Through an analysis of the solutions included in the special issue, we are able to broadly describe how the typical challenge participant approached modeling. Organizers described a four-step process (Salganik et al., 2019):

- *Feature engineering.* The raw data needed significant processing before it could be used in modeling, a stage that organizers deemed "data preparation," but that we include as part of feature engineering (Section 2.1). The main tasks in this step include replacing or imputing missing values, encoding categorical variables, and constructing new variables from other variables. The data exhibited complicated patterns of "missingness," due to skip patterns, nonresponse, and data collection errors. Salganik et al. (2019) report that participants "spent large amounts of time converting the data into a format more suitable for analysis" and that "anecdotally, many participants spent a lot of time addressing missing data."

- *Feature selection.* The feature matrix that resulted from the feature engineering process was usually very high-dimensional. With tens of thousands of features, but only two thousand training observations, most learning algorithms require a dimensionality reduction step such as feature selection. Participants used a variety of approaches, including manual or automated selection using LASSO or mutual information.

- *ML Modeling.* When the feature matrix was ready for ML modeling, participants used a variety of learning algorithms, such as linear regression models, with and without regularization, as well as tree-based models including decision trees, random forests, and gradient-boosted trees.

- *Evaluation.* The final step was evaluation, or "model interpretation," wherein participants aimed to use their best performing predictive models to better understand the predictability of life outcomes, pursuant to the goals of the challenge. They interpreted regression coefficients or computed variable importance, depending on the type of model used.

After the challenge had closed, organizers scored all submissions using the held-out test dataset. It turned out that even the winning submissions were not very accurate in predicting life outcomes. Organizers computed the metric R^2_{Holdout}, a scaled version of the mean squared error that took the value 1 for perfect predictions, the value 0 for predicting the mean of the training dataset, and was unbounded below. The most predictable outcomes were material hardship and GPA, with an $R^2_{\text{Holdout}} = 0.2$, while the other four outcomes had $R^2_{\text{Holdout}} \approx 0.05$. In other words, these winning scores were only slightly more accurate than predicting the mean of the training dataset. This partly arises from the significant class/outcome imbalance in the data — most families did not experience adverse events such as eviction and layoff. Thus, predicting the mode (that the event did not occur) for every family leads to a model that performs reasonably well on the chosen mean-squared error metric, which does not account for outcome imbalance.

Part I

Collaborative and open data science

Chapter 3

Ballet: a framework for collaborative, open-source data science

3.1 Introduction

The open-source software development model has led to successful, large-scale collaborations in building software libraries, software systems, chess engines, scientific analyses, and more (Raymond, 1999; Linux; GNU; Stockfish; Bos et al., 2007). For these projects, hundreds or even thousands of collaborators contribute code to shared repositories using well-defined software development processes.

Collaboration is also required during many steps of the data science process. For example, in feature engineering within predictive modeling, data scientists and domain experts collaborate so that creative ideas for features can be expressed and incorporated into a feature engineering pipeline.

However, workflows in predictive modeling more often emphasize independent work, and data science collaborations tend to be smaller in scale (Choi and Tausczik, 2017), especially in the context of open-source projects (Table 2.1).

Given this state of affairs, we ask: *Can we support larger collaborations in predictive modeling projects by applying successful open-source development models?*

In this chapter, we show that we can successfully adapt and extend the pull request development model to support collaboration during important steps within the data science process by introducing a new development workflow and ML programming model. Our approach, the Ballet framework, is based on decomposing steps in the data science process into modular data science "patches" that can then be intelligently combined, representing objects like "feature definition," "labeling function," or "slice function." Prospective collaborators work in parallel to write patches and submit them to a shared repository. Ballet provides the underlying functionality to support interactive development, test and merge high-quality contributions, and compose the accepted contributions into a single product. Projects built with Ballet are structured and organized by these modular patches, yielding additional benefits including reusability, maintainability, reproducibility, and automated analysis. Our lightweight framework does not require any computing infrastructure beyond that which is freely available in open-source software development.

While data science and predictive modeling have many steps, we identify feature engineering as an important one that could benefit from a more collaborative approach. We thus instantiate these ideas in *Ballet*,[1] a lightweight software framework for collaborative data science that supports collaborative feature engineering on tabular data. Data scientists can use Ballet to grow a shared feature engineering pipeline by contributing feature definitions, which are each subjected to software and ML performance validation. Together with *Assemblé* — a data science development environment customized for Ballet — even novice developers can contribute to large collaborations.

Having provided background on data science, collaborative data work, and open-source software development in Chapter 2, the remainder of this chapter proceeds as follows. We first describe a conceptual framework for collaboration in data science projects in Section 3.2, which we then apply to create the Ballet framework in Section 3.3. We next describe key components of Ballet's support for collaborative feature engineering, such as the feature definition and feature engineering pipeline abstractions, in Section 3.4. We present acceptance procedures for feature definitions, including the use streaming feature definition selection algorithms in Section 3.5. Fi-

[1] `https://ballet.github.io` and `https://github.com/ballet/ballet`

nally, in Section 3.6, we introduce the Assemblé development environment, which supports data scientists in collaborating and contributing code entirely from within a notebook setting.

In the subsequent chapter (Chapter 4), we will present a case study analysis of a predictive model built by 27 collaborators using Ballet. We discuss our work and results in Chapter 5, including future directions for designers and researchers in collaborative data science frameworks.

3.2 Conceptual framework

Having noticed the success of open-source software development along with the challenges in collaborative data science, we set out to understand whether these two paradigms could complement each other, as well as to better grasp the current state of large-scale collaboration in data science. In this section, we describe the formation of key design concepts that underlie the creation of Ballet. Our methods reflect an iterative and informal design process that played out over the time we have worked on this problem as well as through two preliminary user studies (Section 3.7).

The pull request model (Section 2.3) has been particularly successful in enabling integration of proposed changes in shared repositories, and is already used for well over one million shared repositories on GitHub (Gousios et al., 2015, 2016). We informally summarize this development model using the concepts of *product*, *patch*, and *acceptance procedure*. A software artifact is created in a shared repository (product). An improvement to the product is provided in a standalone source code contribution proposed as a pull request (patch). Not every contribution is worthy of inclusion, so high-quality and low-quality contributions must be distinguished (acceptance procedure). If accepted, the pull request can be merged.

Given the success of open-source development processes like the pull request model, we ask: *Can we apply the pull request model to data science projects in order to collaborate at a larger scale?*

3.2.1 Challenges

When we set out to apply the pull request model to data science projects, we found the model was not a natural fit, and discovered key challenges to address, which we describe here. As people embedded in data science work, we built on our own experience developing and researching feature engineering pipelines and other data science steps from a machine learning perspective. We also uncovered and investigated these challenges in preliminary user studies with prototypes of our framework (Section 3.7).

We synthesize these challenges in the context of the literature on collaborative data work and machine learning workflows. Previous work outside the context of open-source development has identified challenges in communication, coordination, observability, and algorithmic aspects (Section 2.2). In addition, Brooks Jr (1995) observed that the number of possible direct communication channels in a collaborative software project scales quadratically with the number of developers. As a result, at small scales, data science teams may use phone calls or video chats, with 74% communicating synchronously and in person (Choi and Tausczik, 2017). At larger scales, like those made possible by the open-source development process, communication can take place more effectively through coordination around a shared work product, or through discussion threads and chat rooms.

Ultimately, we list four challenges for a collaborative framework to address. While not exhaustive, this list comprises the challenges we mainly focus on in this work, though we review and discuss additional ones in Chapters 2 and 5.

C1 *Task management.* Working alone, data scientists often write end-to-end scripts that prepare the data, extract features, build and train model models, and tune hyperparameters (Subramanian et al., 2020; Rule et al., 2018; Muller et al., 2019). How can this large task be broken down so that all collaborators can coordinate with each other and contribute without duplicating work?

C2 *Tool mismatch.* Data scientists are accustomed to working in computational notebooks, and have varying expertise with version control tools like git (Subramanian et al., 2020; Chattopadhyay et al., 2020; Kery et al., 2018;

challenge	*design concept*	*components of Ballet*
task management (C1)	data science patches (D1)	feature definition abstraction (3.4.1), feature engineering language (3.4), patch development in Assemblé (3.6)
tool mismatch (C2)	data science products in open-source workflows (D2)	feature engineering pipeline abstraction (3.4.5), patch contribution in Assemblé (3.6), CLI for project administration (3.3.1)
evaluating contributions (C3)	software and statistical acceptance procedures (D3)	feature API validation (3.5.1), streaming feature definition selection (3.5.2), continuous integration (3.3.1), Ballet Bot (3.3.1)
maintaining infrastructure (C4)	decentralized development (D4)	F/OSS package (3.3.1), free infrastructure and services (3.3.1), bring your own compute (3.3.2)

Table 3.1: Addressing challenges in collaborative data science development by applying our design concepts in the Ballet framework.

Rule et al., 2018). How can these workflows be adapted to use a shared codebase and build a single product?

C3 *Evaluating contributions.* Prospective collaborators may submit code to a shared codebase. Some code may introduce errors or decrease the performance of the ML model (Smith et al., 2017; Renggli et al., 2019; Karlaš et al., 2020; Kang et al., 2020). How can code contributions be evaluated?

C4 *Maintaining infrastructure.* Data science requires careful management of data and computation (Sculley et al., 2015; Smith et al., 2017). Will it be necessary to establish shared data stores and computing infrastructure? Would this be expensive and require significant technical and DevOps expertise? Is this appropriate for the open-source setting?

3.2.2 Design concepts

To address these challenges, we think creatively about how certain data science steps might fit into a modified open-source development process. Our starting point is to look for processes in which some important functionality can be decomposed into smaller, similarly-structured patches that can be evaluated using standardized measures. Through our experience researching and developing feature engineering pipelines and systems, as well as our review of the requirements and key characteristics of the feature engineering process, we found that we could extend and adapt the pull request model to facilitate collaborative development in data science by following a series of four corresponding design concepts (Table 3.1), which form the basis for our framework.

D1 *Data science patches.* We identify steps of the data science process that can be broken down into many *patches* — modular source code units — which can be developed and contributed separately in an incremental process. For example, given a feature engineering pipeline, a patch could be a new feature definition added to the pipeline.

D2 *Data science products in open-source workflows.* A usable data science artifact forms a *product* that is stored in an open-source repository. For example, when solving a feature engineering task, the product is an executable feature engineering pipeline. The composition of many patches from different collaborators forms a product that is stored in a repository on a source code host in which patches are proposed as individual pull requests. We design this process to accommodate collaborators of all backgrounds by providing multiple development interfaces. Notebook-based workflows are popular among data scientists, so our framework supports creation and submission of patches entirely within the notebook.

D3 *Software and statistical acceptance procedures.* ML products have the usual software quality measures along with statistical/ML performance metrics. Collaborators receive feedback on the quality of their work from both of these points of view.

D4 *Decentralized development.* A lightweight approach is needed for managing code, data, and computation. In our decentralized model, each collaborator uses their own storage and compute, and we leverage existing community infrastructure for source code management and patch acceptance.

Besides feature engineering, how and when can this framework be used? Several conditions must be met. First, the data science product must be able to be decomposed into small, similarly-structured patches. Otherwise, the framework has a limited ability to integrate contributions. Second, human knowledge and expertise must be relevant to the generation of the data science patches. Otherwise, automation or learning alone may suffice. Third, measures of statistical and ML performance, or good proxies thereof, must be definable at the level of individual patches. Otherwise, it is difficult for maintainers to reason about how and whether to integrate patches. Finally, dataset size and evaluation time requirements must not be excessive. Otherwise, we could not use existing services that are free for open-source development.[2]

So while we focus on feature engineering, this framework can apply to other steps in data science pipelines — for example, data programming with labeling functions and slicing functions (Ratner et al., 2016; Chen et al., 2019). Indeed, we present a speculative discussion of applying Ballet to data programming projects in Section 9.1.

In the next section, we apply these design principles to describe a framework for collaboration on predictive modeling projects, referring back to these challenges and design concepts as they appear. Then in Section 3.4, we implement this general approach more specifically for collaborative feature engineering on tabular data.

3.3 An overview of Ballet

Ballet extends the open-source development process to support collaborative data science by applying the concepts of data science patches, data science products in open-source workflows, software and statistical acceptance procedures, and decentralized development. As this process is complex, we illustrate how Ballet works by showing the experience of using it from three perspectives — maintainer, collaborator,

[2] As a rough guideline, running the evaluation procedure on the validation data should take no more than five minutes in order to facilitate interactivity.

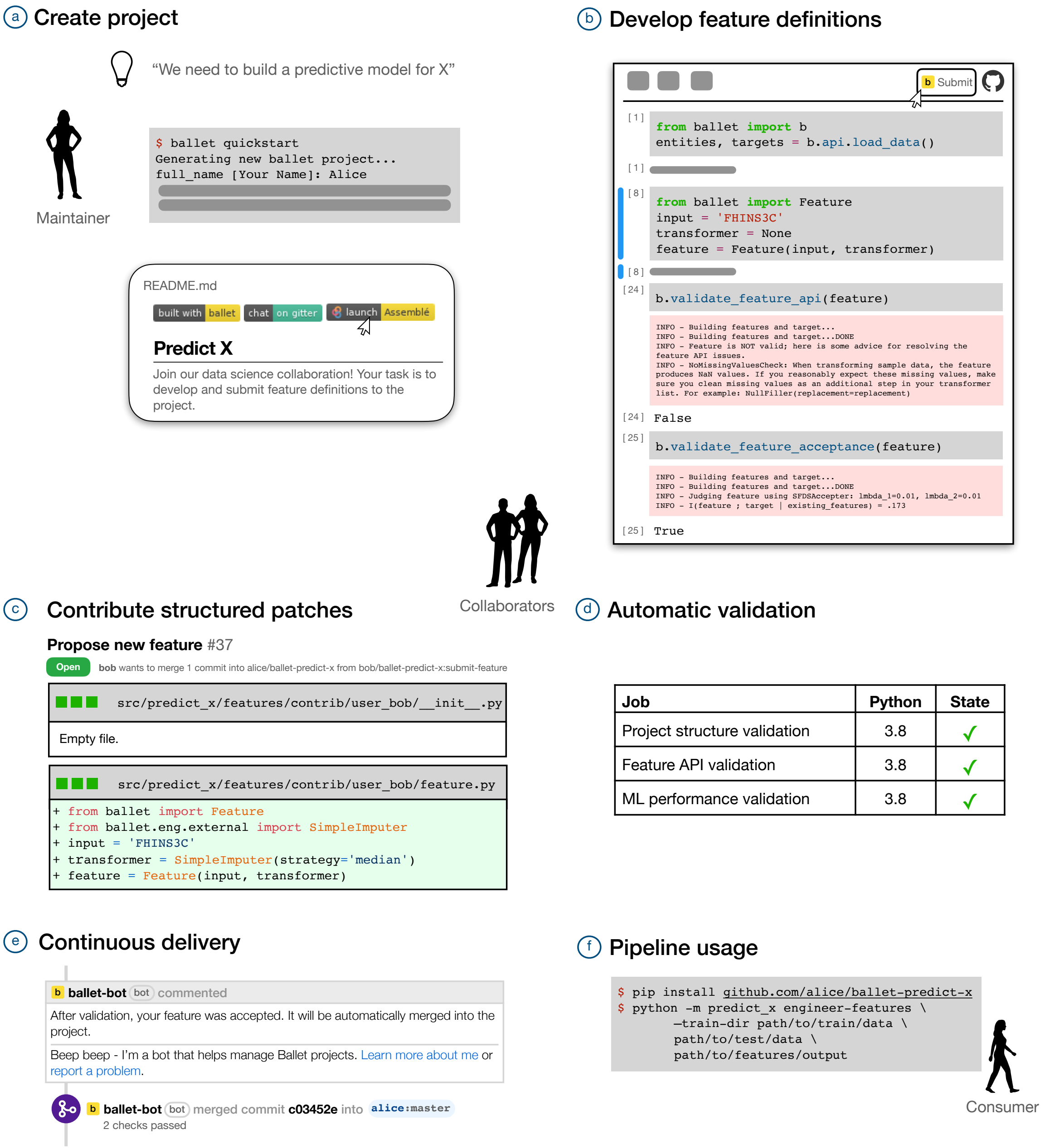
and consumer — building on existing work that investigates different users' roles in open source development and ecosystems (Yu and Ramaswamy, 2007; Berdou, 2010; Roberts et al., 2006; Barcellini et al., 2014; Hauge et al., 2010). This development cycle is illustrated in Figure 3.1. In Section 3.4, we present a more concrete example of feature engineering on tabular datasets.

3.3.1 Maintainer

A maintainer wants to build a predictive model. They first define the prediction goal and upload their dataset. They install the Ballet package, which includes the core framework libraries and command line interface (CLI). Next, they use the CLI to automatically render a new repository from the provided project template, which contains the minimal files and structure required for their project, such as directory organization, configuration files, and problem metadata. They define a task for collaborators: create and submit a data science patch that performs well (C1/D1) — for example, a feature definition that has high predictive power. The resulting repository contains a usable (if, at first, empty) data science pipeline (C2/D2). After pushing to GitHub and enabling our CI tools and bots, the maintainer begins recruiting collaborators.

Collaborators working in parallel submit patches as pull requests with a careful structure provided by Ballet. Not every patch is worthy of inclusion in the product. As patches arrive from collaborators in the form of pull requests, the CI service is repurposed to run Ballet's acceptance procedure such that only high-quality patches are accepted (C3/D3). This "working pipeline invariant" aligns data science pipelines with the aim of continuous delivery in software development (Humble and Farley, 2010). In feature engineering, the acceptance procedure is a feature validation suite (Section 3.5) which marks individual feature definitions as accepted/rejected, and the resulting feature engineering pipeline on the default branch can always be executed to engineer feature values from new data instances.

One challenge for maintainers is to integrate data science patches as they begin to stream in. Unlike software projects where contributions can take any form, these



```
$ ballet quickstart
Generating new ballet project...
full_name [Your Name]: Alice
```

Predict X

Join our data science collaboration! Your task is to develop and submit feature definitions to the project.

```
[1]  from ballet import b
     entities, targets = b.api.load_data()

[8]  from ballet import Feature
     input = 'FHINS3C'
     transformer = None
     feature = Feature(input, transformer)

[24] b.validate_feature_api(feature)

INFO - Building features and target...
INFO - Building features and target...DONE
INFO - Feature is NOT valid; here is some advice for resolving the
feature API issues.
INFO - NoMissingValuesCheck: When transforming sample data, the feature
produces NaN values. If you reasonably expect these missing values, make
sure you clean missing values as an additional step in your transformer
list. For example: NullFiller(replacement=replacement)

[24] False

[25] b.validate_feature_acceptance(feature)

INFO - Building features and target...
INFO - Building features and target...DONE
INFO - Judging feature using SFDSAccepter: lmbda_1=0.01, lmbda_2=0.01
INFO - I(feature ; target | existing_features) = .173

[25] True
```

Propose new feature #37

Open **bob** wants to merge 1 commit into alice/ballet-predict-x from bob/ballet-predict-x:submit-feature

```
src/predict_x/features/contrib/user_bob/__init__.py
```

Empty file.

```
src/predict_x/features/contrib/user_bob/feature.py
+ from ballet import Feature
+ from ballet.eng.external import SimpleImputer
+ input = 'FHINS3C'
+ transformer = SimpleImputer(strategy='median')
+ feature = Feature(input, transformer)
```

Job	Python	State
Project structure validation	3.8	✓
Feature API validation	3.8	✓
ML performance validation	3.8	✓

ballet-bot bot commented

After validation, your feature was accepted. It will be automatically merged into the project.

Beep beep - I'm a bot that helps manage Ballet projects. Learn more about me or report a problem.

ballet-bot bot merged commit **c03452e** into alice:master

2 checks passed

```
$ pip install github.com/alice/ballet-predict-x
$ python -m predict_x engineer-features \
      —train-dir path/to/train/data \
      path/to/test/data \
      path/to/features/output
```

Figure 3.1: An overview of collaborative data science development with the Ballet framework for a feature engineering project. (Continued on the following page.)

Figure 3.1: An overview of collaborative data science development with the Ballet framework for a feature engineering project. (a) A maintainer with a dataset wants to mobilize the power of the open data science community to solve a predictive modeling task. They use the Ballet CLI to render a new project from a provided template and push to GitHub. (b) Data scientists interested in collaborating on the project are tasked with writing feature definitions (defining `Feature` instances). They can launch the project in Assemblé, a custom development environment built on Binder and JupyterLab. Ballet's high-level client supports them in automatically detecting the project configuration, exploring the data, developing candidate feature definitions, and validating feature definitions to surface any API and ML performance issues. Once issues are fixed, the collaborator can submit the feature definition alone by selecting the code cell and using Assemblé's submit button. (c) The selected code is automatically extracted and processed as a pull request following the project structure imposed by Ballet. (d) In continuous integration, Ballet runs feature API and ML performance validation on this one feature definition (e) Feature definitions that pass can be automatically and safely merged by the Ballet Bot. (f) Ballet will collect and compose this new feature definition into the existing feature engineering pipeline, which can be used by the community to model their own raw data.

types of patches are all structured similarly, and if they validate successfully, they may be safely merged without further review. To support maintainers, the *Ballet Bot*[3] can automatically manage contributions, performing tasks such as merging pull requests of accepted patches and closing rejected ones. The process continues until either the performance of the ML product exceeds some threshold, or improvements are exhausted.

Ballet projects are lightweight, as our framework is distributed as a free and open-source Python package, and use only lightweight infrastructure that is freely available to open-source projects, like GitHub, Travis, and Binder (C4/D4). This avoids spinning up data stores or servers — or relying on large commercial sponsors to do the same.

3.3.2 Collaborators

A data scientist is interested in the project and wants to contribute. They find the task description and begin learning about the project and about Ballet. They

[3] `https://github.com/ballet/ballet-bot`

can review and learn from existing patches contributed by others and discuss ideas in an integrated chatroom. They begin developing a new patch in their preferred development environment (*patch development task*). When they are satisfied with its performance, they propose to add it to the upstream project at a specific location in the directory structure using the pull request model (*patch contribution task*). In designing Ballet, we aimed to make it as easy as possible for data scientists with varying backgrounds to accomplish the patch development and patch contribution tasks within open-source workflows.

The Ballet interactive client, included in the core library, supports collaborators in loading data, exploring and analyzing existing patches, validating the performance of their work, and accessing functionality provided by the shared project. It also decreases the time to beginning development by automatically detecting and loading a Ballet project's configuration. Use of the client is shown in Figure 3.1, Panel B.

We enable several interfaces for collaborators to develop and submit patches like feature definitions, where different interfaces are appropriate for collaborators with different types of development expertise, relaxing requirements on development style. Collaborators who are experienced in open-source development processes can use their preferred tools and workflow to submit their patch as a pull request, supported by the Ballet CLI — the project is still just a layer built on top of familiar technologies like git. However, in preliminary user studies (Section 3.7), we found that adapting from usual data science workflows was a huge obstacle. Many data scientists we worked with had never successfully used open-source development processes to contribute to any shared project.

We addressed this by centering all development in the notebook with *Assemblé*, a cloud-based workflow and development environment for contribution to Ballet projects (C1/D1). We created a custom experience on top of community tooling that enables data scientists to develop and submit features entirely within the notebook. We describe Assemblé in detail in Section 3.6.

The submitted feature definitions are marked as accepted or rejected, and data scientists can proceed accordingly, either moving on to their next idea or reviewing diagnostic information and trying to fix a rejected submission.

3.3.3 Consumer

Ballet project consumers — members of the wider data science community — are now free to use the data science product however they desire, such as by executing the feature engineering pipeline to extract features from new raw data instances, making predictions for their own datasets. The project can easily be installed using a package manager like `pip` as a versioned dependency, and ML engineers can extract the machine-readable feature definitions into a feature store or other environment for further analysis and deployment. This "pipeline as code"/"pipeline as package" approach makes it easy to use and re-use the pipeline and helps address data lineage/versioning issues.

For example, the Ballet client for feature engineering projects exposes a method that fits the feature engineering pipeline on training data and can then engineer features from new data instances, and an instance of a pipeline that is already fitted on data from of the upstream project. These can be easily used in other library code.

3.4 A language for feature engineering

We now describe in detail the design and implementation of a feature engineering "mini-language" within Ballet to enable collaborative feature engineering projects. While we spoke in general terms about data science patches and products and the statistical acceptance procedure, here we define these concepts in a "plugin" for feature engineering.

We start from the insight that feature engineering can be represented as a dataflow graph over individual features. We structure code that extracts a group of feature values as a patch, calling these *feature definitions* and representing them with a `Feature` interface. Feature definitions are composed into a feature engineering pipeline product. Newly contributed feature definitions are accepted if they pass a two-stage acceptance procedure that tests both the feature API and its contribution to ML performance. Finally, the plugin specifies the organization of modules within a repository to allow features to be collected programmatically.

In Ballet, we create a flexible and powerful language for feature engineering that is embedded within the larger framework. It supports functionality such as learned feature transformations, supervised feature transformations, nested transformer steps, syntactic sugar for functional transformations, data frame-style transformations, and recovery from errors due to type incompatibility.

```python
from ballet import Feature
from ballet.eng import ConditionalTransformer
from ballet.eng.external import SimpleImputer
import numpy as np

input = 'Lot Area'
transformer = [
    ConditionalTransformer(
        lambda ser: ser.skew() > 0.75,
        lambda ser: np.log1p(ser)),
    SimpleImputer(strategy='mean'),
]
name = 'Lot area unskewed'
feature = Feature(input, transformer, name=name)
```

Figure 3.2: A feature definition that conditionally unskews lot area (for a house price prediction problem) by applying a log transformation only if skew is present in the training data and then mean-imputing missing values.

```python
from ballet import Feature
from ballet.eng.external import SimpleImputer
import numpy as np

input = 'JWAP'  # Time of arrival at work
transformer = [
    SimpleImputer(missing_values=np.nan, strategy='constant', fill_value=0.0),
    lambda df: np.where((df >= 70) & (df <= 124), 1, 0),
]
name = 'If job has a morning start time'
description = 'Return 1 if the Work arrival time >=6:30AM and <=10:30AM'
feature = Feature(input, transformer, name=name, description=description)
```

Figure 3.3: A feature definition that defines a transformation of work arrival time (for a personal income prediction problem) by filling missing values and then applying a custom function.

3.4.1 Feature definitions

A *feature definition* is the code that is used to extract semantically related feature values from raw data. Let us observe data instances $\mathcal{D} = (\mathbf{v}_i, \mathbf{y}_i)_{i=1}^N$, where $\mathbf{v}_i \in \mathcal{V}$ are the raw variables and $\mathbf{y}_i \in \mathcal{Y}$ is the target. In this formulation, the raw variable domain $\mathcal{V}$ includes strings, missing values, categories, and other non-numeric types that cannot typically be inputted to learning algorithms. Thus our goal in feature engineering is to develop a learned map from $\mathcal{V}$ to $\mathcal{X}$ where $\mathcal{X} \subseteq \mathbb{R}^n$ is a real-valued feature space.

Definition 1. *A* feature function *is a learned map from raw variables in one data instance to feature values, $f : (\mathcal{V}, \mathcal{Y}) \to \mathcal{V} \to \mathcal{X}$.*

We indicate the map learned from a specific dataset $\mathcal{D}$ by $f^{\mathcal{D}}$, i.e., $f^D(v) = f(D)(v)$.

A feature function can produce output of different dimensionality. Let $q(f)$ be the dimensionality of the feature space $\mathcal{X}$ for a feature f. We call f a *scalar-valued feature* if $q(f) = 1$ or a *vector-valued feature* if $q(f) > 1$. For example, the embedding of a categorical variable, such as a one-hot encoding, would result in a vector-valued feature.

We can decompose a feature function into two parts, its *input projection* and its *transformer steps*. The input projection is the subspace of the variable space that it operates on, and the transformer steps, when composed together, equal the learned map on this subspace.

Definition 2. *A* feature input projection *is a projection from the full variable space to the* feature input space*, the set of variables that are used in a feature function, $\pi : \mathcal{V} \to \mathcal{V}$.*

Definition 3. *A* feature transformer step *is a learned map from the variable space to the variable space, $f_i : (\mathcal{V}, \mathcal{Y}) \to \mathcal{V} \to \mathcal{V}$.*

We require that individual feature transformer steps compose together to yield the feature function, where the first step applies the input projection and the last step maps to $\mathcal{X}$ rather than $\mathcal{V}$. That is, each transformer step applies some arbitrary transformation as long as the final step maps to allowed feature values.

$$\begin{aligned}
f_0 &: (V, Y) \mapsto \pi \\
f_i \circ f_{i-1} &: (V, Y) \mapsto f_i(f_{i-1}(\dots, Y)(V), Y) \\
f_n &: (\mathcal{V}, \mathcal{Y}) \to \mathcal{V} \to \mathcal{X} \\
f &: (V, Y) \mapsto f_n(\dots(f_1(f_0(V, Y)(V), Y)\dots), Y)
\end{aligned}$$

The `Feature` class in Ballet is a way to express a feature function in code. It is a tuple (`input`, `transformer`). The input declares the variable(s) from $\mathcal{V}$ that are needed by the feature, which will be passed to `transformer`, one or more transformer steps. Each transformer step implements the learned map via `fit` and `transform` methods, a standard interface in machine learning pipelines (Buitinck et al., 2013). A data scientist then simply provides values for the input and transformer of a `Feature` object in their code. Additional metadata, including `name`, `description`, `output`, and `source`, is also exposed by the `Feature` abstraction. For example, the feature `output` is a column name (or set of column names) for the feature value (or feature values) in the resulting feature matrix; if it is not provided by the data scientist, it can be inferred by Ballet using various heuristics.

Two example feature definitions are shown in Figures 3.2 and 3.3.

3.4.2 Learned feature transformations

In machine learning, we estimate the generalization performance of a model by evaluating it on a set of test observations that are unseen by the model during training. *Leakage* is a problem in which information about the test set is accidentally exposed to the model during training, artificially inflating its performance on the test set and thus underestimating generalization error.

Each feature function learns a specific map $\mathcal{V} \to \mathcal{X}$ from $\mathcal{D}$, such that any parameters it uses, such as variable means and variances, are learned from the development (training) dataset. This formalizes the separation between development and testing data to avoid any leakage of information during the feature engineering process.

As in the common pattern, a feature engineering pipeline by itself or within a model has two stages within training: a fit stage and a transform stage. During the fit stage, parameters are learned from the training data and stored within the individual transformer steps. During the transform stage, the learned parameters are used to transform the raw variables into a feature matrix. The same parameters are also used at prediction time.

3.4.3 Nested feature definitions

Feature definitions or feature functions can also be nested within the `transformer` field of another feature. If an existing feature is used as one transformer step in another feature, when the new feature function is executed, the nested feature is executed in a sub-procedure and the resulting feature values are available to the new feature for further transformation. Data scientists can also introspect an existing feature to access its own `input` and `transformer` attributes and use them directly within a new feature.

Through its support for nested feature definitions, Ballet allows collaborating data scientists to define an arbitrary directed acyclic dataflow graph from the raw variables to the feature matrix.

3.4.4 Feature engineering primitives

Many features exhibit common patterns, such as scaling or imputing variables using simple procedures. And while some features are relatively simple and have no learned parameters, others are more involved to express in a fit/transform style. Data scientists commonly extract these more advanced features by manipulating development and test tables directly using popular data frame libraries, often leading to leakage. In preliminary studies (Section 3.7), we found that data scientists sometimes struggled to create features one at a time, given their familiarity with writing long processing scripts. Responding to this feedback, we provided a library of *feature engineering primitives* that implements many common utilities and learned transformations.

Definition 4. *A* feature engineering primitive *is a class that can be instantiated within a sequence of transformer steps to express a common feature engineering pattern.*

This library, `ballet.eng`, includes primitives like `ConditionalTransformer`, which applies a secondary transformation depending on whether a condition is satisfied on the development data, and `GroupwiseTransformer`, which learns a transformer separately for each group of a group-by aggregation on the development set. We also organize and re-export 77 primitives[4] from six popular Python libraries for feature engineering, such as scikit-learn's `SimpleImputer` (Table 3.2).

Table 3.2: Feature engineering primitives implemented or re-exported in `ballet.eng`, by library.

Library	Number of primitives
`ballet`	16
`category_encoders`	17
`feature_engine`	29
`featuretools`	1
`skits`	10
`scikit-learn`	19
`tsfresh`	1

3.4.5 Feature engineering pipelines

Features are then composed together in a feature engineering pipeline.

Definition 5. *Let $f_1, \ldots, f_m$ be a collection of feature functions, $\mathcal{D}$ be a development dataset, and $\mathcal{D}' = (V', Y')$ be a collection of new data instances. A* feature engineering pipeline *$\mathcal{F} = \{f_i\}_{i=1}^m$ applies each feature function to the new data instances and concatenates the result, yielding the feature matrix*

[4] As of ballet v0.19.

$$X = \mathcal{F}^{\mathcal{D}}(V') = f_1^{\mathcal{D}}(V') \oplus \cdots \oplus f_m^{\mathcal{D}}(V').$$

A feature engineering pipeline can be thought of as similar to a collection of feature functions. It is implemented in Ballet in the `FeatureEngineeringPipeline` class.

In Ballet's standard configuration, only feature functions that have been explicitly defined by data scientists (and accepted by the feature validation) are included in the feature engineering pipeline. Thus, raw variables are not outputted by the pipeline unless they are explicitly requested (i.e., by a data scientist developing a feature definition that applies the identity transformation to a raw variable). In alternative configurations, project maintainers can define a set of fixed feature definitions to include in the pipeline, which can include a set of important raw variables with the identity transformation or other transformations applied.

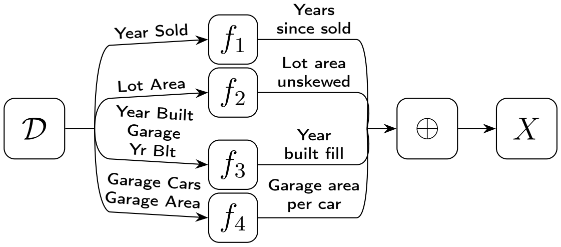


Figure 3.4: A feature engineering pipeline for a house price prediction problem with four feature functions operating on six raw variables.

3.4.6 Feature execution engine

Ballet's feature execution engine is responsible for applying the full feature engineering pipeline or an individual feature to extract feature values from a given set of data instances. Each feature function within the pipeline is passed the input columns it requires, which it then transforms appropriately, internally using one or more transformer steps (Figure 3.4). It operates as follows, starting from a set of `Feature` objects.

1. The transformer steps of each feature are postprocessed in a single step. First, any syntactic sugar is replaced with the appropriate objects. For example, an

anonymous function is replaced by a `FunctionTransformer` object that applies the function, or a tuple of an input and another transformer is replaced by an `SubsetTransformer` object that applies the transformer on the given subset of the input and passes through the remaining columns unchanged. Second, the transformer steps are all wrapped in functionality that allows them to recover from any errors that are due to type incompatibility. For example, if the underlying transformation expects a 1-d array (column vector), but receives as input a 2-d array with a single column, the wrapper will catch the error, convert the 2-d array to a 1-d array, and retry the transformation. The wrapper pre-defines a set of these "conversion approaches" (one of which is the identity transformation), which will be tried in sequence until one is successful. The successful approach is stored so that it can be re-used during subsequent applications of the feature.

2. The features are composed together into a feature engineering pipeline object.

3. The fit stage of the feature engineering pipeline is executed. For each feature, the execution engine indexes out the declared input columns from the raw data and passes them to the wrapped `fit` method of the feature's transformer. (This stage only occurs during training.)

4. The transform stage of the feature engineering pipeline is executed. For each feature, the execution engine indexes out the declared input columns from the raw data and passes them to the wrapped `transform` method of the feature's transformer.

This process can also be parallelized across features. Since support for nested feature definitions (Section 3.4.3) means that if features were executed independently there may be redundant computation if there were dependencies between features, this would necessitate a more careful approach in which the features are first sorted topologically and then resulting feature values are cached after first computation. For very large feature sets or datasets, full-featured dataflow engines should be considered.

3.5 Acceptance procedures for feature definitions

Contributions of feature engineering code, just like other code contributions, must be evaluated for quality before being accepted in order to mitigate the risk of introducing errors, malicious behavior, or design flaws. For example, a feature function that produces non-numeric values can result in an unusable feature engineering pipeline. Large feature engineering collaborations can also be susceptible to “feature spam,” a high volume of low-quality feature definitions (submitted either intentionally or unintentionally) that harm the collaboration (Smith et al., 2017). Modeling performance can suffer and require an additional feature selection step — violating the working pipeline invariant — and the experience of other collaborators can be harmed if they are not able to assume that existing feature definitions are high-quality.

To address these possibilities, we extensively validate feature definition contributions for software quality and ML performance. Validation is implemented as a test suite that is both exposed by the Ballet client and executed in CI for every pull request. Thus, the same method that is used in CI for validating feature contributions is available to data scientists for debugging and performance evaluation in their development environment. Ballet Bot can automatically merge pull requests corresponding to accepted feature definitions and close pull requests corresponding to rejected feature definitions.

This automatic acceptance procedure is defined for the addition of new feature definitions only, while acceptance procedures for edits or deletions of feature definitions is important future work.

3.5.1 Feature API validation

User-contributed feature definitions should satisfy the `Feature` interface and successfully deal with common error situations, such as intermediate computations producing missing values. We fit the feature function to a separate subsampled training dataset in an isolated environment and extract feature values from subsampled training and validation datasets, failing immediately on any implementation errors. We then con-

`IsFeatureCheck`	`HasCorrectInputTypeCheck`	`HasCorrectOutputDimensionsCheck`
`HasTransformerInterfaceCheck`	`CanFitCheck`	`CanFitOneRowCheck`
`CanTransformCheck`	`CanTransformNewRowsCheck`	`CanTransformOneRowCheck`
`CanFitTransformCheck`	`CanMakeMapperCheck`	`NoMissingValuesCheck`
`NoInfiniteValuesCheck`	`CanDeepcopyCheck`	`CanPickleCheck`

Table 3.3: Feature API validation suite in (`ballet.validation.feature_api.checks`) that ensures the proper functioning of the shared feature engineering pipeline.

duct a battery of 15 tests to increase confidence that the feature function would also extract acceptable feature values on unseen inputs (Table 3.3). Each test is paired with "advice" that can be surfaced back to the user to fix any issues (Figure 3.1).

Another part of feature API validation is an analysis of the changes introduced in a proposed PR to ensure that the required project structure is preserved and that the collaborator has not accidentally included irrelevant code that would need to be evaluated separately.[5] A feature contribution is valid if it consists of the addition of a valid source file within the project's `src/features/contrib` subdirectory that also follows a specified naming convention using the user's login name and the given feature name. The introduced module must define exactly one object — an instance of `Feature` — which will then be imported by the framework.

3.5.2 ML performance validation

A complementary aspect of the acceptance procedure is validating a feature contribution in terms of its impact on machine learning performance, which we cast as a streaming feature definition selection (SFDS) problem. This is a variant of streaming feature selection where we select from among feature definitions rather than feature values. Features that improve ML performance will pass this step; otherwise, the contribution will be rejected. Not only does this discourage low-quality contributions, but it provides a way for collaborators to evaluate their performance, incentivizing more deliberate and creative feature engineering.

We first compile requirements for an SFDS algorithm to be deployed in our setting, including that the algorithm should be stateless, support real-world data types

[5] This "project structure validation" is only relevant in CI and is not exposed by the Ballet client.

(mixed discrete and continuous), and be robust to over-submission. While there has been a wealth of research into streaming feature selection (Zhou et al., 2005; Wu et al., 2013; Wang et al., 2015; Yu et al., 2016), no existing algorithm satisfies all requirements. Instead, we extend prior work to apply to our situation. Our SFDS algorithm proceeds in two stages.[6] In the *acceptance* stage, we compute the conditional mutual information of the new feature values with the target, conditional on the existing feature matrix, and accept the feature if it is above a dynamic threshold. In the *pruning* stage, existing features that have been made newly redundant by accepted features can be pruned. Full details are presented in the following section.

3.5.3 Streaming feature definition selection

Feature selection is a classic problem in machine learning and statistics (Guyon and Elisseeff, 2003). The problem of feature selection is to select a subset of the available feature values such that a learning algorithm that is run on the subset generates a predictive model with the best performance according to some measure.

Definition 6. *The* feature selection problem *is to select a subset of feature values that maximizes some utility,*

$$X^* = \underset{X' \in \mathcal{P}(X)}{\arg\max}\, U(X'), \tag{3.1}$$

where $\mathcal{P}(A)$ denotes the power set of A. For example, U could measure the empirical risk of a model trained on X'.

If there exists a group structure in X, then this formulation ignores the group structure and allows feature values to be subselected from within groups. In some cases, like ours, this may not be desirable, such as if it is necessary to preserve the coherence and interpretability of each feature group. In the case of feature engineering using feature functions, it further conflicts with the understanding of each feature function as extracting a semantically related set of feature values.

[6] Indeed, we abbreviate the general problem of streaming feature definition selection as SFDS, and also call our algorithm to solve this problem SFDS. We trust that readers can disambiguate based on context.

Thus we instead consider the related problem of feature definition selection.

Definition 7. *The* feature definition selection *problem is to select a subset of feature definitions that maximizes some utility,*

$$\mathcal{F}^* = \operatorname*{arg\,max}_{\mathcal{F}' \in \mathcal{P}(\mathcal{F})} U(\mathcal{F}'), \tag{3.2}$$

This constrains the feature selection problem to select either all of or none of the feature values extracted by a given feature.

In Ballet, as collaborators develop new features, each feature arrives at the project in a streaming fashion, at which point it must be accepted or rejected immediately. Streaming feature definition selection is a streaming extension of feature definition selection.

Definition 8. *Let* Γ *be a feature definition stream of unknown size, let* $\mathcal{F}$ *be the set of features accepted as of some time, and let* $f \in \Gamma$ *arrive next. The* streaming feature definition selection *problem is to select a subset of feature definitions that maximizes some utility,*

$$\mathcal{F}^* = \operatorname*{arg\,max}_{\mathcal{F}' \in \mathcal{P}(\mathcal{F} \cup f)} U(\mathcal{F}'). \tag{3.3}$$

Streaming feature definition selection consists of two decision problems, considered as sub-procedures. The *streaming feature definition acceptance* decision problem is to *accept* f, setting $\mathcal{F} \leftarrow \mathcal{F} \cup f$, or *reject*, leaving $\mathcal{F}$ unchanged. The *streaming feature pruning* decision problem is to remove a subset $\mathcal{F}_0 \subset \mathcal{F}$ of low-quality features, setting $\mathcal{F} = \mathcal{F} \setminus \mathcal{F}_0$.

Design criteria

Streaming feature definition selection algorithms must be carefully designed to best support collaborations in Ballet. We consider the following design criteria, motivated by engineering challenges, security risks, and experience from system prototypes:

1. *Definitions, not values.* The algorithm should have first-class support for feature definitions (or feature groups) rather than selecting individual feature values.

2. *Stateless.* The algorithm should require as inputs only the current state of the Ballet project (i.e., the problem data and accepted features) and the pull request details (i.e., the proposed feature). Otherwise, each Ballet project (i.e., its GitHub repository) would require additional infrastructure to securely store the algorithm state.

3. *Robust to over-submission.* The algorithm should be robust to processing many more feature submissions than raw variables present in the data (i.e., $|\Gamma| \gg |\mathcal{V}|$). Otherwise malicious (or careless) contributors can automatically submit many features, unacceptably increasing the dimensionality of the resulting feature matrix.

4. *Support real-world data.* The algorithm should support mixed continuous- and discrete-valued features, common in real-world data.

Surprisingly, there is no existing algorithm that satisfies these design criteria. Algorithms for feature value selection might only support discrete data, algorithms for feature group selection might require persistent storage of decision parameters, etc. And the robustness criterion remains important given the results of Smith et al. (2017), in which users of a collaborative feature engineering system programmatically submitted thousands of irrelevant features, constraining modeling performance. These factors motivate us to create our own algorithm.

Feature definition alpha-investing

As a first (unsuccessful) approach, we consider *feature definition alpha-investing.* Alpha-investing (Zhou et al., 2005) is one algorithm for streaming feature selection. It maintains a time-varying parameter, α_t, which controls the algorithm's false-positive rate and conducts a likelihood ratio test to compare the current features with the resulting features if the new feature is added.

We can extend this method to support feature definitions rather than feature values as follows. Compute the likelihood ratio $T = -2(\log \hat{L}(\mathcal{F}) - \log \hat{L}(\mathcal{F} \cup f))$, where $\hat{L}(\cdot)$ is the maximum likelihood of a linear model. Then $T \sim \chi^2(q(f))$ and we compute a p-value accordingly. If $p < \alpha_t$, then f is accepted; otherwise it is rejected. α_t is adjusted according to an update rule that is a function of the sequence of accepts/rejects (Zhou et al., 2005).

Unfortunately, the feature definition alpha-investing algorithm does not satisfy the design criteria of Ballet because it is neither stateless nor robust to over-submission. The pitfalls are that α_t must be securely stored somewhere and that it is affected by rejected features — adversaries could repeatedly submit noisy features that are liable to be rejected, artificially lowering the threshold for high-quality features.

SFDS

Instead, we present a new algorithm, SFDS, for streaming feature definition selection based on mutual information criteria. It extends the GFSSF algorithm (Li et al., 2013) both to support feature definitions rather than feature values and to support real-world tabular datasets with a mix of continuous and discrete variables.

The algorithm (Algorithm 1) works as follows. In the acceptance stage, we first determine if a new feature f is *strongly relevant*; that is, whether the information $f(\mathcal{D})$ provides about Y above and beyond the information that is already provided by $\mathcal{F}(\mathcal{D})$ is above some threshold governed by hyperparameters λ_1 and λ_2, which penalize the number of features and the number of feature values, respectively. If so, we accept it immediately. Otherwise, the feature may still be *weakly relevant*, in which case we consider whether f and some other feature $f' \in \mathcal{F}$ provide similar information about Y. If f is determined to be superior to such an f', then f can be accepted. Later, in the pruning stage, f' and any other redundant features are pruned.

CMI estimation

In the SFDS algorithm, we compute several quantities of the form $I(f(\mathcal{D}), Y|\mathcal{F}(\mathcal{D}))$, i.e., the conditional mutual information (CMI) of the proposed feature and the target, given the set of accepted features. Since we do not know the true joint distribution of feature values and target, we must derive an estimator for this quantity. Let $Z = f(\mathcal{D})$

```
Algorithm 1: SFDS
input  : feature stream $\Gamma$, evaluation dataset $\mathcal{D}$
output : accepted feature set $\mathcal{F}$

$\mathcal{F} \leftarrow \varnothing$
while $\Gamma$ has new features do
    $f \leftarrow$ get next feature from $\Gamma$
    if $accept(\mathcal{F}, f, \mathcal{D})$ then
        $\mathcal{F} \leftarrow prune(\mathcal{F}, f, \mathcal{D})$
        $\mathcal{F} \leftarrow \mathcal{F} \cup f$
    end
end
return $\mathcal{F}$
```

```
Procedure accept($\mathcal{F}$, $f$, $\mathcal{D}$)
input  : accepted feature set $\mathcal{F}$, proposed feature $f$, evaluation dataset $\mathcal{D}$
params : penalty on number of feature definitions $\lambda_1$, penalty on number of
         feature values $\lambda_2$
output : accept/reject

if $I(f(\mathcal{D}); Y|\mathcal{F}(\mathcal{D})) > \lambda_1 + \lambda_2 \times q(f)$ then
    return true
end
for $f' \in \mathcal{F}$ do
    $\mathcal{F}' \leftarrow \mathcal{F} \setminus f'$
    if $I(f(\mathcal{D}); Y|\mathcal{F}'(\mathcal{D})) - I(f'(\mathcal{D}); Y|\mathcal{F}'(\mathcal{D})) > \lambda_1 + \lambda_2 \times (q(f) - q(f'))$ then
        return true
    end
end
return false
```

```
Procedure prune($\mathcal{F}$, $f$, $\mathcal{D}$)
input  : previously accepted feature set $\mathcal{F}$, newly accepted feature $f$, evaluation
         dataset $\mathcal{D}$
params : penalty on number of feature definitions $\lambda_1$, penalty on number of
         feature values $\lambda_2$
output : pruned feature set $\mathcal{F}$

for $f' \in \mathcal{F}$ do
    $\mathcal{F}' \leftarrow \mathcal{F} \setminus f' \cup f$
    if $I(f'(\mathcal{D}); Y|\mathcal{F}'(\mathcal{D})) < \lambda_1 + \lambda_2 \times q(f')$ then
        $\mathcal{F} \leftarrow \mathcal{F} \setminus f'$
    end
end
return $\mathcal{F}$
```

Figure 3.5: SFDS algorithm for streaming feature definition selection. It relies on two lower-level procedures, `accept` and `prune` to accept new feature definitions and to possibly prune newly redundant feature definitions.

and $X = \mathcal{F}(\mathcal{D})$, i.e., the feature values extracted by feature f and feature set $\mathcal{F}$, respectively. Then CMI is given by $I(Z;Y|X) = H(Z|X) + H(Y|X) - H(Z,Y|X)$.

We represent feature values as joint random variables with separate discrete and continuous components, i.e., $Z = (Z^d, Z^c)$ and $X = (X^d, X^c)$. This poses a challenge in estimation due to the mixed variable types. To address this, we adapt prior work (Kraskov et al., 2004) on mutual information estimation to handle the calculation of CMI in the setting of mixed tabular datasets.

Let $\mathcal{F}$ be the set of already accepted features with corresponding feature values $X = \mathcal{F}(\mathcal{D})$. Then a new feature arrives, f, with corresponding feature values $Z = f(\mathcal{D})$.

The conditional mutual information (CMI) is given by:

$$I(Z;Y|X) = H(Z|X) + H(Y|X) - H(Z,Y|X) \tag{3.4}$$

Applying the chain rule of entropy, $H(A,B) = H(A) + H(B|A)$, we have:

$$\begin{aligned} I(Z;Y|X) =& H(Z,X) - H(X) + H(Y,X) \\ & - H(X) - H(Z,Y,X) + H(X) \\ =& H(Z,X) + H(Y,X) \\ & - H(Z,Y,X) - H(X) \end{aligned} \tag{3.5}$$

We represent feature values in separate components of discrete and continuous random variables, i.e., $X = (X^d, X^c)$:

$$\begin{aligned} I(Z;Y|X) =& H(Z^d, Z^c, X^d, X^c) + H(Y, X^d, X^c) \\ & - H(Z^d, Z^c, Y, X^d, X^c) - H(X^d, X^c) \end{aligned} \tag{3.6}$$

We expand the entropy terms again using the chain rule of entropy to condition on the discrete components of the random variables:

$$\begin{aligned} I(Z;Y|X) =& H(Z^c, X^c|Z^d, X^d) + H(Z^d, X^d) \\ &+ H(Y, X^c|X^d) + H(X^d) \\ &- H(Z^c, Y, X^c|Z^d, X^d) - H(Z^d, X^d) \\ &- H(X^c|X^d) - H(X^d) \end{aligned} \tag{3.7}$$

After cancelling terms:

$$\begin{aligned} I(Z;Y|X) =& H(Z^c, X^c|Z^d, X^d) + H(Y, X^c|X^d) \\ &- H(Z^c, Y, X^c|Z^d, X^d) - H(X^c|X^d) \end{aligned} \tag{3.8}$$

We use the definition of conditional entropy and take the weighted sum of the continuous entropies conditional on the unique discrete values. Let Z^d have support U and X^d have support V.

$$\begin{aligned} &I(Z;Y|X) = \\ &\sum_{u\in U, v\in V} p_{Z^d,X^d}(u,v) H(Z^c, X^c|Z^d = u, X^d = v) \\ &+ \sum_{v\in V} p_{X^d}(v) H(Y, X^c|X^d = v) \\ &- \sum_{u\in U, v\in V} p_{Z^d,X^d}(u,v) H(Z^c, Y, X^c|Z^d = u, X^d = v) \\ &- \sum_{v\in V} p_{X^d}(v) H(X^c|X^d = v) \end{aligned} \tag{3.9}$$

Unfortunately, we cannot perform this calculation directly as we do not know the joint distribution of X, Y, and Z. Thus we will need to estimate the quantities p and H based on samples from their joint distribution observed in $\mathcal{D}$. For this, we make use of two existing estimators.

Kraskov entropy estimation Kraskov et al. (2004) present estimators for mutual information (MI) based on nearest-neighbor statistics. From the assumption that the log density around each point is approximately constant within a ball of small radius, simple formulas for MI and entropy can be derived. The radius $\epsilon(i)/2$ is found as the distance from point i to its kth nearest neighbor. Unfortunately, their MI estimator cannot be used for CMI estimation and also cannot directly handle mixed discrete and continuous datasets. However, we can adapt their entropy estimator for our own CMI estimation.

The Kraskov entropy estimator $\hat{H}^{\text{KSG}}$ for a variable A is given by:

$$\begin{aligned}\hat{H}^{\text{KSG}}(A) =& \frac{-1}{N}\sum_{i=1}^{N-1}\psi(n_a(i)+1)+\psi(N)\\ &+\log(c_{d_A})+\frac{d_A}{N}\sum_{i=1}^{N}\log(\epsilon_k(i)),\end{aligned} \tag{3.10}$$

where N is the number of data instances, ψ is the digamma function, $n_a(i)$ is the number of points within distance $\epsilon_k(i)/2$ from point i, and c_{d_A} is the volume of a unit ball with dimensionality d_A.

Consider the joint random variable $W = (X, Y, Z)$. Then $\epsilon_k^W(i)$ is twice the distance from the ith sample of W to its kth nearest neighbor.

The entropy of W is then given by

$$\begin{aligned}\hat{H}^{\text{KSG}}(W) =& \psi(k)+\psi(N)+\log(c_{d_X}c_{d_Y}c_{d_Z})\\ &+\frac{d_X+d_Y+d_Z}{N}\sum_{i=1}^{N}\log(\epsilon_k^W(i)),\end{aligned} \tag{3.11}$$

Empirical probability estimation Let A be a discrete random variable with an unknown probability mass function p_A. Suppose we observe realizations $a_1, \ldots, a_n$.

Then the empirical probability mass function is given by

$$\hat{p}_A(A = a) = \frac{1}{n}\sum_{i=1}^{n}\mathbf{1}^{\{a_i=a\}}. \tag{3.12}$$

CMI Estimator Formula Now we can substitute our estimators $\hat{p}$ from Equation (3.12) and $\hat{H}^{\text{KSG}}$ from Equation (3.11) into Equation (3.9).

Finally, we can use estimators for p and H to estimate I:

$$
\begin{aligned}
&\hat{I}(Z;Y|X) = \\
&\sum_{u\in U,v\in V} \hat{p}(u,v)\hat{H}^{\text{KSG}}(Z^c, X^c|Z^d = u, X^d = v) \\
&+\sum_{v\in V} \hat{p}(v)\hat{H}^{\text{KSG}}(Y, X^c|X^d = v) \\
&-\sum_{u\in U,v\in V} \hat{p}(u,v)\hat{H}^{\text{KSG}}(Z^c, Y, X^c|Z^d = u, X^d = v) \\
&-\sum_{v\in V} \hat{p}(v)\hat{H}^{\text{KSG}}(X^c|X^d = v)
\end{aligned} \tag{3.13}
$$

Alternative validators

Maintainers of Ballet projects are free to configure alternative ML performance validation algorithms given the needs of their own projects. While we use SFDS for the *predict-census-income* project, Ballet provides implementations of the following alternative validators: `AlwaysAccepter` (accept every feature definition), `MutualInformationAccepter` (accept feature definitions where the mutual information of the extracted feature values with the prediction target is above a threshold), `VarianceThresholdAccepter` (accept feature definitions where the variance of each feature value is above a threshold), and `CompoundAccepter` (accept feature definitions based on the conjunction or disjunction of the results of multiple underlying validators). Additional validators can be easily created by defining a subclass of `ballet.validation.base.FeatureAccepter` and/or `ballet.validation.base.FeaturePruner`.

3.6 An interactive development environment for data science collaborations

In our discussion of Ballet so far, we have largely focused on the software engineering processes and technical details of feature engineering. However, the development environment that data scientists use in a Ballet collaboration can be an important factor in their experience and performance. In this section, we consider more carefully a development environment for Ballet projects and the interactions it supports.

Typically, a data scientist contributing to a Ballet project (or other kinds of data science projects) does exploratory work in a notebook before finally identifying a worthwhile patch to contribute. By this time, their notebook may be "messy" (Head et al., 2019), and the process of extracting the relevant patch and translating it into a well-structured contribution to a shared repository becomes challenging. Data scientists usually need to rely on a completely separate set of tools for this process, jettisoning the notebook for command line or GUI tools targeting team-based version control. This *patch contribution task* is difficult even for data scientists experienced with open-source practices (Gousios et al., 2015), and this difficulty is only more acute for data scientists who are less familiar with open-source development workflows.

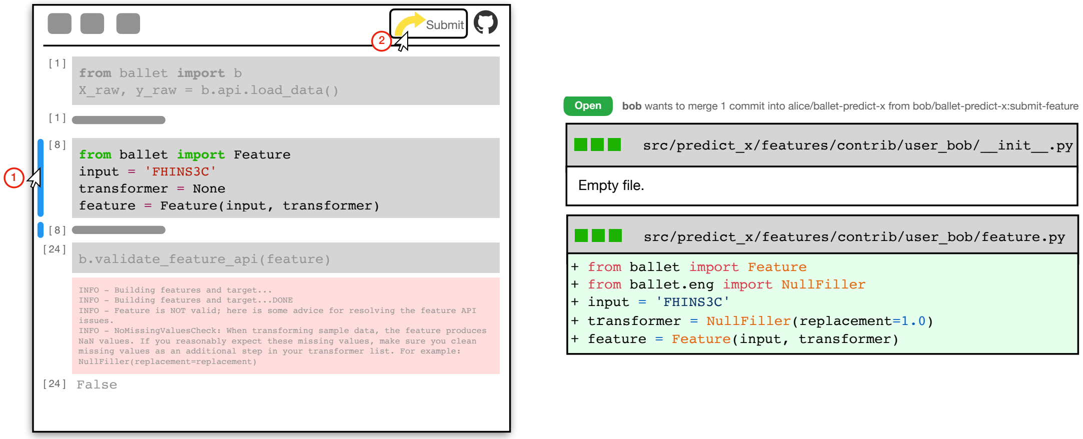
To address this challenge, we propose a novel development environment, Assemblé.[7,8] Assemblé solves the patch contribution task for data science collaborations that use Ballet[9] by providing a higher-level interface for contributing code snippets within a larger notebook to an upstream repository — meeting data scientists where they are most comfortable. Rather than asking data scientists to productionize their exploratory notebooks, Assemblé enables data scientists to both develop and contribute back their code without leaving the notebook. A code fragment selected by a data scientist can be automatically formulated as a pull request to an upstream GitHub repository using an interface situated within the notebook environment itself,

[7] `https://github.com/ballet/ballet-assemble`

[8] *Assemblé* is a ballet move that involves lifting off the floor on one leg and landing on two.

[9] Assemblé targets contributions to Ballet projects because of the structure that these projects impose on code contributions, but can be extended to support other settings as well.

automating and abstracting away use of low-level tools for testing and team-based development. It integrates tightly with Binder,[10] a community service for cloud-hosted notebooks, so that developers can get started with no setup required.



```
[1]  from ballet import b
     X_raw, y_raw = b.api.load_data()
[1]

[8]  from ballet import Feature
     input = 'FHINS3C'
     transformer = None
     feature = Feature(input, transformer)
[8]
[24] b.validate_feature_api(feature)

     INFO - Building features and target...
     INFO - Building features and target...DONE
     INFO - Feature is NOT valid; here is some advice for resolving the feature API
     issues.
     INFO - NoMissingValuesCheck: When transforming sample data, the feature produces
     NaN values. If you reasonably expect these missing values, make sure you clean
     missing values as an additional step in your transformer list. For example:
     NullFiller(replacement=replacement)
[24] False
```

Open **bob** wants to merge 1 commit into alice/ballet-predict-x from bob/ballet-predict-x:submit-feature

```
src/predict_x/features/contrib/user_bob/__init__.py
```

Empty file.

```
src/predict_x/features/contrib/user_bob/feature.py
+ from ballet import Feature
+ from ballet.eng import NullFiller
+ input = 'FHINS3C'
+ transformer = NullFiller(replacement=1.0)
+ feature = Feature(input, transformer)
```

Figure 3.6: An overview of the Assemblé development environment. Assemblé's frontend (left) extends JupyterLab to add a Submit button and a GitHub authentication button to the Notebook toolbar (top right). Users first authenticate Assemblé with GitHub using a supported OAuth flow. Then, after developing a patch within a larger, messy notebook, users select the code cell containing their desired patch using existing Notebook interactions (1), and press Assemblé's Submit button (2) to cause it to be automatically formulated as a pull request by the backend. The backend performs lightweight static analysis and validation of the intended submission and then creates a well-structured PR containing the patch (right). Taken together, the components of Assemblé support the *patch contribution task* for notebook-based developers.

We here describe the ideation, design, and implementation of a development environment that supports notebook-based collaborative data science. We will later report on a user study of 23 data scientists who used Assemblé in a data science collaboration case study (Section 4.3.5).

3.6.1 Design

To investigate development workflow issues in Ballet, we first conducted a formative study with eight data scientists recruited from a laboratory mailing list at MIT. We asked them to write and submit feature definitions for a collaborative project

[10] `https://mybinder.org/`

based around predicting the incidence rates of dengue fever in two different regions. Although participants created feature definitions successfully, we observed that they struggled to contribute them to the shared repository using the pull request model, with only two creating a pull request at all. In interviews, participants acknowledged that a lack of familiarity and experience with the pull request-based model of open source development was an obstacle to contributing the code that they had written, especially in the context of team-based development (Gousios et al., 2015).

In this study, and in other experiments with Ballet, we observed that data scientists predominately used notebooks to develop feature definitions before turning to entirely different environments and tools to extract the smallest relevant patch and create a pull request. We thus identified the *patch contribution task* as an important interface problem to address in order to improve collaborative data science. Once working code has been written, we may be able to automate the entire process of code contribution according to the requirements of the specific project the user is working on.

With this in mind, we elicited the following design requirements to support patch contribution in a collaborative data science environment.

R1 *Make code easy to contribute.* Once a patch has been identified, it should be easy to immediately contribute it without a separate process to productionize it.

R2 *Hide low-level tools.* Unfamiliarity and difficulty with low-level tooling and processes, such as `git` and the pull request model, tend to interrupt data scientists' ability to collaborate on a shared repository. Any patch submission solution should not include manual use of these tools.

R3 *Minimize setup and installation friction.* Finally, the solution should fit seamlessly within users' existing development workflows, and should be easy to set up and install.

Based on these requirements, we propose a design that extends the notebook interface to support submission of individual code cells as pull requests. By focusing on individual code cells, we allow data scientists to easily isolate relevant code to submit. Once a user has selected a code cell using existing Notebook interactions, pressing a simple, one-click "Submit" button added to the Notebook Toolbar panel spurs the creation and submission of a patch according to the configuration of the underlying project.

By abstracting away the low-level details of this process, we lose the ability to identify some code quality issues that would otherwise be identified by the tooling. To address this, we run an initial server-side validation using static analysis before forwarding on the patch, in order to immediately surface relevant problems to users within the notebook context. If submission is successful, the data scientist can view their new PR in a matter of seconds. Assemblé is tightly integrated with Binder such that it can be launched from every Ballet project via a README badge. Installation of the extension is handled automatically and the project settings are automatically detected so that data scientists can get right to work. An in-notebook, OAuth-based authentication flow also allows users to easily authenticate with GitHub without difficult configuration.

In summary, we design Assemblé to provide the following functionalities:

- isolate relevant code snippets from a messy notebook;
- transparently provide access to take actions on GitHub;
- automatically formulate an isolated snippet as a PR to an upstream data science project without exposing any git details.

3.6.2 Implementation

Assemblé is implemented in three components: a JupyterLab frontend extension, a JupyterLab server extension, and an OAuth proxy server.

The frontend extension is implemented in TypeScript on JupyterLab 2. It adds two buttons to the Notebook Panel toolbar. The GitHub button allows the user to initiate an authentication flow with GitHub. The Submit button identifies the currently selected code cell from the active notebook and extracts the source. It then posts the contents to the server to be submitted (R1). If the submission is successful, it displays a link to the GitHub pull request view. Otherwise, it shows a relevant error message — usually a Python traceback due to syntax errors in the user's code.

The server extension is implemented in Python on Tornado 6. It adds routes to the Jupyter Server under the `/assemble` prefix. These include `/assemble/submit` to receive the code to be submitted, and three routes under `/assemble/auth` to handle the authentication flow with GitHub. Upon extension initialization, it detects a Ballet project by ascending the file system, via the current working directory looking for the `ballet.yml` file and loading the project using the `ballet` library according to that configuration.

When the server extension receives the code to be submitted, it first runs a static analysis using Python's `ast` module to ensure that it does not have syntax errors or undefined symbols, and automatically cleans/reformats the code to the target project's preferred style. It then prepares to submit it as a pull request. The upstream repository is determined from the project's settings and is forked, if needed, via the `pygithub` interface to the GitHub API with the user's OAuth token, and cloned to a temporary directory. Using the Ballet client library, Assemblé can create an empty file at the correct path in the directory structure that will contain the proposed contribution, and writes to and commits this file. Depending on whether the user has contributed in the past, Assemblé may then also need to create additional files/folders to preserve the Python package structure (i.e.,`__init__.py` files). It then pushes to a new branch on the fork, and creates a pull request with a default description. Finally, it returns the pull request view link. This replaces what is usually 5–7 manual git operations with a robust and automated process (R2).

The final piece of the puzzle is authentication with GitHub, such that the server can act on GitHub as the user to create a new pull request. Most extensions that provide similar functionality (i.e., take some actions with an external service on behalf of a user that require authentication) ask the user to acquire a personal access token from the external service and provide it as a configuration variable, and in some cases register a web application using a developer console (Project Jupyter Contributors, a,b).

For our purposes, this is not acceptable, due to the high cost of setup for non-expert software developers (R2, R3). Instead, we would like to use OAuth (OAuth Working Group, 2012) to allow the user to enter their username and password for the service, and exchange them for a token that the server can use. However, this cannot be accomplished directly using the OAuth protocol because OAuth applications on GitHub (or elsewhere) must register a static callback URL. Instead, Assemblé might be running at any address, because with its Binder integration, the URLs assigned to Binder sessions are dynamic and on different domains.[11] To address this, we create `github-oauth-gateway`, a simple proxy server for GitHub OAuth.[12] We host a reference deployment and register it as an OAuth application with GitHub. Before the user can submit their code, they click the GitHub icon in the toolbar (Figure 3.6). This launches the OAuth flow. First the server creates a secret "state" at random. Then it redirects the user to the GitHub OAuth login page. The user is prompted to enter their username and password, and if the sign-in is successful, GitHub responds to the gateway with the token and the state created previously. The server polls the gateway for a token associated with its unique state, and receives the token in response when it is available.

3.7 Preliminary studies

We conducted several preliminary studies and evaluation steps during the iterative design process for Ballet. These preliminary studies informed the design and implementation of all of the components of Ballet that have been presented in this chapter.

[11] For example, launching the same repository in a Binder can result in first a `hub.gke.mybinder.org` URL and then an `notebooks.gesis.org` URL, depending on the BinderHub deployment selected by the MyBinder load balancer.

[12] `https://github.com/ballet/github-oauth-gateway`

Disease incidence prediction

We first evaluated an initial prototype of Ballet in a user study with eight data scientists. All participants had at least basic knowledge of collaborative software engineering and open-source development practices (i.e., using git and pull requests). We explained the framework and gave a brief tutorial on how to write feature definitions. Participants were then tasked with writing feature definitions to help predict the incidence of dengue fever given historical data from Iquitos, Peru and San Juan, Puerto Rico (Epidemic Prediction Initiative), for which they were allotted 30 minutes. Three participants were successfully able to merge their first feature definition within this period, while the remainder produced features with errors or were unable to write one. In interviews, participants suggested that they found the Ballet framework helpful for structuring contributions and validating features, but were unfamiliar with writing feature engineering code in terms of feature definitions with separate fit/transform behavior (Section 3.4.1), and struggled to translate exploratory work in notebooks all the way to pull requests to a shared project. Based on this feedback, we created the `ballet.eng` library of feature engineering primitives (Section 3.4.4) and created tutorial materials for new collaborators. We also began the design process that became the Assemblé environment that supports notebook-based developers (Section 3.6).

House price prediction

We evaluated a subsequent version of Ballet in a user study with 13 researchers and data scientists. This version included changes made since the first preliminary study and introduced an alpha version of Assemblé that did not yet include server-side or in-notebook validation functionality. Five of the participants had little to no prior experience contributing to open-source projects, six reported contributing occasionally, and two contributed frequently. All self-reported as intermediate or expert data scientists and Python developers. Participants were given a starter notebook that guided the development and contribution of feature definitions, and documentation on the framework. They were tasked with writing feature definitions to help predict the selling price of a house given administrative data collected in Ames, Iowa (De Cock, 2011). After contributing, participants completed a short survey with a usability evaluation and provided semi-structured free-text feedback. Participants reported that they were moderately successful at learning to write and submit feature definitions but wanted more code examples. They also reported that they wanted to validate their features within their notebook using the same methods that were used in the automated testing in CI. Based on this feedback, among other improvements, we expanded and improved our feature engineering guide and the starter notebook. We also made methods for feature API validation and ML performance validation available in the interactive client (Section 3.5) and expanded the Assemblé server-side validation to catch common issues. Various simulation studies for this same dataset are conducted in (Lu, 2019).

Chapter 4

Understanding data science collaborations

4.1 Introduction

There is great potential for large-scale, collaborative data science to address societal problems through community-driven analyses of public datasets (Choi and Tausczik, 2017; Hou and Wang, 2017). For example, the Fragile Families Challenge tasked researchers and data scientists with predicting outcomes, including GPA and eviction, for a set of disadvantaged children and their families (Salganik et al., 2020), and *crash-model* is an application for predicting car crashes and thereby directing safety interventions (Insight Lane). Such projects, which involve complex and unwieldy datasets, attract scores of interested citizen scientists and developers whose knowledge, insight, and intuition can be significant if they are able to contribute and collaborate.

To make progress toward this outcome, we must first better understand the capabilities and challenges of collaborative data science as projects scale beyond small teams in open-source settings. Although much research has focused on elucidating the diverse challenges involved in data science development (Chattopadhyay et al., 2020; Yang et al., 2018; Subramanian et al., 2020; Sculley et al., 2015; Choi and Tausczik, 2017; Zhang et al., 2020; Muller et al., 2019), little attention has been given to large, open-source collaborations, partly due to the lack of real-world examples available for study.

Leveraging Ballet as a probe, we create and conduct an analysis of *predict-census-income*, a collaborative effort to predict personal income through engineering features from raw individual survey responses to the U.S. Census American Community Survey (ACS). We use a mixed-method software engineering case study approach to study the experiences of 27 developers collaborating on this task, focusing on understanding the experience and performance of participants from varying backgrounds, the characteristics of collaboratively built feature engineering code, and the performance of the resulting model compared to alternative approaches.

4.2 Methods

We conduct a study using the versions of Ballet and Assemblé described in Chapter 3. To better understand the characteristics of live collaborative data science projects, we use a mixed-method software engineering case study approach (Runeson and Höst, 2009). The case study approach allows us to study the phenomenon of collaborative data science in its "real-life context." This choice of evaluation methodology allows us to move beyond a laboratory setting and gain deeper insights into how large-scale collaborations function and perform. Through this study, we aim to answer the following four research questions:

RQ1 What are the most important aspects of our collaborative framework to support participant experience and project outcomes?

RQ2 What is the relationship between participant background and participant experience/performance?

RQ3 What are the characteristics of feature engineering code in a collaborative project?

RQ4 How does a collaborative model perform in comparison to other approaches?

These research questions build on our conceptual framework, allowing us to better understand the effects of our design choices as well as to move forward our understanding of collaborative data science projects in general.

4.2.1 General procedures

We created an open-source project using Ballet, *predict-census-income*,[1] to produce a feature engineering pipeline for personal income prediction. After invited participants consented to the research study terms, we asked them to fill out a pre-participation survey with background information about themselves, which served as the independent variables of our study. Next, they were directed to the public repository containing the collaborative project and asked to complete the task described in the project README. They were instructed to use either their preferred development environment or Assemblé. After they completed this task, we surveyed them about their experience.

4.2.2 Participants

In recruiting participants, we wanted to ensure that our study included beginners and experts in statistical and ML modeling, software development, and survey data analysis (the problem domain). To achieve this, we compiled personal contacts with various backgrounds. After reaching these contacts, we then used snowball sampling to recruit more participants with similar backgrounds. We expanded our outreach by posting to relevant forums and mailing lists in data science development, Python programming, and survey data analysis. Participants were entered into a drawing for several nominal prizes but were not otherwise compensated.

4.2.3 Dataset

The input data is the raw survey responses to the 2018 U.S. Census American Community Survey (ACS) for Massachusetts (Table 4.1). This "Public Use Microdata Sam-

[1] `https://github.com/ballet/predict-census-income`

ple" (PUMS) has anonymized individual-level responses. Unlike the classic ML "adult census" dataset (Kohavi, 1996) which is highly preprocessed, raw ACS responses are a realistic form for a dataset used in an open data science project. Following Kohavi (1996), we define the prediction target as whether an individual respondent will earn more than $84,770 in 2018 (adjusting the original "adult census" prediction target of $50,000 for inflation), and filter a set of "reasonable" rows by keeping people older than 16 with personal income greater than $100 with hours worked in a typical week greater than zero. We merged the "household" and "person" parts of the survey to get compound records and split the survey responses into a development set and a held-out test set.

	Development	Test
Number of rows	30085	10029
Entity columns	494	494
High income	7532	2521
Low income	22553	7508

Table 4.1: ACS dataset used in *predict-census-income* project.

4.2.4 Research instruments

Our mixed-method study synthesizes and triangulates data from five sources:

- *Pre-participation survey.* Participants provided background information about themselves, such as their education; occupation; self-reported background with ML modeling, feature engineering, Python programming, open-source development, analysis of survey data, and familiarity with the U.S. Census/ACS specifically; and preferred development environment. Participants were also asked to opt in to telemetry data collection.

- *Assemblé telemetry.* To better understand the experience of participants who use Assemblé on Binder, we instrumented the extension and installed an instrumented version of Ballet to collect usage statistics and some intermediate outputs. Once participants authenticated with GitHub, we checked with our telemetry server to see whether they had opted in to telemetry data collection. If they did so, we sent and recorded the buffered telemetry events.

- *Post-participation survey.* Participants who attempted and/or completed the task were asked to fill out a survey about their experience, including the development environment they used, how much time they spent on each sub-task, and which activities they did and functionality they used as part of the task and which of these were most important. They were also asked to provide open-ended feedback on different aspects, and to report how demanding the task was using the NASA-TLX Task Load Index (Hart and Staveland, 1988), a workload assessment that is widely used in usability evaluations in software engineering and other domains (Cook et al., 2005; Salman and Turhan, 2018). Participants indicate on a scale the temporal demand, mental demand, and effort required by the task, their perceived performance, and their frustration. The TLX score is a weighted average of responses (0=very low task demand, 100=very high task demand).

- *Code contributions.* For participants who progressed in the task to the point of submitting a feature definition to the upstream *predict-census-income* project, we analyze the submitted source code as well as the performance characteristics of the submission.

- *Expert and AutoML baselines.* To obtain comparisons to solutions born from Ballet collaborations, we also obtain baseline solutions to the personal income prediction problem from outside data science experts and from a cloud provider's AutoML service. First, we asked two outside data science experts working independently to solve the combined feature engineering and modeling task (without knowledge of the collaborative project).[2] These experts were asked to work until they were satisfied with the performance of their predictive model, but not to exceed four hours, and were not compensated. Second, we used

[2] Replication files are available at `https://github.com/micahjsmith/ballet-cscw-2021`.

Google Cloud AutoML Tables,[3] an AutoML service for tabular data, which supports structured data "as found in the wild," to automatically solve the task, and ran it with its default settings until convergence.

The study description, pre-participation survey, and post-participation survey can be found in the supplementary material to Smith et al. (2021a).

4.2.5 Analysis

After linking our data sources together, we performed a quantitative analysis to summarize results (e.g., participant backgrounds, average time spent) and relate measures to each other (e.g., participant expertise to cognitive load). Where appropriate, we also conducted statistical tests to report on significant differences for phenomena of interest. For qualitative analysis, we employed open and axial coding methodology to categorize the free-text responses and relate codes to each other to form emergent themes (Böhm, 2004). Two researchers first coded each response independently, and responses could receive multiple codes, which were then collaboratively discussed. We resolved disagreements by revisiting the responses, potentially introducing new codes in relation to themes discovered in other responses. We later revisited all responses and codes to investigate how they relate to each other, which led us to the emergent themes we present in our results. Finally, to understand the kind of source code that is produced in a collaborative data science setting, we performed lightweight program analysis to extract and quantify the feature engineering primitives used by our participants.

4.3 Results

We present our results by interleaving the outcomes of quantitative and qualitative analysis (including verbatim quotes from free-text responses) to form a coherent narrative around our research questions.

[3] https://cloud.google.com/automl-tables/

In total, 50 people signed up to participate in the case study and 27 people from four global regions completed the task in its entirety. To the best of our knowledge, this makes our project the sixth largest ML modeling collaboration hosted on GitHub in terms of code contributors (Table 2.1). During the case study, 28 features were merged that together extract 32 feature values from the raw data. Of case study participants, 26 submitted at least one feature and 22 had at least one feature merged. As we went through participants' qualitative feedback about their experience, several key themes emerged, which we discuss inline.

4.3.1 RQ1: Collaborative framework design

We identified several themes that relate to the design of frameworks for collaborative data science. We start by connecting these themes to the design decisions we made about Ballet.

Goal Clarity. The project-level goal is clear — to produce a predictive model. In the case of survey data that requires feature engineering, Ballet takes the approach of decomposing this data into individual goals via the feature definition abstraction, and asking collaborators to create and submit a patch that introduces a well-performing feature. Success in this task is validated using statistical tests (Section 3.5). However, the relationship between the individual and project goals may not always appear aligned to all participants. This negatively impacted some participants' experiences by introducing confusion about the direction and goal of their task. Some of the concerns expressed had to do with specific documentation elements, but others indicated a deeper confusion: *"Do the resulting features have to be 'meaningful' for a human or can they be built as combinations that maximize some statistical measure?"* (P2). Using the concept of software and statistical acceptance procedures, many high-quality features were merged into the project. However, the procedure was not fully transparent to the case study participants and may have prevented them from optimizing their features. While a feature that maximizes some statistical measure is best in the short term, it may constrain group productivity overall, as other participants benefit from being able to learn from existing features. And while having specific individual goals incentivizes high-quality feature engineering, participants are then less focused on the project-level goal and maintainers must either implement new project functionality themselves or define additional individual goals. This is a classic tension in designing collaborative mechanisms when it comes to appropriately structuring goals and incentives Ouchi (1979).

Learning by Example. We asked participants to rank the functionalities that were most important for completing the task, focusing both on creating and submitting feature definitions (Figure 4.1). For the patch development task, participants ranked most highly the ability to refer to example code written by fellow participants or project maintainers. This form of implicit collaboration was useful for participants to accelerate the onboarding process, learn new feature engineering techniques, and coordinate their efforts.

Distribution of Work. However, this led to feedback about difficulties in identifying how to effectively participate in the collaboration. Participants wanted the framework to provide more functionality to determine how to partition the input space: *"for better collaboration, different users can get different subsets of variables"* (P1). Some participants specifically asked for methods to review the input variables that had and had not been used and to limit the number of variables that one person would need to consider. This is a promising direction for future work, and similar ideas appear in automatic code reviewer recommendation (Peng et al., 2018). Other participants, however, were satisfied with a more passive approach in which they used the Ballet client to programmatically explore existing feature definitions.

Cloud-Based Workflow. In terms of submitting feature definitions, the most popular element by far was Assemblé. Importantly, all of the nine participants who reported that they "never" contribute to open-source software were able to successfully submit a PR to the *predict-census-income* project with Assemblé— seven in the cloud and the others locally.[4] Attracting participants like these who are not experienced data scientists is critical for sustaining large collaborations, and prioritizing inter-

[4] Local use involves installing JupyterLab and Assemblé on a local machine, rather than using the version running on Binder.

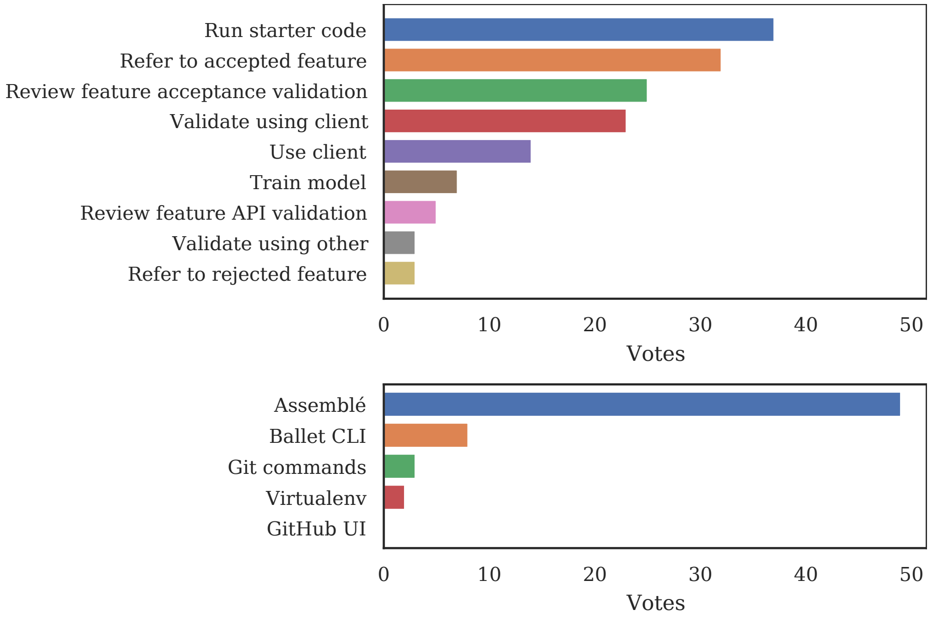


Figure 4.1: Most important functionality within a collaborative feature engineering project for the patch development task (top) and the patch contribution task (bottom), according to participant votes. Participants were asked to rank their top three items for creating feature definitions (awarded three, two, and one points in aggregating votes) and their top two items for submitting feature definitions (awarded two and one points in aggregating votes).

faces that provide first-class support for collaboration can support these developers. The adaptation of the open-source development process reflected in Assemblé shows that concepts of open-source workflows and decentralized development did effectively address the aforementioned challenges for some developers.

In summary, we found that the feature definition abstraction, the cloud-based workflow in Assemblé, and the coordination and learning from referring to shared feature definitions were the aspects that contributed most to the participants' experiences. While the concept of data science patches makes significant progress toward addressing task management challenges, frictions remain around goal clarity and division of work, which should be addressed in future designs.

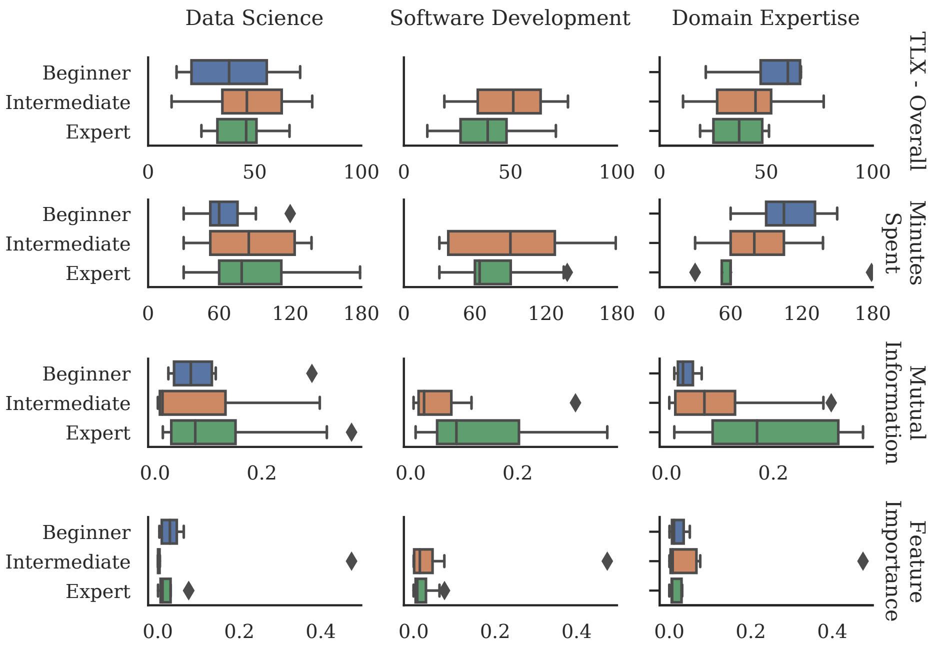


Figure 4.2: Task demand, total minutes spent on task, mutual information of best feature with target on the test set, and total global feature importance assigned by AutoML service on development set, for participants of varying experience sorted by type of background. (Statistical and ML modeling background is labeled as "Data Science.")

4.3.2 RQ2: Participant background, experience, and performance

In considering the relationship between participants' backgrounds, experiences, and performance, we look at six dimensions of participants' backgrounds. Because many are complementary, for purposes of analysis, we collapse them into the broader categories of ML modeling background, software development background, and domain expertise. Our main dependent variables for illustrating participant experience are the overall cognitive load (TLX - Overall) and total minutes spent on the task (Minutes Spent). Our main dependent variables for illustrating participant performance are two measures of the ML performance of each feature: its mutual information with the target and its feature importance as assessed by AutoML. We summarize the relationship between background, experience, and performance measures in Figure 4.2.

Beginners find the task accessible. Beginners found the task to be accessible, as across different backgrounds, beginners had a median task demand of 45.2 (lower is less demanding, p25=28.5, p75=60.4). The groups that found the task most demanding were those with little experience analyzing survey data or developing open-source projects.

Experts find the task less demanding but perform similarly. We found that broadly, participants with increased expertise in any of the background areas perceived the task as less demanding. However, ML modeling and feature engineering experts spent more time working on the task than beginners did. They were not necessarily using this time to fix errors in their feature definitions, as they invoked the Ballet client's validation functions fewer times, according to telemetry data (16 times for experts, 33.5 times for non-experts). They may have been spending more time learning about the project and data without writing code. Then, they may have used their preferred methods to help evaluate their features during development. However, our hypothesis that experts would onboard faster than non-experts when measured by minutes spent learning about Ballet (a component of the total minutes spent) is rejected for ML modeling background (Mann-Whitney U=85.0, Δ medians -6.0 minutes) and for software development background (U=103.0, Δ medians -1.5 minutes).

Domain expertise is critical. Of the different types of participant background, domain expertise had the strongest relationship with better participant outcomes. This is encouraging because it suggests that if collaborative data science projects attract experts in the project domain, these experts can be successful as long as they have data science and software development skills above a certain threshold and are supported by user-friendly tooling like Assemblé. One explanation for the relative importance of domain expertise is that participants can become overwhelmed or confused by *dataset challenges* with the wide and dirty survey dataset: *"There are a lot of values in the data, and I couldn't figure out the meaning of the values, because I didn't know much about the topic"* (P20). We speculate that given the time constraints of the task, participants who were more familiar with survey data analysis were able to allocate time they would have spent here to learning about Ballet or developing features. We find that beginners spent substantially more time

```python
from ballet import Feature
from ballet.eng.external import SimpleImputer

input = ["JWTR", "JWRIP", "JWMNP"]

def calculate_travel_budget(df):
    if (df["JWTR"] == 1.0).all():
        return df["JWMNP"] * df["JWRIP"]
    return df["JWMNP"] * df["JWTR"]

transformer = [
    calculate_travel_budget,
    SimpleImputer(strategy="mean"),
]
name = "work_travel_combined"
description = "Combine data for time to travel to work with vehicle. Lower value,
↪  the most likely they have higher income"
feature = Feature(input, transformer, name=name, description=description)
```

Figure 4.3: A feature definition that computes a cleaned measure of vehicle commute time (for the *predict-census-income* project).

learning about the prediction problem and data — a median of 36 minutes vs. 13.6 minutes for intermediate and expert participants (Mann-Whitney U=36.5, p=0.064, n_1=6, n_2=21).

4.3.3 RQ3: Collaborative feature engineering code

We were interested in understanding the kind of feature engineering code that participants write in this collaborative setting. Participants in the case study contributed 28 feature definitions to the project, which together extract 32 feature values. The features had 47 transformers, with most feature functions applying a single transformer to their input but some applying up to four transformers sequentially. Two examples of feature definitions developed by participants are shown in Figures 3.3 and 4.3.

Feature engineering primitives. Participants collectively used 10 different feature engineering primitives (Section 3.4.4). Our source code analysis shows that 17/47 transformers were `FunctionTransformer` primitives that can wrap standard statistical functions or are used by Ballet to automatically wrap anonymous functions. Use of these was broadly split between simple functions to process variables that needed minimal cleaning/transformation vs. complex functions that extracted custom mappings from ordinal or categorical variables based on a careful reading of the survey codebook.

Feature characteristics. These feature functions consumed 137 distinct variables from the raw ACS responses, out of a total of 494 present in the entities table. Most of these variables were consumed by just one feature, but several were transformed in different ways, such as `SCHL` (educational attainment), which was an input to five different features. Thus 357 variables, or 72%, were ignored by the collaborators. Some were ignored because they are not predictive of personal income. For example, the end-to-end AutoML model that operates directly on the raw ACS responses assigns a feature importance of less than 0.001 to 418 variables (where the feature importance values sum to one). However, there may still be missed opportunities by the collaborators, as the AutoML model assigns feature importance of greater than 0.01 to seven variables that were not used by any of the participants' features — such as `RELP`, which indicates the person's relationship to the "reference person" in the household and is an intuitive predictor of income because it allows the modeler to differentiate between adults who are dependents of their parents. This suggests an opportunity for developers of collaborative frameworks like Ballet to provide more formal direction about where to invest feature engineering effort — for example, by providing methods to summarize the inputs that have or have not been included in patches, in line with the *distribution of work* theme that emerged from participant responses and the challenge of task management. Of the features, 11/28 had a learned transformer while the remainder did not learn any feature engineering-specific parameters from the training data, and 14/47 transformers were learned transformers.

Feature definition abstraction. The `Feature` abstraction of Ballet yields a one-to-one correspondence between the task and feature definitions. This new programming paradigm required participants to adjust their usual feature engineering toolbox. For many respondents, this was a positive change, with benefits for reusability, shareability, and tracking prior features: *"It allows for a better level of abstraction*

Feature Engineering	Modeling	Accuracy	Precision	Recall	F1	Failure rate
Ballet	AutoML	**0.876**	**0.838**	0.830	**0.834**	0.000
AutoML	AutoML	0.462	0.440	0.423	0.431	0.475
Ballet	Expert 1	0.828	0.799	0.707	0.734	0.000
Ballet	Expert 2	0.840	0.793	0.858	0.811	0.000
Expert 1	Expert 1	0.814	0.775	0.686	0.710	0.000
Expert 2	Expert 2	0.857	0.809	**0.867**	0.828	0.000

Table 4.2: ML Performance of Ballet and alternatives. The AutoML feature engineering is not robust to changes from the development set and fails with errors on almost half of the test rows. But when using the feature definitions produced by the Ballet collaboration, the AutoML method outperforms human experts.

as it raises Features up to their own entity instead of just being a standalone column" (P16). For others, it was difficult to adjust, and participants noted challenges in learning how to express their ideas using transformers and feature engineering primitives and how to debug failures.

4.3.4 RQ4: Comparative performance

While we focus on better understanding how data scientists work together in a collaborative setting, ultimately one important measure of the success of a collaborative model is its ability to demonstrate good ML performance. To evaluate this, we compare the performance of the feature engineering pipeline built by the case study participants against several alternatives built from our baseline solutions we obtained from outside data science experts and a commercial AutoML service, Google Cloud AutoML Tables (Section 4.2.4).

We found that among these alternatives, the best ML performance came from using the Ballet feature engineering pipeline and passing the extracted feature values to AutoML Tables (Table 4.2). This hybrid human-AI approach outperformed end-to-end AutoML Tables and both of the outside experts. This finding also confirms previous results suggesting that feature engineering is sometimes difficult to automate, and that advances in AutoML have led to expert- or super-expert performance on clean, well-defined inputs.

Qualitative differences. The three approaches to the task varied widely. Due to Ballet's structure, participants spent all of their development effort on creating a small set of high-quality features. AutoML Tables performs basic feature engineering according to the inferred variable type (normalize and bucketize numeric variables, create one-hot encoding and embeddings for categorical variables) but spends most of its runtime budget searching and tuning models, resulting in a gradient-boosted decision tree for solving the census problem. The experts similarly performed minimal feature engineering (encoding and imputing); the resulting models were a minority class oversampling step followed by a tuned AdaBoost classifier (Expert 1) and a custom greedy forward feature selection step followed by a linear probability model (Expert 2).

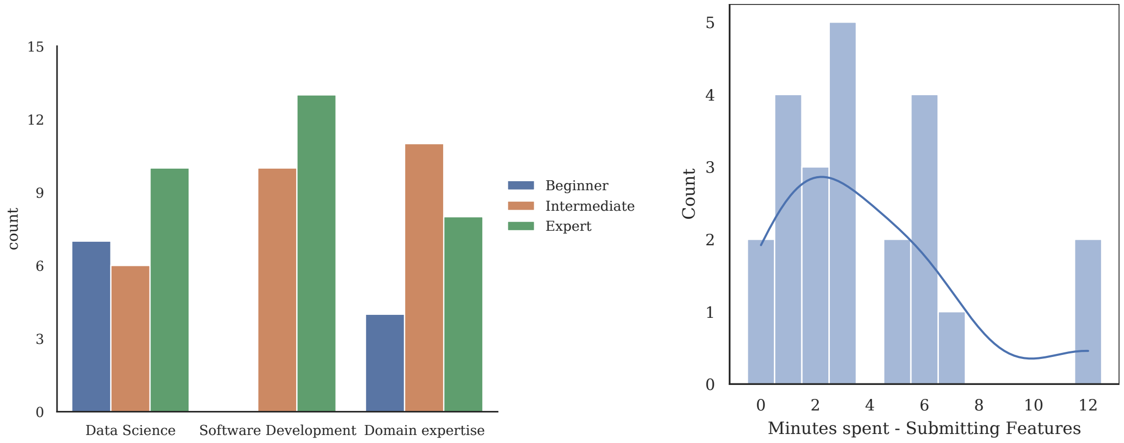
4.3.5 Evaluation of Assemblé

As part of the *predict-census-income* case study, we conduct a nested evaluation of Assemblé by studying participants who used it. We aim to assess the ability of users to successfully create pull requests for code snippets within a messy notebook, and to identify key themes from participants' experiences.

Procedures

Of 27 data scientists who participated in the case study, 23 participants used Assemblé (v0.7.2) to develop their code and submit it to the shared repository.

Recall from Section 4.2.4 that participants first completed a short questionnaire in which they self-reported their background in data science and open-source software development and their preferred development environments for data science tasks. Participants were also asked to consent to telemetry data collection. If they did, we instrumented Assemblé to collect detailed usage data on their development sessions, their use of the submit button functionality, and their use of the Ballet client library. After completing their feature development, participants completed a short survey from which we isolated responses relating to their use of Assemblé, including its



(a) Background of 23 developers using Assemblé in a study involving predicting personal income.

(b) Distribution of total minutes spent submitting features to upstream repository.

Figure 4.4: Assemblé user study results.

features, their overall experience with the project, and any free-response feedback.

Results

Only five participants reported a preference for performing data science activities and Python development in notebook environments before the study, with 10 instead preferring IDEs and four preferring text editors. Seven participants had never contributed to open-source projects at all, while the remainder reported contributing approximately yearly (eight), monthly (four), or weekly (four). Fifteen participants opted into telemetry data collection, generating an average of 33 telemetry events each. A summary of participant background is shown in Figure 4.4.

Quantitative Result Our main finding is that even with their diverse backgrounds and initial preferences, *all participants in the study successfully used Assemblé to create one or more pull requests to the upstream project repository.* According to telemetry data, the modal user pressed the submit button just once. Since the user study task was to submit a single feature, this suggests that users were immediately successful at creating a pull request for their desired contribution. We also find that participants were able to do this fairly quickly — half were able to create a pull request using Assemblé in three minutes or less (Figure 4.4b). In 16 out of 45 submit events captured in the telemetry data (belonging to five unique users), Assemblé's static analysis identified syntax errors in the intended submissions, each of which would have led to a pull request that would have failed Ballet's automated test suite. In all of these cases, users were able to quickly resolve these errors and submit again.

Qualitative Results From a qualitative perspective, we identified two major themes from the free text responses in our post-participation survey.

Keep It Simple While Introducing Better Affordances. Users overwhelmingly noted the simplicity with which they were able to submit their features, with one participant noting *"The process of integrating the new feature was very smooth"* and another saying *"[Submitting a feature] was extremely and [surprisingly] easy! Most rewarding part."* However, some participants noted that while the submission process was seamless, affordances could be better highlighted, e.g.: *"Maybe highlight a bit more that you need to select the feature cell before hitting submit — I got confused after I missed this part."* Indeed, in the few cases where participants were not able to submit their feature on their first attempt, we see in our telemetry data that they either selected the wrong cell or introduced a syntax error.

Tensions between Abstraction and Submission Transparency. Another theme that emerged in our analysis was submission transparency. While we achieved our goal of hiding the lower-level procedures required in the pull request model, some participants were curious about the underlying process. Several wanted to know how their feature was evaluated, both in server-side validation and in continuous integration after pull request creation: *"It was not clear whether my feature was actually good, especially compared to other features."* Others expressed a lack of understanding of what was going on "under the hood": *"I didn't fully understand how Assemblé was working on the backend to actually develop the feature with relatively straightforward commands, but it seemed to work pretty well."* This feedback highlights the tension between abstraction and transparency. While users clearly appreciated the simplicity facilitated by the submission mechanism, they missed the traceability and feedback a more classical pull request model would have provided. We see this as an opportunity to introduce optionally available traces detailing the steps of the underlying process, partly as a way of onboarding non-experts into the open-source development workflow.

Chapter 5

Discussion of Ballet

In this section, we reflect on Ballet, Assemblé, and the *predict-census-income* case study with a particular eye toward scale, human factors, security, privacy, and the limitations of our research. We also discuss future areas of focus for HCI researchers and designers of collaborative frameworks.

5.1 Effects of scale

Although Ballet makes strides in scaling collaborative data science projects beyond small teams, we expect additional challenges to arise as collaborations are scaled even further.

The number of possible direct communication channels in a project scales quadratically with the number of developers (Brooks Jr, 1995). At the scale of our case study, communication among collaborators can take place effectively through discussion threads, chat rooms, and shared work products. But projects with hundreds or thousands of developers require other strategies, such as search, filtering, and recommendation of relevant content. The metadata exposed by feature definitions (Section 3.4.1) makes it possible to explore these functionalities in future work.

A task management challenge that goes hand-in-hand with communication is distribution of work, a theme from our qualitative analysis in Section 4.3. Even at the scale of our case study, some collaborators wanted Ballet itself to support them in the distribution of feature engineering work. At larger scales, this need becomes more pressing if redundant work is to be avoided. In addition to strategies like partitioning the variable space and surfacing unused variables for developers, other solutions may include ticketing systems, clustering of variables and partitioning of clusters, and algorithms to rank variables by their impact after transformations have been applied.

5.2 Effects of culture

Data science teams are often made up of like-minded people from similar backgrounds. For example, Choi and Tausczik (2017) report that most of the open data analysis projects they reviewed were comprised of people who already knew each other — partly because teammates wanted to be confident that everyone there had the required expertise.

Our more formalized and structured notion of collaboration may allow data science developers with few or no personal connections to form more diverse, cross-cultural teams. For example, the *predict-census-income* project included collaborators from four different global regions (North America, Europe, Asia, and the Middle East). The support for validating contributions like feature definitions with statistical and software quality measures may allow teammates to have confidence in each other even without knowing each other's backgrounds or specific expertise.

5.3 Security

Any software project that receives untrusted code must be mindful of security considerations. The primary threat model for Ballet projects is a well-meaning collaborator that submits poorly-performing feature definitions or inadvertently "breaks" the feature engineering pipeline, a consideration that partly informed the acceptance procedure in Section 3.5. Ballet's support for automatic merging of accepted features presents a risk that harmful code may be embedded within otherwise relevant features. While requiring a maintainer to give final approval for accepted features is a practical defense, defending against malicious contributions is an ongoing struggle for open-source projects (Payne, 2002; Decan et al., 2016; Baldwin, 2018).

5.4 Privacy

Data is, to no surprise, central to data science. This can pose challenges for open data projects if the data they want to use is sensitive or confidential — for example, if it contains personally identifiable information. The main way to address this issue is to secure the dataset but open the codebase. In this formulation, access to the data is limited to those who have undergone training or signed a restricted use agreement. But at the same time, the entirety of the code, including the feature definitions, can be developed publicly without revealing any non-public information about the data. With this strategy, developers and maintainers must monitor submissions to ensure that data is not accidentally copied into source code files — a process that can be automated, similar to scanning for secure tokens and credentials (Meli et al., 2019; Glanz et al., 2020).

One alternative is to make the entire repository private, ensuring that only people who have been approved have access to the code and data. However, this curtails most of the benefits of open data science and makes it more difficult to attract collaborators.

Another alternative is to anonymize data or use synthetic data for development while keeping the actual data private and secure. Recent advances in synthetic data generation (Xu et al., 2019; Patki et al., 2016) allow a synthetic dataset to be generated with the same schema and joint distribution as the real dataset, even for complex tables. This may be sufficient to allow data science developers to discover patterns and create feature definitions that can then be executed on the real, unseen dataset. This follows work releasing sensitive datasets for analysis in a privacy-preserving way using techniques like differential privacy (Dwork, 2008). Indeed, the U.S. Census is now using differential privacy techniques in the release of data products such as the ACS (Abowd et al., 2020). Analyses developed in an open setting could then be re-run privately on the original data according to the privacy budget of each researcher.

5.5 Interpretability and documentation

Zhang et al. (2020) observe that data science workers rarely create documentation about their work during feature engineering, suggesting that human decision-making may be reflected in the data pipeline while "simultaneously becoming invisible." This poses a risk for replicability, maintenance, and interpretability.

In Ballet, the structure provided by our feature definition abstraction means that the resulting feature values have clear provenance and are interpretable, in the sense that for each column in the feature matrix, the raw variables used and the exact transformations applied are easily surfaced and understood. Feature value names (columns in the feature matrix) can be provided by data scientists when they create feature definitions, or reasonable names can be inferred by Ballet from the available metadata and through lightweight program analysis.

5.6 Feature stores

Feature stores, or applications that ingest, store, and serve feature values for offline model training and online training and inference, are rapidly becoming part of the machine learning engineering toolkit. Open-source systems like Feast[1] are emerging to complement the proprietary systems that are known to be used at large technology companies, such as Zipline within AirBnb's BigHead platform (Brumbaugh et al., 2019) or Michelangelo at Uber (Hermann and Del Balso, 2017). However, such feature stores do not support feature engineering, feature discovery, or feature validation, but instead focus on the data systems aspect of features (as their name indicates). Thus, the human process of developing new features and discovering and improving existing ones remains an area in need of framework support. These two problems — of developing features, then using them in production systems — remain complementary.

[1] https://github.com/feast-dev/feast

5.7 Feature maintenance

Just as software libraries require maintenance to fix bugs and make updates in response to changing APIs or dependencies, so too do feature definitions and feature engineering pipelines. Feature maintenance may be required in several situations. First, components from libraries used in a feature definition, such as the name or behavior of an imputation primitive, could change. Second, the schema of the target dataset could change, such as if a survey is conducted in a new year, with certain questions from prior years replaced with new ones.[2] Third, feature maintenance may be required due to distribution shift, in which new observations following the same schema have a different data distribution, causing the assumptions reflected in a feature definition to be invalidated.

Though we have focused mainly on the scale of a collaboration in terms of the number of code contributors, another important measure of scale is the length of time the project remains in a developed, maintained state, and as such is useful to consumers. As projects age, these secondary issues of feature maintenance, as well as dataset and model versioning and changing usage scenarios, become more salient.

A similar development workflow to the one presented in this thesis could also be used for feature maintenance, and researchers have pointed out that the open-source model is particularly well suited for ensuring software is maintained (Johnson, 2006). Currently, Ballet focuses on supporting the addition of new features; to support the modification of existing features would require additional design considerations, such as how developers using Assemblé could indicate which feature should be updated/removed by their pull request. Automatically detecting the need for maintenance due to distribution shift or otherwise is an important research direction, and can be supported in the meantime by *ad hoc* statistical tests created by project maintainers.

[2] For example, the U.S. Census has modified the language used to ask about respondents' race several times in response to an evolving understanding of this construct. A changelog (American Community Survey Office, 2019) of a recently conducted survey compared to the prior year contained 42 entries.

5.8 Higher-order features

While feature definitions allow data scientists to express complex transformations of their raw variables, the process can become tedious if they have many variables to process. For example, as we will see in Chapter 8 for the Fragile Families Challenge data, even with a highly-collaborative feature engineering effort, it is difficult to process many thousands of variables using Ballet's existing functionality. However, in many prediction problems, some variables are quite similar to each other and require similar processing. This motivates support for *higher-order features* that generalize feature definitions to operate on functions on variables, rather than on variables themselves. That is, while a feature might operate on a single variable, a higher-order feature might operate on a set of variables, that each satisfy some condition, by applying the same feature to each individual variable. The input to a higher-order feature could be a set of variables, a function from the entities data frame to a set of variables, a function that returns a boolean for each variable indicating whether it should be operated on, or a data type or other meta-information about a variable. Higher-order features could be developed and contributed by data scientists alongside of the development of normal features.

5.9 Combining human and automated feature engineering

In some prediction tasks, automated feature engineering algorithms like DFS (Kanter and Veeramachaneni, 2015) and Cognito (Khurana et al., 2016) can perform well by themselves with minimal human oversight. And in other prediction tasks, many simple features are trivial to develop. There is promise in combining together human-driven and machine-driven (automated) feature engineering approaches. One advantage of Ballet is that it simply expects that code contributions to a shared project introduce new feature definitions, but leaves open the question of whether the feature definitions are developed by humans or machines, and whether the code is submitted through a graphical user interface, a development environment like Assemblé, or through an automated process. As a result, human-generated and machine-generated feature definitions can co-exist peacefully within a single project, and the same feature validation method can be used for both types of features. Future research in this area should consider how interfaces can expose automated feature engineering algorithms to support data scientists developing new features, and whether acceptance procedures for features need to be customized when both human and machine features are being contributed.

5.10 Ethical considerations

As the field of machine learning rapidly advances, more and more ethical considerations are being raised, including of recent models (Bender et al., 2021; Bolukbasi et al., 2016; Strubell et al., 2019). The same set of concerns could also be raised about any model developed using Ballet. Addressing the underlying issues is beyond the scope of our work. However, we emphasize that Ballet provides several benefits from an ethical perspective. The open-source setting means that models are open and transparent from the outset. Similarly, we focus on the development of models that aim to address societal problems, such as vehicle fatality prediction and government survey optimization.

5.11 Data source support

We described the application of Ballet to a disease incidence forecasting problem, a house price prediction problem, and a personal income prediction problem, and will describe the application to a life outcomes prediction problem in Chapter 8. These tasks are similar in the sense that they use structured data in a single table.

Ballet could also support the following data sources as inputs to its collaborative feature engineering process:

- Multi-table, relational data that has been denormalized into single-table form.

- NoSQL/NewSQL collections that are flattened into a data frame.
- Survey data from various providers, such as Qualtrics, Google Forms, and Survey Monkey.

To better support these alternative data sources, Ballet could implement "connectors" that transform data from one of these initial forms into the single-table data frame that Ballet currently supports.

Moreover, Ballet could be extended to support querying on multi-table relational data directly. The feature definition abstraction requires data science developers to write a tuple of input and transformer. In the case of a data frame, it is easy to interpret the input as an index into the data frame's column index and the transformer as operations on rectangular data. However, these same concepts could apply to multi-table data. The input could be a set of tables within a relational database and the transformer could be an SQL query written over the database. Ballet's feature execution engine could be modified to rewrite queries to ensure they do not introduce leakage. The queries could be written in SQL directly, in a Python-based object-relational mapper (ORM) such as SQLAlchemy, or in an in-memory representation of a relational database such as a `featuretools.EntitySet`.

5.12 Assemblé

To allow developers to select code to submit, we rely upon simple existing interactions provided by Jupyter (i.e. select one cell, select multiple cells). However, some developers requested *better affordances*, and other interactions could be incorporated. For example, code gathering tools (Head et al., 2019) could allow users to more easily select code to be submitted while staying within the notebook environment.

One reason (of many) that powerful developer tools exist for team-based version control is to avoid and/or resolve merge conflicts when contributions are scattered across multiple files. With Assemblé, we can avoid such merge conflicts by tightly coupling with Ballet projects, in the sense that we can make assumptions about the structure those projects impose on contributions, such as that contributions are in single Python modules at well-defined locations in the directory structure. By relaxing these assumption, or by defining such structures for other settings, Assemblé could be used more generally to contribute patches to central locations. For example, the ML Bazaar framework (Chapter 6) organizes data science pipelines into a graph of "ML primitives," each a JSON annotation of some underlying implementation that an expert or experts must create and validate in a notebook. Assemblé could be used to extract the completed primitive and submit it to the project's curated catalog of community primitives. As another example, an educator running an introductory programming class could invite students to submit their implementations of a basic algorithm to a joint hosting repository, such that they could share in the code review process and learn from the implementations of others. Similarly, a Python language extension for sharing simple functions (Fast and Bernstein, 2016) could use the functionality of the development environment to share these functions, rather than requiring the manual addition of function decorators.

5.13 Earlier visions of collaboration

In earlier work preceding the developing of Ballet, we created FeatureHub, a cloud-hosted feature engineering platform (Section 2.1). Through the experience gained in that project, we identified drawbacks and challenges that can occur when collaboration is facilitated through hosted platforms and called for the development of new collaborative paradigms:

> *I propose the development of a new paradigm for platform-less collaborative data science, with a focus on feature engineering. Under this approach collaborators will develop feature engineering source code on their own machines, in their own preferred environments. They will submit their source code to an authoritative repository that will use still other services to verify that the proposed source code is syntactically and semantically valid and to evaluate performance on an unseen test set. If tests pass and performance is sufficient, the proposed code can be merged into the repository of features comprising the machine learning model.*
>
> (Smith, 2018, page 100)

Our work on Ballet fully realizes this earlier vision. The *authoritative repository* is the project hosted on GitHub. The *still other services* are the continuous integration providers like Travis CI. The *syntactically and semantically valid* condition is enforced by the feature API validation. The *evaluated performance* is given by the ML performance validation using streaming feature definition selection algorithms. The *proposed code can be merged* automatically by the Ballet Bot.

Ballet fully supports collaborators in developing feature definitions using their *preferred environments*. However, the earlier vision did not fully grasp the importance of the development environment itself, and its support for the patch contribution task. With Ballet, we have found that providing data scientists with tools to solve the patch contribution task within a notebook environment was critical for facilitating collaborations among different data science personas.

5.14 Limitations

There are several limitations to our approach. Feature engineering is a complex process, and we have not yet provided support for several common practices (or potential new practices). For example, many features are trivial to specify and can be enumerated by automated approaches (Kanter and Veeramachaneni, 2015), and some data cleaning and preparation can be performed automatically. We have referred the responsibility for adding these techniques to the feature engineering pipeline to individual project maintainers, even as we consider a hybrid approach (Section 5.9). Similarly, feature engineering with higher-level features (Section 5.8) could enhance developer productivity.

Feature engineering is only one part of the larger data science process, albeit an important one. Indeed, many domains, including computer vision and natural language processing, have largely replaced manually engineered features with learned ones extracted by deep neural networks. Applying our conceptual framework to other aspects of data science, like data programming or ensembling in developing predictive models, can increase the impact of collaborations. Similarly, improving collaboration in other aspects of data work — like data journalism, exploratory data analysis, causal modeling, and neural network architecture design — remains an important challenge.

Part II

Automated data science

Chapter 6

The Machine Learning Bazaar

6.1 Introduction

Once limited to conventional commercial applications, machine learning (ML) is now 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 systems, as key functionality becomes fragmented across ML-specific or domain-specific software libraries created by independent communities. In addition, the process of building problem-specific end-to-end systems continues to be marked by ML and data management challenges, such as formulating achievable learning problems (Kanter et al., 2016), managing and cleaning data and metadata (Miao et al., 2017; van der Weide et al., 2017; Bhardwaj et al., 2015), scaling tuning procedures (Falkner et al., 2018; Li et al., 2020), and deploying models and serving predictions (Baylor et al., 2017; Crankshaw et al., 2015). In practice, engineers and data scientists often spend significant effort developing ad hoc programs for new problems: writing "glue code" to connect components from different software libraries, processing different forms of raw input, and interfacing with external systems. These steps are tedious and error-prone, and lead to the emergence of brittle "pipeline jungles" (Sculley et al., 2015).

In the Ballet framework, we support collaboration in feature engineering within predictive machine learning modeling pipelines (Chapter 3). However, this is only one

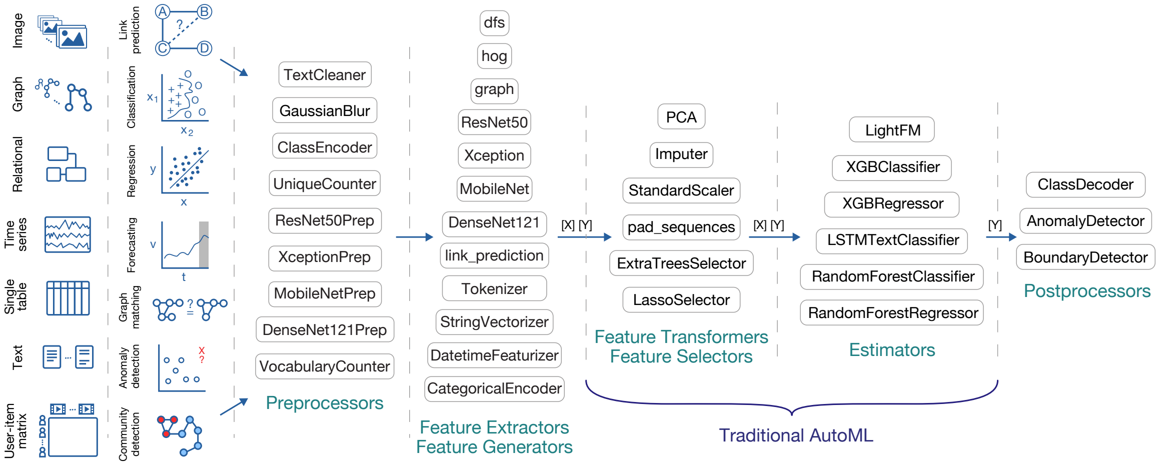


Figure 6.1: Various ML task types that can be solved in *ML Bazaar* by combining ML primitives (abbreviated here from fully-qualified names). Primitives are categorized into preprocessors, feature processors, estimators, and postprocessors, and are drawn from many different ML libraries, such as Ballet, scikit-learn, Keras, OpenCV, and NetworkX, as well as custom implementations. Many additional primitives and pipelines are available in our curated catalog.

step of the larger data science process. If data scientists are spending more time on feature engineering, they in turn have less time to spend on other aspects of creating an end-to-end modeling solution.

These points raise the question, *how can we make it easier to buildML systems in practical settings?* A new approach is needed to designing and developing software systems that solve specific ML tasks. Such an approach should address a wide variety of input data modalities, such as images, text, audio, signals, tables, and graphs; and many learning problem types, such as regression, classification, clustering, anomaly detection, community detection, and graph matching; it should cover the intermediate stages involved, such as data preprocessing, munging, featurization, modeling, and evaluation; and it should fine-tune solutions through AutoML functionality, such as hyperparameter tuning and algorithm selection. Moreover, it should offer coherent APIs, fast iteration on ideas, and easy integration of new ML innovations. Combining these elements would allow almost all end-to-end learning problems to be solved or built using a single ambitious framework.

To address these challenges, we present the *Machine Learning Bazaar*,[1] a frame-

[1] Just as one open-source community was described as "a great babbling bazaar of different agen-

work for designing and developing ML and AutoML systems. We organize the ML ecosystem into composable software components, ranging from basic building blocks like individual classifiers, to feature engineering pipelines creating using Ballet, to full AutoML systems. With our design, a user specifies a task, provides a raw dataset, and either composes an end-to-end pipeline out of pre-existing, annotated, ML primitives or requests a curated pipeline for their task (Figure 6.1). The resulting pipelines can be easily evaluated and deployed across a variety of software and hardware settings, and tuned using a hierarchy of AutoML approaches. Using our own framework, we have created an AutoML system which we entered into DARPA's Data-Driven Discovery of Models (D3M) program; ours was the first end-to-end, modular, publicly released system designed to meet the program's goal.

As an example of what can be developed using our framework, we highlight the Orion project, an MIT-based endeavor that tackles anomaly detection in the field of satellite telemetry (Figure 6.2), as one of several successful real-world applications that use *ML Bazaar* for effective ML system development (Section 7.1). The Orion pipeline processes a telemetry signal using several custom preprocessors, an LSTM predictor, and a dynamic thresholding postprocessor to identify anomalies. The entire pipeline can be represented by a short Python snippet. Custom processing steps are easily implemented as modular components, two external libraries are integrated without glue code, and the pipeline can be tuned using composable AutoML functionality.

Contributions in this chapter include:

A composable framework for representing and developing ML and AutoML systems. Our framework enables users to specify a pipeline for any ML task, from image classification to graph matching, through a unified API (Sections 6.2 and 6.3).

The first general-purpose automated machine learning system. Our system, AutoBazaar, is to the best of our knowledge the first open-source, publicly-available sys-

das and approaches" (Raymond, 1999), our framework is characterized by the availability of many compatible alternatives, a wide variety of libraries and custom solutions, a space for new contributions, and more.

tem with the ability to reliably compose end-to-end, automatically-tuned solutions for 15 data modalities and problem types (Section 6.4.1).

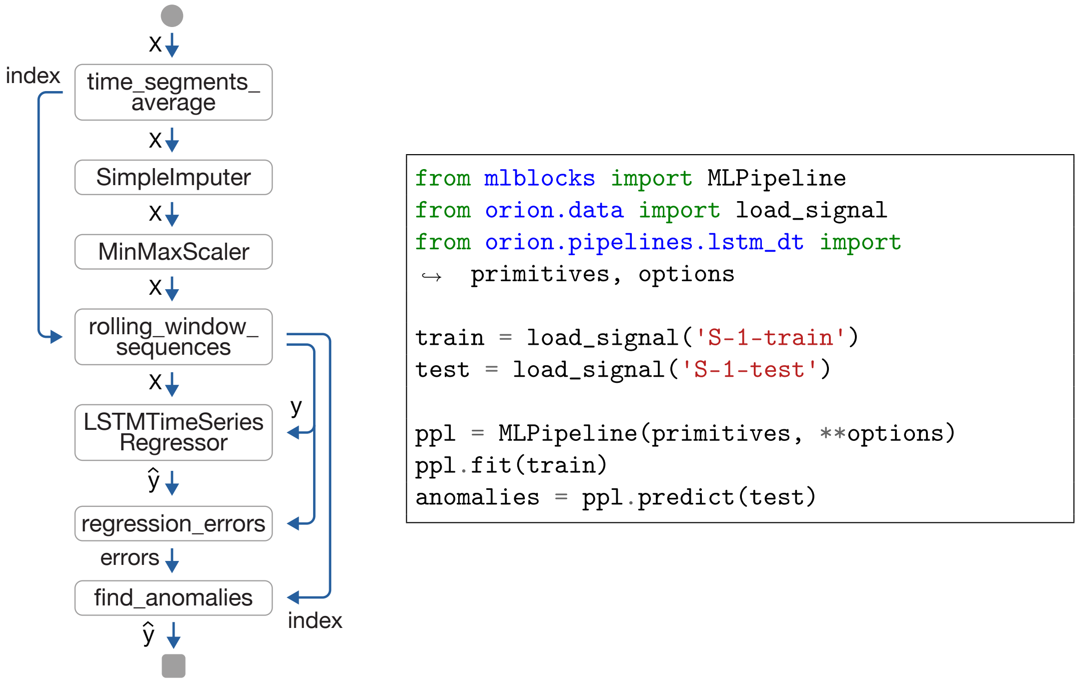
Industry applications. We describe 5 successful applications of our framework to real-world problems (Section 7.1).

A comprehensive evaluation. We evaluated our AutoML system against a suite of 456 ML tasks/datasets covering 15 ML task types, and analyzed 2.5 million scored pipelines (Section 7.2).

```
primitives = [
    'mlprimitives.custom.ts_preprocessing.time_segments_average',
    'sklearn.impute.SimpleImputer',
    'sklearn.preprocessing.MinMaxScaler',
    'mlprimitives.custom.ts_preprocessing.rolling_window_sequences',
    'keras.Sequential.LSTMTimeSeriesRegressor',
    'mlprimitives.custom.ts_anomalies.regression_errors',
    'mlprimitives.custom.ts_anomalies.find_anomalies',
]
```

```
options = {
    'init_params': {
        'mlprimitives.custom.ts_preprocessing.time_segments_average#1': {
            'time_column': 'timestamp',
            'interval': 21600,
        },
        'sklearn.preprocessing.MinMaxScaler#1': {'feature_range': [-1, 1]},
        'mlprimitives.custom.ts_preprocessing.rolling_window_sequences#1': {
            'target_column': 0,
            'window_size': 250,
        },
        'keras.Sequential.LSTMTimeSeriesRegressor': {'epochs': 35},
    },
    'input_names': {
        'mlprimitives.custom.ts_anomalies.find_anomalies#1': {
            'index': 'target_index'
        },
    },
    'output_names': {
        'keras.Sequential.LSTMTimeSeriesRegressor#1': {'y': 'y_hat'},
    },
}
```

(a) Python representation.



```python
from mlblocks import MLPipeline
from orion.data import load_signal
from orion.pipelines.lstm_dt import
↪  primitives, options

train = load_signal('S-1-train')
test = load_signal('S-1-test')

ppl = MLPipeline(primitives, **options)
ppl.fit(train)
anomalies = ppl.predict(test)
```

(b) Graph representation.

(c) Usage with Python SDK.

Figure 6.2: Representation and usage of the Orion pipeline for anomaly detection using the *ML Bazaar* framework. ML system developers or researchers describe the pipeline in a short Python snippet by a sequence of primitives annotated from several libraries (and optional additional parameters). Our framework compiles this into a graph representation (Section 6.2.2) by consulting meta-information associated with the underlying primitives (Section 6.2.1). Developers can then use our Python SDK to train the pipeline on "normal" signals, and identify anomalies in test signals. The `MLPipeline` provides a familiar interface but enables more general data engineering and ML processing. It also can expose the entire underlying hyperparameter configuration space for tuning by our AutoML libraries or others (Section 6.3).

Open-source libraries. Components of our framework have been released as the open-source libraries MLPrimitives, MLBlocks, BTB, piex, and AutoBazaar.

6.2 A framework for machine learning pipelines

The *ML Bazaar* is a composable framework for developing ML and AutoML systems based on a hierarchical organization of and unified API for the ecosystem of ML software and algorithms. It is possible to use curated or custom software components for every aspect of the practical ML process, from featurizers for relational datasets to signal processing transformers to neural networks to pre-trained embeddings. From these *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.

6.2.1 ML primitives

A *primitive* is a reusable, self-contained software component for ML paired with the structured *annotation* of its metadata. It has a well-defined `fit`/`produce` interface, wherein it receives input data in one of several formats or types, performs computations, and returns the data in another format or type. With this categorization and abstraction, the widely varying functionalities required to construct ML pipelines can be collected in a single location. Primitives can be reused in chained computations while minimizing glue code written by callers. Example primitive annotations are shown in Figures 6.3 and 6.4.

Primitives encapsulate different types of functionality. Many have a learning component, such as a random forest classifier. Some, categorized as transformers, may only have a `produce` method, but are very important nonetheless. For example, the Hilbert and Hadamard transforms from signal processing would be important primitives to include while building an ML system to solve a task in Internet-of-Things.

Some primitives do not change values in the data, but simply prepare or reshape it. These *glue primitives* are intended to reduce the glue code that would otherwise be required to connect primitives into a full system. An example of this type of primitive is `pandas.DataFrame.unstack`.

Annotations

Each primitive is annotated with machine-readable metadata that enables it to be used and automatically integrated within an execution engine. Annotations allow us

```json
{
  "name": "cv2.GaussianBlur",
  "contributors": [
    "Carles Sala <csala@csail.mit.edu>"
  ],
  "description": "Blur an image using a Gaussian filter.",
  "classifiers":
    {"type": "preprocessor", "subtype": "transformer"},
  "modalities": ["image"],
  "primitive": "mlprimitives.adapters.cv2.GaussianBlur",
  "produce": {
    "args": [{"name": "X", "type": "ndarray"}],
    "output": [{"name": "X", "type": "ndarray"}]
  },
  "hyperparameters": {
    "fixed": {
      "ksize_width": {"type": "int", "default": 3},
      "ksize_height": {"type": "int", "default": 3},
      "sigma_x": {"type": "float", "default": 0.0},
      "sigma_y": {"type": "float", "default": 0.0}
    },
    "tunable": {}
  }
}
```

Figure 6.3: Annotation of the `GaussianBlur` transformer primitive following the MLPrimitives schema. (Some fields are abbreviated or elided.) This primitive does not annotate any *tunable hyperparameters*, but such a section marks hyperparameter types, defaults, and feasible values.

to unify a variety of primitives from disparate libraries, reduce the need for glue code, and provide information about the tunable hyperparameters. This full annotation[2] is provided in a single JSON file, and has three major sections:

- *Meta-information.* This section has the name of the primitive, the fully-qualified name of the underlying implementation as a Python object, and other detailed metadata, such as the author, description, documentation URL, categorization, and what data modalities it is most used for. This information enables searching and indexing primitives.

- *Information required for execution.* This section has the names of the methods pertaining to `fit`/`produce` in the underlying implementation, as well as the data

[2] The primitive annotation specification is described and documented in full in the associated MLPrimitives library.

```
{
  "name": "ballet.engineer_features",
  "contributors": ["Micah Smith <micahs@mit.edu>"],
  "documentation": "https://ballet.github.io/ballet/mlp_reference
  ↪  .html#ballet-engineer-features",
  "description": "Applies the feature engineering pipeline from the given Ballet
  ↪  project",
  "classifiers": {"type": "preprocessor", "subtype": "transformer"},
  "primitive": "ballet.mlprimitives.make_engineer_features",
  "fit": {
    "method": "fit",
    "args": [
      {"name": "X", "type": "pandas.DataFrame"},
      {"name": "y", "type": "pandas.DataFrame"}
    ]
  },
  "produce": {
    "method": "transform",
    "args": [{"name": "X", "type": "pandas.DataFrame"}],
    "output": [{"name": "X", "type": "pandas.DataFrame"}]
  },
  "hyperparameters": {}
}
```

Figure 6.4: Annotation of the `ballet.engineer_features` learning primitive following the MLPrimitives schema. (Some fields are abbreviated or elided.)

types of the primitive's inputs and outputs. When applicable, for each primitive, we annotate the *ML data types* of declared inputs and outputs; i.e., recurring objects in ML that have a well-defined semantic meaning, such as a feature matrix X, a target vector y, or a space of class labels `classes`. We provide a mapping between ML data types and synonyms used by specific libraries as necessary. This logical structure will help dramatically decrease the amount of glue code developers must write (Section 6.2.2).

- *Information about hyperparameters.* The third section details all the hyperparameters of the primitive — their names, descriptions, data types, ranges, and whether they are *tunable* or *fixed* (not appropriate to tune during model development, such as a parameter indicating how many CPUs/GPUs are available to use for training). It also captures any conditional dependencies between hyperparameters.

Source	Count	Source	Count
scikit-learn	41	XGBoost	2
MLPrimitives (custom)	27	LightFM	1
Keras	25	OpenCV	1
pandas	17	python-louvain	1
Featuretools	4	scikit-image	1
NumPy	3	statsmodels	1
NetworkX	2		

Table 6.1: Primitives in the curated catalog of MLPrimitives, by library source. Catalogs maintained by individual projects may contain more primitives.

We have developed the open-source *MLPrimitives*[3] library, which contains a number of primitives adapted from different libraries (Table 6.1). For libraries that already provide a `fit`/`produce` interface or similar (e.g., scikit-learn), a primitive developer has to write the JSON specification and point to the underlying estimator class.

To support the integration 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. These adapter modules then allow us to integrate many functionalities as primitives from the library without having to write a separate object for each — thus requiring us to write only an annotation file for each primitive. Keras is an example of such a library.

For developers, domain experts, and researchers, MLPrimitives enables the easy *contribution* of new primitives in several ways by providing primitive templates, example annotations, and detailed tutorials and documentation. We also provide procedures for validating proposed primitives against the formal specification and a unit test suite. Finally, data scientists can also write custom primitives.

Currently, MLPrimitives maintains a curated *catalog* of high-quality, useful primitives from 13 libraries,[4] as well as custom primitives that we have created (Table 6.1). Each primitive is identified by a fully-qualified name to differentiate primitives across catalogs. The JSON annotations can then be mined for additional insights.

[3] `https://github.com/MLBazaar/MLPrimitives`

[4] As of MLPrimitives v0.3.

Designing for contributions

We considered multiple alternatives to the primitives API, such as representing all primitives as Python data structures or classes regardless of their type (i.e., transformers or estimators). One disadvantage of these alternatives is that it makes it more difficult for domain experts to contribute primitives. We have found that domain experts, such as engineers and scientists in the satellite industry, prefer writing functions to other constructs such as classes. We have also found that many domain-specific processing methods are simply transformers, without a learning component.

Lightweight integration

Another option we considered was to enforce that every primitive — whether brought over from a library with a compatible API or otherwise — be integrated via a Python class with wrapper methods. We opted against this approach as it led to excessive wrapper code and created redundancy, which made it more difficult to write primitives. Instead, for libraries that are compatible, our design only requires that we create the annotation file.

Language independence

In this work, we focus on the wealth of ML functionality that exists in the Python ecosystem. Through *ML Bazaar*'s careful design, we could also support other common languages in data science, including R, MATLAB, and Julia, and enable multi-language pipelines. Starting from our JSON primitive annotation format, a multi-language pipeline execution backend would be built that uses language-specific kernels or containers and relies on an interoperable data format such as Apache Arrow. A language-independent format like JSON provides several additional advantages: It is both machine- and human- readable and writeable, and it is also a natural format for storage and querying in NoSQL document stores — allowing developers to easily query a knowledge base of primitives for the subset appropriate for a specific ML task type, for example.

6.2.2 ML pipelines

To solve practical 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 developers can easily compose primitives without sacrificing flexibility. We aim to support end users 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. 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. As one realization of these ideas, we have implemented *MLBlocks*,[5] a library for composing, training, and deploying end-to-end ML pipelines.

```
from mlblocks import MLPipeline, load_pipeline
from mlblocks.datasets import load_umls

dataset = load_umls()
X_train, X_test, y_train, y_test = dataset.get_splits(1)
graph = dataset.graph
node_columns = ['source', 'target']

pipeline = MLPipeline(load_pipeline('graph.link_prediction.nx.xgb'))
pipeline.fit(X_train, y_train, graph=graph, node_columns=node_columns)
y_pred = pipeline.predict(X_test, graph=graph, node_columns=node_columns)
```

Figure 6.5: Usage of MLBlocks for a graph link prediction task. Curated pipelines in the MLPrimitives library can be easily loaded. Pipelines provide a familiar API but enable more general data engineering and ML.

We introduce *ML pipelines*, which collect multiple primitives into a single computational graph. Each primitive in the graph is instantiated in a *pipeline step*, which loads and interprets the underlying primitive and provides a common interface to run a step in a larger program.

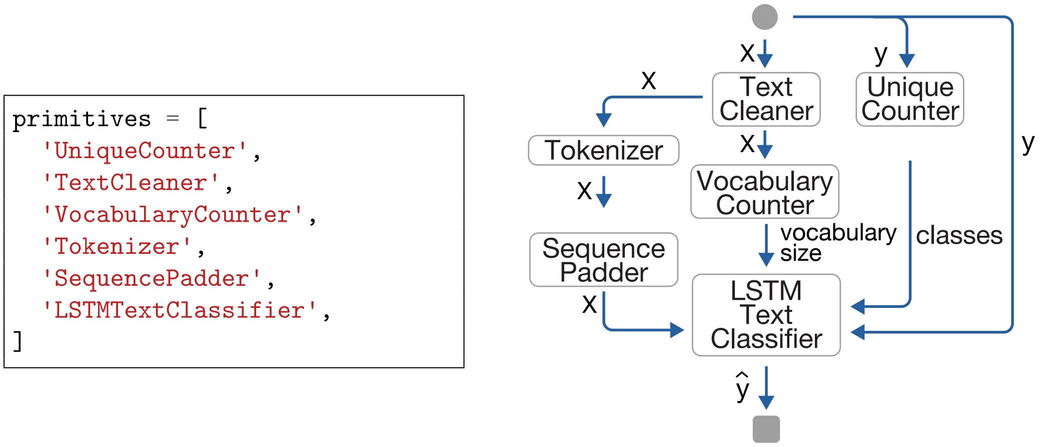
We define a *pipeline* as a directed acyclic multigraph $L = \langle V, E, \lambda \rangle$, where V is a collection of pipeline steps, E are the directed edges between steps representing data flow, and λ is a joint hyperparameter vector for the underlying primitives. A valid

[5] https://github.com/MLBazaar/MLBlocks

pipeline — and its generalizations (Section 6.3.1) — must also satisfy acceptability constraints that require the inputs to each step to be satisfied by the outputs of another step connected by a directed edge.

The term "pipeline" is used in the literature to refer to a ML-specific sequence of operations, and sometimes abused (as we do here) to refer to a more general computational graph or analysis. In our conception, we bring foundational data processing operations of raw inputs into this scope, including 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 type and spanning the entire ML process beginning with the raw dataset.

Pipeline description interface



```
primitives = [
  'UniqueCounter',
  'TextCleaner',
  'VocabularyCounter',
  'Tokenizer',
  'SequencePadder',
  'LSTMTextClassifier',
]
```

(a) Python representation. (b) Graph representation.

Figure 6.6: Recovery of ML computational graph from pipeline description for a text classification pipeline. The ML data types that enable extraction of the graph, and stand for data flow, are labeled along edges.

Large graph-structured workloads can be difficult to specify for end-users due to the complexity of the data structure, and such workloads are an active area of research in data management. In *ML Bazaar*, we consider three aspects of pipeline representation: ease of composition, readability, and computational issues. First, we prioritize easy composition of complex ML pipelines by providing a *pipeline description interface* (PDI) in which developers specify only the topological ordering of all pipeline steps in the pipeline without requiring any explicit dependency declarations. These steps can be passed to our libraries as Python data structures or loaded from JSON files. Full training-time (`fit`) and inference-time (`produce`) computational graphs can then be recovered (Algorithm 2). This is made possible by the meta-information provided in the primitive annotations, in particular the ML data types of the primitive inputs and outputs. We leverage the observation that steps that modify the same ML data type can be grouped into the same subpath. In cases where this information does not uniquely identify a graph, the user can additionally provide an *input-output map* which serves to explicitly add edges to the graph, as well as other parameters to customize the pipeline.

Though it may be more difficult to read and understand these pipelines from the PDI alone as the edges are not shown nor labeled, it is easy to accompany them with the recovered graph representation (Figures 6.2 and 6.6).

The resulting graphs describe abstract computational workloads, but we must be able to actually execute them for purposes of learning and inference. From the recovered graphs, we could repurpose many existing data engineering systems as backends for scheduling and executing the workloads (Rocklin, 2015; Zaharia et al., 2016; Palkar et al., 2018). In our MLBlocks execution engine, a collection of objects and a metadata tracker in a key-value store are iteratively transformed through sequential processing of pipeline steps. The Orion pipeline would be executed using MLBlocks as shown in Figure 6.2c.

6.2.3 Discussion

Why not scikit-learn?

Several alternatives exist to our new ML pipeline abstraction (Section 6.2.2), such as scikit-learn's `Pipeline` (Buitinck et al., 2013). Ultimately, while our pipeline is inspired by these alternatives, it aims to provide more general data engineering and ML

Algorithm 2: Pipeline-Graph Recovery

```
input  : pipeline description $S = (v_1, \ldots, v_n)$, source node $v_0$, sink node $v_{n+1}$
output : directed acyclic multigraph $\langle V, E \rangle$
$S \leftarrow v_0 \cup S \cup v_{n+1}$
$V \leftarrow \varnothing$, $E \leftarrow \varnothing$
$U \leftarrow \varnothing$                                   // unsatisfied inputs
while $S \neq \varnothing$ do
    $v \leftarrow \text{popright}(S)$                        // last pipeline step remaining
    $M \leftarrow \text{popmatches}(U, \text{outputs}(v))$
    if $M \neq \varnothing$ then
        $V \leftarrow V \cup \{v\}$
        for $(v', \sigma) \in M$ do
            $E \leftarrow E \cup \{(v, v', \sigma)\}$
        end
        for $\sigma \in \text{inputs}(v)$ do                  // unsatisfied inputs of $v$
            $U \leftarrow U \cup \{(v, \sigma)\}$
        end
    else                                                     // isolated node
        return INVALID
    end
end
if $U \neq \varnothing$ then                                  // unsatisfied inputs remain
    return INVALID
end
return $\langle V, E \rangle$
```

Figure 6.7: Pipeline steps are added to the graph in reverse order and edges are iteratively added when the step under consideration produces an output that is required by an existing step. Exactly one graph is recovered if a valid graph exists. In cases where multiple graphs have the same topological ordering, the user can additionally provide an *input-output map* (which modifies the result of inputs(v)/outputs(v) above) to explicitly add edges and thereby select from among several possible graphs.

functionality. While the scikit-learn pipeline sequentially applies a list of transformers to X and y only before outputting a prediction, our pipeline supports general computational graphs, simultaneously accepts multiple data modalities as input, produces multiple outputs, manages evolving metadata, and can use software from outside the scikit-learn ecosystem/design paradigm. For example, we can use our pipeline to construct entity sets (Kanter and Veeramachaneni, 2015) from multi-table relational data for input to other pipeline steps. We can also support pipelines in an unsupervised learning paradigm, such as in Orion, where we create the target y “on-the-fly” (Figure 6.6).

Where’d the glue go?

To connect learning components from different libraries with incompatible APIs, data scientists end up writing “glue code.” Typically, this glue code is written within pipeline bodies. In *ML Bazaar*, we mitigate the need for this glue by pushing the need for API adaptation down to the level of primitive annotations, which are written once and reside in central locations, amortizing the adaptation cost. Moreover, the need for glue code arises during data shaping and the creation of intermediate outputs. We created a number of primitives that support these common programming patterns and miscellaneous needs during the development of an ML pipeline. These are, for example, data reshaping primitives like `pandas.DataFrame.unstack`, data preparation primitives like `pad_sequences` required for Keras-based LSTMs, and utilities like `UniqueCounter` that count the number of unique classes.

Interactive development

Interactivity is an important aspect of data science development for beginners and experts alike, as they build understanding of the data and iterate on different modeling ideas. In *ML Bazaar*, the level of interactivity possible depends on the specific runtime library. For example, our MLBlocks library supports interactive development in a shell or notebook environment by allowing for the inspection of intermediate pipeline outputs and by allowing pipelines to be iteratively expanded starting from a loaded pipeline description. Alternatively, ML primitives could be used as a backend pipeline representation for software that provides more advanced interactivity, such as drag-and-drop. For interfaces that require low latency pipeline scoring to provide user feedback such as Crotty et al. (2015), *ML Bazaar*’s performance depends mainly on the underlying primitive implementations (Section 7.2).

Supporting new task types

While *ML Bazaar* handles 15 ML task types (Table 7.3), there are many more task types for which we do not currently provide pipelines in our default catalog (Section 7.2.5). To extend our approach to support new task types, it is generally sufficient to write several new primitive annotations for pre-processing input and post-processing output — no changes are needed to the core *ML Bazaar* software libraries such as MLPrimitives and MLBlocks. For example, for the anomaly detection task type from the Orion project, several new simple primitives were implemented: `rolling_window_sequences`, `regression_errors`, and `find_anomalies`. Indeed, support for a certain task type is predicated on the availability of a pipeline for that task type rather than on any characteristics of our software libraries.

Primitive versioning

The default catalog of primitives from the MLPrimitives library is versioned together, and library conflicts are resolved manually by maintainers through careful specification of minimum and maximum dependencies. This strategy ensures that the default catalog can always be used, even if there are incompatible updates to the underlying libraries. Automated tools can be integrated to aid both end-users and maintainers in understanding potential conflicts and safely bumping library-wide versions.

6.3 An automated machine learning framework

From the components of the *ML Bazaar*, data scientists can easily and effectively build ML pipelines with fixed hyperparameters for their specific problems. To improve the performance of these solutions, we introduce the more general *pipeline templates* and *pipeline hypertemplates* and then present the design and implementation of AutoML primitives which facilitate hyperparameter tuning and model selection, either using our own library for Bayesian optimization or external AutoML libraries. Finally, we describe AutoBazaar, one specific AutoML system we have built on top of these components.

6.3.1 Pipeline templates and hypertemplates

Frequently, pipelines require hyperparameters to be specified at several places. Unless these values are fixed at annotation time, hyperparameters must be exposed in a machine-friendly interface. This motivates pipeline templates and pipeline hypertemplates, which generalize pipelines by allowing a hierarchical tunable hyperparameter configuration space and provide first-class tuning support.

We define a *pipeline template* as a directed acyclic multigraph $T = \langle V, E, \Lambda \rangle$, where Λ is the joint hyperparameter configuration space for the underlying primitives. By providing values $\lambda \in \Lambda$ for the unset hyperparameters of a pipeline template, a specific 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 pipeline hypertemplates.

We define a *pipeline hypertemplate* as a directed acyclic multigraph $H = \langle V, E, \bigcup_j \Lambda_j \rangle$, where V is a collection of pipeline steps, E are directed edges between steps, and Λ_j is the hyperparameter configuration space for pipeline template T_j. A number of pipeline templates can be derived from one pipeline hypertemplate by fixing the conditional hyperparameters.

6.3.2 Tuners and selectors

Just as primitives are the components of ML computation, AutoML primitives represent components of an AutoML system. We separate AutoML primitives into *tuners* and *selectors*. In our extensible AutoML library for developing AutoML systems, *BTB*,[6] we provide various instances of these AutoML primitives.

Given a pipeline template, an AutoML system must find a specific pipeline with fully-specified hyperparameter values to maximize some utility. Given pipeline tem-

[6] `https://github.com/MLBazaar/BTB`

plate T and a function f that assigns a performance score to pipeline L_λ with hyperparameters $\lambda \in \Lambda$, the tuning problem is defined as

$$\lambda^* = \arg\max_{\lambda \in \Lambda} f(L_\lambda). \tag{6.1}$$

We introduce *tuner*s, AutoML primitives which provide a `record`/`propose` interface in which evaluation results are recorded to the tuner by the user or by an AutoML controller and new hyperparameters are proposed in return.

Hyperparameter tuning is widely studied and its effective use is instrumental to maximizing the performance of ML systems (Bergstra et al., 2011; Bergstra and Bengio, 2012; Feurer et al., 2015; Snoek et al., 2012). One widely used approach to hyperparameter tuning is Bayesian optimization (BO), a black-box optimization technique in which expensive evaluations of f are kept to a minimum 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. We structure these meta-models and acquisition functions as separate, BO-specific AutoML primitives that can be combined together to form a tuner. Researchers have argued for different formulations of meta-models and acquisition functions (Oh et al., 2018; Wang et al., 2017; Snoek et al., 2012). In our BTB library for AutoML, we implement the `GP-EI` tuner, which uses a Gaussian Process meta-model primitive and an Expected Improvement (EI) acquisition function primitive, among several other tuners. Many other tuning paradigms exist, such as those based on evolutionary strategies (Loshchilov and Hutter, 2016; Olson et al., 2016), adaptive execution (Jamieson and Talwalkar, 2016; Li et al., 2017), meta-learning (Gomes et al., 2012), or reinforcement learning (Drori et al., 2018). Though we have not provided implementations of these in BTB, one could do so using our common API.

For many ML task types, there may be multiple pipeline templates or pipeline hypertemplates available, each with their own tunable hyperparameters. The aim is to balance the exploration-exploitation tradeoff while selecting promising pipeline templates to tune. For a set of pipeline templates $\mathcal{T}$, we define the selection problem as

$$T^* = \operatorname*{arg\,max}_{T \in \mathcal{T}} \max_{\lambda_T \in \Lambda_T} f(L_{\lambda_T}). \tag{6.2}$$

We introduce *selector*s, AutoML primitives which provide a `compute_rewards`/`select` API.

Algorithm selection is often treated as a multi-armed bandit problem where the score returned from a selected template can be assumed to come from an unknown underlying probability distribution. In BTB, we implement the `UCB1` selector, which uses the upper confidence bound method (Auer et al., 2002), among several other selectors. Users or AutoML controllers can use selectors and tuners together to perform joint algorithm selection and hyperparameter tuning.

6.4 AutoML systems

6.4.1 AutoBazaar

Using the ML Bazaar framework, we have built *AutoBazaar*,[7] an open-source, end-to-end, general-purpose, multi-task, automated machine learning system. It consists of several components: an AutoML controller; a pipeline execution engine; data stores for metadata and pipeline evaluation results; loaders and configuration for ML tasks, primitives, etc.; a Python language client; and a command-line interface. AutoBazaar is an open-source variant of the AutoML system we have developed for the DARPA D3M program.

We focus here on the core pipeline search and evaluation algorithms (Algorithm 3). The input to the search is a computational budget and an ML task, which consists of the raw data and task and dataset metadata — dataset resources, problem type, dataset partition specifications, and an evaluation procedure for scoring. Based on these inputs, AutoBazaar searches through its catalog of primitives and pipeline templates for the most suitable pipeline that it can build. First, the controller loads the

[7] `https://github.com/MLBazaar/AutoBazaar`

train and test dataset partitions, $\mathcal{D}^{(train)}$ and $\mathcal{D}^{(test)}$, following the metadata specifications. Next, it loads from its default catalog and the user's custom catalog a collection of candidate pipeline templates suitable for the ML task type. Using the BTB library, it initializes a `UCB1` selector and a collection of `GP-EI` tuners for joint algorithm selection and hyperparameter tuning. The search process begins and continues for as long as the computation budget has not been exhausted. In each iteration, the selector is queried to select a template, the corresponding tuner is queried to propose a hyperparameter configuration, a pipeline is generated and scored using cross validation over $\mathcal{D}^{(train)}$, and the score is reported back to the selector and tuner. The best overall pipeline found during the search, L^*, is re-fit on $\mathcal{D}^{(train)}$ and scored over $\mathcal{D}^{(test)}$. Its specification is returned to the user alongside the score obtained, s^*.

Algorithm 3: AutoBazaar Pipeline Search

```
input  : task $t = (M, f, \mathcal{D}^{(train)}, \mathcal{D}^{(test)})$, budget $B$
output : best pipeline $L^*$, best score $s^*$
$\mathcal{T} \leftarrow$ load_available_templates($M$)
A $\leftarrow$ init_automl($\mathcal{T}$)                       // bookkeeping
$s^* \leftarrow +\infty, L^* \leftarrow \varnothing$
while $B > 0$ do
    $T \leftarrow$ select($A$)                             // uses selector.select
    $\lambda \leftarrow$ propose($A, T$)                   // uses $T$'s tuner.propose
    $L \leftarrow (T, \lambda)$
    $s \leftarrow$ cross_validate_score($f, L, \mathcal{D}^{(train)}$)
    record(A, $L, s$)                                      // update selector and tuners
    if $s < s^*$ then
        $s^* \leftarrow s$, $L^* \leftarrow L$
    end
    decrease($B$)
end
$s^* \leftarrow$ fit_and_score($f, L^*, \mathcal{D}^{(train)}, \mathcal{D}^{(test)}$)
return $L^*, s^*$
```

Figure 6.8: Search and evaluation of pipelines in AutoBazaar. Detailed task metadata M is used by the system to load relevant pipeline templates and scorer function f is used to score pipelines.

Chapter 7

Evaluations of ML Bazaar

In this section, we report on evaluating ML Bazaar in two dimensions: real-world applications of ML Bazaar and extensive experimentation on a benchmark corpus.

7.1 Applications

In Chapter 6, we claimed that *ML Bazaar* makes it easier to develop ML systems. We now provide evidence for this claim in this section by describing 5 real-world use cases in which *ML Bazaar* is currently used to create both ML and AutoML systems. Through these industrial applications we examine the following questions: Does *ML Bazaar* support the needs of ML system developers? If not, how easy was it to extend?

7.1.1 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 their satellites and identify anomalies, which might indicate a looming failure severely affecting the satellite's coverage. This time series/anomaly detection task was not initially supported by any of the pipelines in our curated catalog. Our collaborators were able to easily implement a recently developed end-to-end anomaly detection method (Hundman et al., 2018) using pre-existing transformation primitives in *ML Bazaar* and by adding several new primitives: a primitive for the specific LSTM architecture used in the paper and new time series anomaly detection postprocessing primitives, which take as input a time series and time series forecast, and produce as output a list of anomalies, identified by intervals $\{[t_i, t_{i+1}]\}$. This design enabled rapid experimentation through substituting different time series forecasting primitives and comparing the results. In subsequent work, they develop a new GAN-based anomaly detection model as an ML primitive (`orion.primitives.tadgan.TadGAN`) and evaluate it within the anomaly detection pipeline on 11 datasets (Geiger et al., 2020). The work has been released as the open-source Orion project.[1]

7.1.2 Predicting clinical outcomes from electronic health records

Cardea is an open-source, automated framework for predictive modeling in health care on electronic health records following the FHIR schema (Alnegheimish et al., 2020). Its developers formulated a number of prediction problems including predicting length of hospital stay, missed appointments, and hospital readmission. All tasks in Cardea are multitable regression or classification. From *ML Bazaar*, Cardea uses the `featuretools.dfs` primitive to automatically engineer features for this highly-relational data and multiple other primitives for classification and regression. The framework also presents examples on a publicly available patient no-show prediction problem.

7.1.3 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 the time series classification ML task type. *ML Bazaar* has several time series classification pipelines available in its catalog and they enable usage of time series from 140 turbines to develop multiple pipelines, tune them, and produce prediction results. Multiple

[1] `https://github.com/signals-dev/Orion`

outcomes are predicted, ranging from stoppage and pitch failure to less common issues, such as gearbox failure. This library is released as the open-source GreenGuard project.[2]

7.1.4 Leaks and crack detection in water distribution systems

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

7.1.5 DARPA D3M program

DARPA's Data-Driven Discovery of Models (D3M) program, of which we are participants, aims to spur development of automated systems for model discovery for use by non-experts. Among other goals, participants aim to design and implement AutoML systems that can produce solutions to arbitrary ML tasks without any human involvement. We used *ML Bazaar* to create an AutoML system to be evaluated against other teams from US academic institutions. Participants include ourselves (MIT), CMU, UC Berkeley, Brown, Stanford, TAMU, and others. Our system relies on AutoML primitives (Section 6.3) and other features of our framework, but does *not* use our primitive and pipeline implementations (neither MLPrimitives nor MLBlocks).

We present results comparing our system against other teams in the program. DARPA organizes an evaluation every six months (Winter and Summer). During evaluation, AutoML systems submitted by participants are run by DARPA on 95 tasks spanning several task types for three hours per task. At the end of the run, the best pipeline identified by the AutoML system is evaluated on held-out test data. Results are also compared against two independently-developed expert baselines (MIT Lincoln Laboratory and Exline).

[2] `https://github.com/signals-dev/GreenGuard`

System	Top pipeline	Beats Expert 1	Beats Expert 2	Rank
System 1	29	57	31	1
ML Bazaar	18	56	28	2
System 3	15	47	22	3
System 4	14	46	21	4
System 5	10	42	14	5
System 6	8	43	15	6
System 7	8	33	12	7
System 8	6	24	11	8
System 9	4	25	13	9
System 10	2	27	12	10

Table 7.1: Results from the DARPA D3M Summer 2019 evaluation (the latest evaluation as of the publication of Smith et al. 2020). Entries represent the number of ML tasks. "Top pipeline" is the number of tasks for which a system created a winning pipeline. "Beats Expert 1" and "Beats Expert 2" are the number of tasks for which a system beat the two expert team baselines. We highlight Systems 6 and 7 as they belong to the same teams as Shang et al. (2019) and Drori et al. (2018), respectively. (We are unable to comment on other systems as they have not yet provided public reports.) Rank is given based on number of top pipeline lines produced. The top 4 teams are consistent in their ranking even if a different column is chosen.

Results from one such evaluation from Spring 2018 were presented by Shang et al. (2019). We make comparisons from the Summer 2019 evaluation, the results of which were released in August 2019 — the latest evaluation as of the publication of Smith et al. (2020). Table 7.1 compares our AutoML system against nine other teams. Given the same tasks and same machine learning primitives, this comparison highlights the efficacy of the AutoML primitives (BTB) in *ML Bazaar* only — it does not provide any evaluation of our other libraries. In its implementation, our system uses a `GP-MAX` tuner and a `UCB1` selector. Across all metrics, our system places 2nd out of the 10 teams.

7.1.6 Discussion

Through these applications using the components of the *ML Bazaar*, several advantages surfaced.

Composability

One important aspect of *ML Bazaar* is that it does not restrict the user to use a single monolithic system, rather users can pick and choose parts of the framework they want to use. For example, Orion uses only MLPrimitives/MLBlocks, Cardea uses MLPrimitives but integrates the hyperopt library for hyperparameter tuning, our D3M AutoML system submission mainly uses AutoML primitives and BTB, and AutoBazaar uses every component.

Focus on infrastructure

The ease of developing ML systems for the task at hand freed up time for teams to think through and design a comprehensive ML infrastructure. In the case of Orion and GreenGuard, this led to the development of a database that catalogues the metadata from every ML experiment run using *ML Bazaar*. This had several positive effects: it allowed for easy sharing between team members, and it allowed the company to transfer the knowledge of what worked from one system to another system. For example, the satellite company plans to use the pipelines that worked on a previous generation of the satellites on the newer ones from the beginning. With multiple entities finding uses for such a database, creation of such infrastructure could be templatized.

Multiple use cases

Our framework allowed the water technology company to solve many different ML task types using the same framework and API.

Fast experimentation

Once a baseline pipeline has been designed to solve a problem, we notice that users can quickly shift focus to developing and improving primitives that are responsible for learning.

Production ready

A fitted pipeline maintains all the learned parameters as well as all the data manipulations. A user is able to serialize the pipeline and load it into production. This reduces the development-to-production lifecycle.

7.2 Experimental evaluation

In this section, we experimentally evaluate *ML Bazaar* along several dimensions. We also leverage our evaluation results to perform several case studies in which we show how a general-purpose evaluation setting can be used to assess the value of specific ML and AutoML primitives.

7.2.1 ML task suite

The *ML Bazaar* Task Suite is a comprehensive corpus of tasks and datasets to be used for evaluation, experimentation, and diagnostics. It consists of 456 ML tasks spanning 15 task types. Tasks, which encompass raw datasets and annotated task descriptions, are assembled from a variety of sources, including MIT Lincoln Laboratory, Kaggle, OpenML, Quandl, and Crowdflower. We create train/test splits and organize the folder structure, but otherwise do no preprocessing (sampling, outlier detection, imputation, featurization, scaling, encoding, etc.), instead presenting data in its raw form as it would be ingested by end-to-end pipelines. Our publicly available task suite can be browsed online[3] or through *piex*,[4] our library for exploration and meta-analysis of ML tasks and pipelines. The covered task types are shown in Table 7.3 and a summary of the tasks is shown in Table 7.2.

We made every effort to curate a corpus that was evenly balanced across ML task types. Unfortunately, in practice, available datasets are heavily skewed toward traditional ML problems of single-table classification, and our task suite reflects this deficiency, although 49% of our tasks are not single-table classification. Indeed, among

[3] `https://mlbazaar.github.io`

[4] `https://github.com/MLBazaar/piex`

	min	p25	p50	p75	max
Number of examples	7	202	599	3,634	6,095,521
Number of classes†	2	2	3	6	115
Columns of X	1	3	9	22	10,937
Size (compressed)	3KiB	21KiB	145KiB	2MiB	36GiB
Size (inflated)	22KiB	117KiB	643KiB	7MiB	42GiB

Table 7.2: Summary of tasks in *ML Bazaar* Task Suite (n=456). †for classification tasks

other evaluation suites, the OpenML 100 and the AutoML Benchmark (Bischl et al., 2019; Gijsbers et al., 2019) are both exclusively comprised of single-table classification problems. Similarly, evaluation approaches for AutoML methods usually target the black-box optimization aspect in isolation (Golovin et al., 2017; Guyon et al., 2015; Dewancker et al., 2016) without considering the larger context of an end-to-end pipeline.

7.2.2 Pipeline search

We run the search process for all tasks in parallel on a heterogenous cluster of 400 AWS EC2 nodes. Each ML task is solved independently on a node of its own over a 2-hour time limit. Metadata and fine-grained details about every pipeline evaluated are stored in a MongoDB document store. After checkpoints at 10, 30, 60, and 120 minutes of search, the best pipelines for each task are selected by considering the cross-validation score on the training set and are then re-scored on the held-out test set.[5]

7.2.3 Computational bottlenecks

We first evaluate the computational bottlenecks of the AutoBazaar system. To assess these, we instrument AutoBazaar and our framework libraries (MLBlocks, MLPrimitives, BTB) to determine what portion of overall execution time for pipeline search is

[5] Exact replication files and detailed instructions for the experiments in this section are included here: `https://github.com/micahjsmith/ml-bazaar-2019` and can be further analyzed using our piex library.

Data Modality	Problem Type	Tasks	Pipeline Template
graph	community detection	2	CommunityBestPartition
	graph matching	9	link_prediction_feat_extr graph_feat_extr CategoricalEncoder SimpleImputer StandardScaler XGBClassifier
	link prediction	1	link_prediction_feature_extraction CategoricalEncoder SimpleImputer StandardScaler XGBClassifier
	vertex nomination	1	graph_feature_extraction categorical_encoder SimpleImputer StandardScaler XGBClassifier
image	classification	5	ClassEncoder preprocess_input MobileNet XGBClassifier ClassDecoder
	regression	1	preprocess_input MobileNet XGBRegressor
multi table	classification	6	ClassEncoder dfs SimpleImputer StandardScaler XGBClassifier ClassDecoder
	regression	7	dfs SimpleImputer StandardScaler XGBRegressor
single table	classification	234	ClassEncoder dfs SimpleImputer StandardScaler XGBClassifier ClassDecoder
	collaborative filtering	4	dfs LightFM
	regression	87	dfs SimpleImputer StandardScaler XGBRegressor
	timeseries forecasting	35	dfs SimpleImputer StandardScaler XGBRegressor
text	classification	18	UniqueCounter TextCleaner VocabularyCounter Tokenizer pad_sequences LSTMTextClassifier
	regression	9	StringVectorizer SimpleImputer XGBRegressor
timeseries	classification	37	ClassEncoder dfs StandardImputer StandardScaler XGBClassifier ClassDecoder

Table 7.3: ML task types (data modality and problem type pairs) and associated ML tasks counts in the *ML Bazaar* Task Suite, along with default templates from AutoBazaar (i.e., where we have curated appropriate pipeline templates to solve a task).

due to our runtime libraries vs. other factors such as I/O and underlying component implementation. The results are shown in Figure 7.1. Overall, the vast majority of execution time is due to execution of the underlying primitives (p25=90.2%, p50=96.2%, p75=98.3%). A smaller portion is due to the AutoBazaar runtime (p50=3.1%) and a negligible (p50<0.1%) portion of execution time is due to our other framework libraries and I/O. Thus, performance of pipeline execution/search is largely limited by the performance of the underlying physical implementation from the external library.

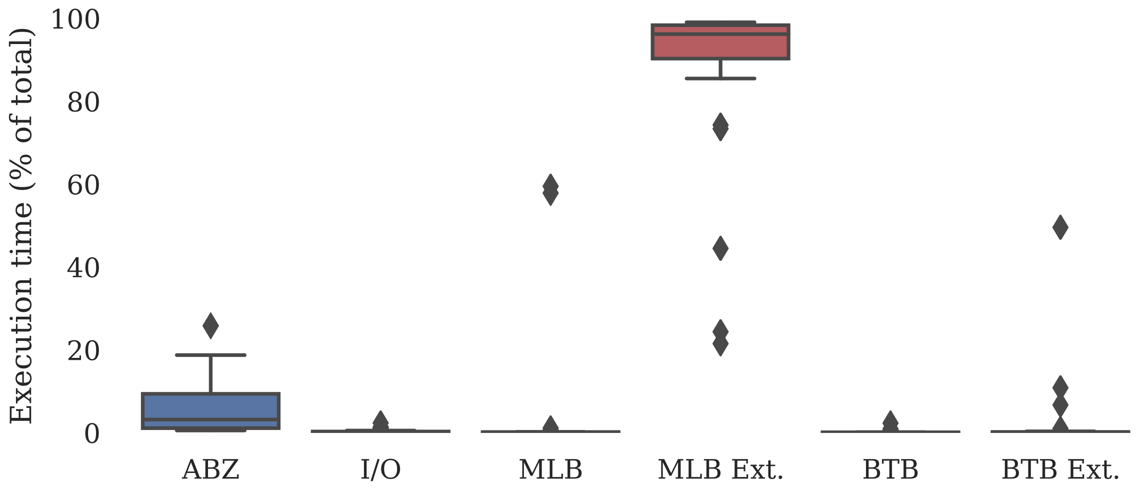


Figure 7.1: Execution time of AutoBazaar pipeline search attributable to different libraries/components. The box plot shows quartiles of the distribution, 1.5× IQR, and outliers. MLB Ext and BTB Ext refer to calls to external libraries providing underlying implementations, like the scikit-learn `GaussianProcessRegressor` used in the `GP-EI` tuner. The vast majority of execution time is attributed to the underlying primitives implemented in external libraries.

7.2.4 AutoML performance

One important attribute of AutoBazaar is the ability to improve pipelines for different tasks through tuning and selection. We measure the improvement in the best pipeline per task, finding that the average task improves its best score by 1.06 standard deviations over the course of tuning, and that 31.7% of tasks improve by more than one standard deviation (Figure 7.2). This demonstrates the effectiveness that a user may expect to obtain from an AutoBazaar pipeline search. However, as we describe in Section 6.3, there are so many AutoML primitives that can be implemented using our tuner/selector APIs that a comprehensive comparison is beyond the scope of this work.

7.2.5 Expressiveness of *ML Bazaar*

To further examine the expressiveness of *ML Bazaar* in solving a wide variety of tasks, we randomly selected 23 Kaggle competitions from 2018, comprising tasks ranging from image and time series classification to object detection and multi-table

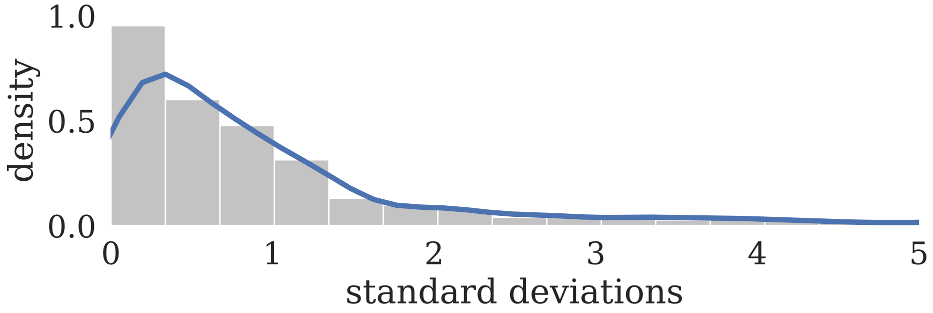


Figure 7.2: Distribution of task performance improvement due to *ML Bazaar* AutoML. Improvement for each task is measured as the score of the best pipeline less the score of the initial default pipeline, in standard deviations of all pipelines evaluated for that task.

regression. For each task, we attempted to develop a solution using existing primitives and catalogs.

Overall, we were able to immediately solve 11 tasks. While we did not support four task types — image matching (two tasks), object detection within images (four tasks), multi-label classification (one task), and video classification (one task) — we could readily support these within our framework by developing new primitives and pipelines. For these tasks, multiple data modalities were provided to participants (i.e., some combination of image, text, and tabular data). To support these tasks, we would need to develop a new "glue" primitive that could concatenate separately-featurized data from each resource to create a single feature matrix. Though our evaluation suite contains many examples of tasks with multiple data resources of different modalities, we had written pipelines customized to operate on certain common subsets (i.e., tabular + graph). While we cannot expect to have *already* implemented pipelines that can work with the innumerable diversity of ML task types, the flexibility of our framework means that we can write new primitives and pipelines that allow it to solve these problems.

7.2.6 Case study: evaluating ML primitives

When new primitives are contributed by the ML community, they can be incorporated into pipeline templates and pipeline hypertemplates, either to replace similar pipeline steps or to form the basis of new topologies. By running the end-to-end system on our evaluation suite, we can assess the impact of the primitive on general-purpose ML workloads (rather than overfit baselines).

In this first case study, we compare two similar primitives: annotations for the XGBoost (`XGB`) and random forest (`RF`) classifiers. We ran two experiments, one in which `RF` is used in pipeline templates and one in which `XGB` is substituted instead.

We consider 1.86×10^6 relevant pipelines to determine the best scores produced for 367 tasks. We find that the `XGB` pipelines substantially outperformed the `RF` pipelines, winning 64.9% 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.

7.2.7 Case study: evaluating AutoML primitives

The design of the *ML Bazaar* AutoML system and our extensive evaluation corpus allows us to easily swap in new AutoML primitives (Section 6.3.2) to see to what extent changes in components like tuners and selectors can improve performance in general settings.

In this case study, we revisit Snoek et al. (2012), which was influential for bringing about widespread use of Bayesian optimization for tuning ML models in practice. Their contributions include: (C1) proposing the usage of the Matérn 5/2 kernel for tuner meta-model, (C2) describing an integrated acquisition function that integrates over uncertainty in the GP hyperparameters, (C3) incorporating a cost model into an EI per second acquisition function, and (C4) explicitly modeling pending parallel trials. How important was each of these contributions to the resulting tuner?

Using *ML Bazaar*, we show how a more thorough *ablation study* (Lipton and Steinhardt, 2019), not present in Snoek et al. (2012), would be conducted to address these questions, by assessing the performance of our general-purpose AutoML system using different combinations of these four contributions. Here we focus on contribution C1. 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, kernel hyperparameters are set by optimizing the marginal likelihood. In this way, we can isolate the contributions of the proposed kernel in the context of general-purpose ML workloads.

In total, 4.31×10^5 pipelines were evaluated to find the best pipelines for a subset of 414 tasks. We find that no improvement comes 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 overperformance 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.

Part III

Looking forward

Chapter 8

Putting the pieces together: collaborative, open-source, and automated data science for the Fragile Families Challenge

8.1 Introduction

The Fragile Families Challenge (Section 2.7) aimed to prompt the development of predictive models for life outcomes from detailed longitudinal data on a set of disadvantaged children and their families. Organizers released anonymized and merged data on a set of 4,242 families with data collected from the birth of the child until age nine. Participants in the challenge were then tasked with predicting six life outcomes of the child or family at age 15: child grade point average, child grit, household eviction, household material hardship, primary caregiver layoff, and primary caregiver participation in job training.

The FFC was run over a four-month period in 2017, and received 160 submissions from social scientists, machine learning practitioners, students, and others. Unfortunately, despite the massive effort to design the challenge and develop predictive models, organizers concluded that "even the best predictions were not very accurate" and that "the best submissions [...] were only somewhat better than the results from a simple benchmark model [...] with four predictor variables selected by a domain expert" (Salganik et al., 2020). Much of this disappointing performance may be due to an inherent unpredictability of outcomes six years into the future. Indeed, it may even be encouraging, in the sense that the measured factors of young children's lives may not predetermine their futures or those of their families.

One limitation of the FFC was that the dataset required extensive *data preparation and feature engineering* in order to be suitable for ML modeling. Overall, 12,942 variables were released in the background data, and 73% of all values were missing (Salganik et al., 2019). Given the nature of the challenge, the small teams that were competing were ill-equipped to handle the data preparation necessary. Participants generally addressed this in one of two ways. First, some teams expended extensive effort on manually preparing the data, often at the expense of experimenting with different modeling techniques. Many such teams duplicated or approximated work done by other teams working independently. Second, many teams used simple automated techniques to arrive at a small set of reasonably clean features. This had the effect of losing out on potentially highly predictive information.

Considering the design and results of the FFC, I ask two questions. First, *what would it take to enable collaboration rather than competition in predictive modelling?* Second, *would new ML development tools and methodologies increase the impact of data science on societal problems?* Rather than working independently, the 160 teams could have pooled their resources to carefully and deliberately prepare the data for analysis in a single data preparation pipeline, while exploring a larger range of manual and automated modeling choices.

In this chapter, we describe a novel collaborative approach to solving the Fragile Families Challenge using the tools of Ballet and ML Bazaar that were presented earlier in this thesis. In our approach, a group of data scientists works closely together to create feature definitions to process the challenge dataset. We embed our shared feature engineering pipeline within an ML pipeline that is tuned automatically. As a result, the human effort involved in our approach is overwhelmingly spent on feature engineering.

8.2 Collaborative modeling

8.2.1 Methods

We created an open-source project using Ballet, *predict-life-outcomes*,[1] to produce a feature engineering pipeline and predictive model for life outcomes.

Dataset

We use the exact dataset used in the FFC, which is archived by Princeton's Office of Population Research. Researchers can request access to the challenge dataset, agreeing to a data access agreement that protects the privacy of the individuals in the FFCWS.

The challenge dataset contains a "background" table of 4,242 rows (one per child in the training set) and 12,942 columns (variables). The "train" split contains 2,121 rows (half of the background set), the "leaderboard" split contains 530 rows, and the "test" split contains 1,591 rows. The background variables represent responses to survey questions asked over five "waves": collected in the hospital at the child's birth, and collected at approximately age one, three, five, and nine of the child. Each wave includes questions asked to different sets of individuals, including the mother, the father, the primary caregiver, the child themselves, a childcare provider, the kindergarten teacher, and the elementary school teacher.

Each split contains the full set of variables plus six prediction targets, which are constructed from survey questions asked during the age 15 survey:

1. *Grit.* Grit is a measure of passion and perseverance of the child on a scale from 1–4. It is constructed from the child's responses to four survey questions, such as whether they agree that they are a hard worker.

[1] `https://github.com/ballet/predict-life-outcomes`

2. *GPA*. Grade point average (GPA) is a measure of academic achievement of the child on a scale from 1.0–4.0, according to the self-reported grades earned by the child in their most recent grading period in four subjects.

3. *Material hardship*. Material hardship is a measure of extreme poverty of the family on a scale from 0–1. It is constructed from answers to 11 survey questions about topics like food insecurity and difficulty paying rent. The number of different ways in which the family experienced hardship are summed and rescaled to the unit interval.

4. *Eviction*. Eviction is an outcome in which a family is forced from their home due to nonpayment of rent or mortgage. This prediction target measures whether the family had been evicted at any point in the six year period between the age nine interview and the age 15 interview.

5. *Layoff*. Layoff is an indicator of whether the family's primary caregiver was laid off from their job at any point in the six year period. Those who had not worked in that time period were coded as missing.

6. *Job training*. Job training is an indicator for whether the primary caregiver had taken any job training in the six year period, such as computer training or literacy classes.

Unlike in many machine learning challenges — but very much like in real-world data science problems — the targets themselves contain many missing values. For the purpose of validating feature contributions to this project with a supervised feature validator, we focus on the *Material Hardship* prediction problem. However, we want our feature definitions to be useful for all six problems.

While Ballet's default ML performance validator uses the SFDS algorithm (Section 3.5.3), in this problem we use a different validator that combines two different feature filtering techniques. The first is a variance threshold filter that ensures that the variance of given feature values is above a threshold. (If the feature is vector-valued, then each feature value must exceed the threshold individually.) The second is a mutual information-based filter that ensures that the mutual information of the feature values with the target is above a threshold. A candidate feature must pass both filters to be accepted.

Collaborators

Collaborators were recruited to join the project from a variety of sources. First, we contacted data scientists who had previously participated in a Ballet project, such as the *predict-census-income* project. Second, we asked additional personal and professional contacts. Third, we reached out to researchers who had competed in the original Fragile Families Challenge in 2017. Importantly, this last set of people had already been granted access to the dataset as part of their original entry and already had strong familiarity with the data.

Collaborators who had not previously worked with the data were asked to apply for data access with Princeton's Office of Population Research. Once access was granted, we generated a unique keypair for each collaborator that would allow collaborators to securely download our copy of the data from secure cloud storage. This copy of the data was identical to the official challenge dataset except that we had split the background table into separate tables corresponding to the train, leaderboard, and test sets. We also restricted access to the leaderboard and test targets. This removed the ability to develop on these held-out datasets and ensured fair comparison with the original competition results.

8.2.2 Feature development

Data scientists collaborating on the project developed features in an iterative process following the workflow described in Section 3.3.2 and Fig. 3.1. After first obtaining access to the data, data scientists were next provided with documentation and tutorial materials describing how to contribute to a Ballet project, how to use Ballet's feature engineering language (Section 3.4), and the background and data details of the FFC. Once they were comfortable with this material, they could browse the set of existing features contributed by their collaborators.

Finally, data scientists were ready to begin developing features. They could choose their own development environment, with Assemblé being a typical choice. They could then step through a notebook-based guide that introduced the use of different API methods to load the dataset, search the metadata repository, discover existing features, and validate a new feature. In this environment, they could write and submit new feature definitions to the shared repository.

Two feature definitions created through this collaboration are shown in Figures 8.1 and 8.2. These features are typical of the features in the project, and show the extensive manipulations required to produce even a single feature definition from such a complex dataset. We can see how:

- The input column names are identified by highly-abbreviated, inscrutable codes that must be interpreted using a codebook or metadata API.
- Categorical input columns have multiple levels, identified by negative numbers that indicate different kinds of missingness.
- Some missing values can be imputed using simple strategies.
- Many columns can be combined together using simple arithmetic operations.
- Many features use complex transformations even if they do not have any learned parameters.
- Detailed metadata, such as a short name, a longer human-readable description, and the exact provenance of the feature values, can be extracted programmatically from the feature definition.

In Sections 4.3.1 and 5.1, we discussed how the theme of *distribution of work* emerged from our analysis of the *predict-census-income* case study. Given the scale of the variable space in the FFC, we propose and implement one solution to the distribution of work problem by introducing the idea of feature development partitions.

```
from ballet import Feature
from ballet.eng import NullFiller
import numpy as np

input = ["cm1hhinc", "cm2hhinc", "cm3hhinc", "cm4hhinc", "cm5hhinc", "m4f3a"]
transformer = [
    ("m4f3a", lambda x: np.where(x < 0, 1, x)),  # impute unanswered with 1
    # average income in all waves
    (
        ["cm1hhinc", "cm2hhinc", "cm3hhinc", "cm4hhinc", "cm5hhinc"],
        lambda df: df.where(df>0, np.nan).mean(axis=1),
        "income",
    ),
    NullFiller(0),
    lambda x: x["income"] / x["m4f3a"],  # ratio
]
name = "HH income ratio"
description = "the ratio of household (HH) income by the number of people in HH
↪  surveyed in wave 4"
feature = Feature(input, transformer, name=name, description=description)
```

Figure 8.1: A feature definition for the *predict-life-outcomes* project that computes the household income ratio (total household income per member of the household) for each family.

A *feature development partition* describes a subset of variables for a data scientist to focus on while developing feature definitions for a project.

In this project, we allow any collaborator to propose a new feature development partition as a ticket (i.e., GitHub Issue) on the shared repository that follows a certain structure. The partition has a name, a specification of the variables that comprise it, and any helpful background about the variables or why this partition is promising for development. While the variable specification can be expressed in any language, including natural language, specifications are usually written in Python for convenience, such that a collaborator working on the partition can get started quickly by running the snippet to access the full variable list in their development environment. Any collaborator, including the one who proposed the partition, can comment on the discussion thread to "claim" the partition, indicating that they are working on it. Multiple data scientists who claim the same partition can communicate with each other directly or follow each other's work. A stylized partition is shown in Figure 8.3.

```
from ballet import Feature
from ballet.eng.external import SimpleImputer

input = ["cf1edu", "cm1edu"]
transformer = [
    lambda df: df.max(axis=1),
    lambda df: df >= 4,
    SimpleImputer(strategy="mean"),
]
name = "college-educated parents"
description = "Whether the father or the mother has a degree of college education
↪  or above in wave 1."
feature = Feature(input, transformer, name=name, description=description)
```

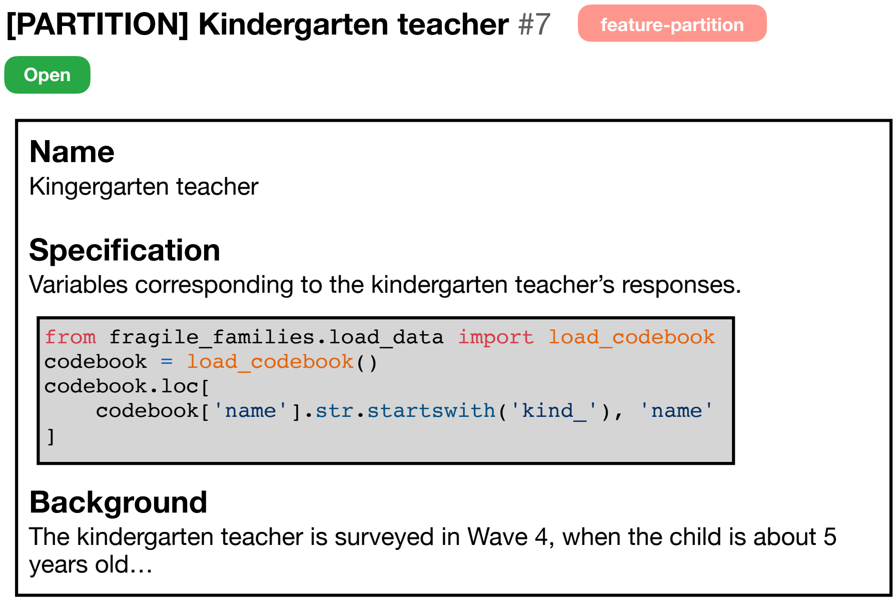
Figure 8.2: A feature definition for the *predict-life-outcomes* project that computes whether either of the parents of the child had a college degree as of the child's birth.

8.2.3 Automated modeling

Our collaboratively developed feature engineering pipeline is embedded within a larger ML pipeline that can be automatically tuned. To do this, we use the ML Bazaar framework in three ways.

First, we create several ML primitives to annotate components in the project. The feature engineering pipeline is annotated in the `ballet.engineer_features` primitives. The target encoder is annotated in the `ballet.encode_target` primitive (which is further modified in the `fragile_families.encode_target` primitive with an argument indicating which prediction target is being considered). Then, the additional primitive `ballet.drop_missing_targets` drops rows with missing targets at runtime, a necessity given missing targets for some families in the FFC data. We pair these primitives with existing primitives from the `MLPrimitives` catalog that define additional preprocessing steps and estimators, such as `sklearn.linear_model.ElasticNet` and `xgboost.XGBRegressor`.

Second, we create multiple pipeline templates (Section 6.3.1) that connect the feature engineering pipeline with different estimators. The pipeline templates are shown in Table 8.1. In this case, we also encode the prediction target (i.e. select a single target at a time from the set of six life outcomes) and drop rows in which the target value is missing. For classification targets, we design pipelines that output



[PARTITION] Kindergarten teacher #7

Name

Kingergarten teacher

Specification

Variables corresponding to the kindergarten teacher's responses.

```
from fragile_families.load_data import load_codebook
codebook = load_codebook()
codebook.loc[
    codebook['name'].str.startswith('kind_'), 'name'
]
```

Background

The kindergarten teacher is surveyed in Wave 4, when the child is about 5 years old...

Figure 8.3: A stylized feature development partition for the *predict-life-outcomes* project. This partition proposes focusing effort on the subset of variables that represent responses by the kindergarten teacher of the child in Wave 4 (when they were five years old). The specification of the partition is a code snippet that outputs the exact variable names.

the predicted probability of the positive class (rather than the most likely class, see Section 8.2.4).

Third, we use the AutoBazaar search algorithm (Algorithm 3) to automatically select from among the pipeline templates and tune hyperparameters in a given ML pipeline. Recall that AutoBazaar uses the BTB library (Section 6.4.1) for its search, and here we use BTB's `UCB1` selector, which uses the upper-confidence bound bandit algorithm, and `GCP-MAX` tuner, which uses a Gaussian copula process meta-model and a predicted score acquisition function.

We ran the AutoML search procedure over our set of pipeline templates for 500 iterations for each of the six targets. We selected the ML pipeline that performed the best on the held-out leaderboard set. We then used the test set to evaluate the best-performing pipeline for each prediction target and pipeline template pair.

Name	Reg	Clf	Pipeline Template
ballet-elasticnet	✓	✓	ballet.engineer_features fragile_families.encode_target ballet.drop_missing_targets sklearn.linear_model.ElasticNet
ballet-randomforest	✓		ballet.engineer_features fragile_families.encode_target ballet.drop_missing_targets sklearn.ensemble.RandomForestRegressor
ballet-randomforest-proba		✓	ballet.engineer_features fragile_families.encode_target ballet.drop_missing_targets sklearn.ensemble.RandomForestClassifier fragile_families.squeeze_predicted_probabilities
ballet-knn	✓		ballet.engineer_features fragile_families.encode_target ballet.drop_missing_targets sklearn.neighbors.KNeighborsRegressor
ballet-knn-proba		✓	ballet.engineer_features fragile_families.encode_target ballet.drop_missing_targets sklearn.neighbors.KNeighborsClassifier fragile_families.squeeze_predicted_probabilities
ballet-xgboost	✓		ballet.engineer_features fragile_families.encode_target ballet.drop_missing_targets xgb.XGBRegressor
ballet-xgboost-proba		✓	ballet.engineer_features fragile_families.encode_target ballet.drop_missing_targets xgb.XGBClassifier fragile_families.squeeze_predicted_probabilities

Table 8.1: Pipeline templates used for automated modeling in the *predict-life-outcomes* project for either regression (Reg) or classification (Clf) targets targets. The difference between regression and classification pipelines is that the classification pipelines predict the probability of each class and then “squeeze” the predictions to emit the probability of the positive class only.

8.2.4 Metrics

We primarily evaluate the predictive performance of our collaborative model against the performance obtained by entrants to the original FFC in 2017. For comparison purposes, we use the same metrics defined by the challenge organizers, mean squared error (MSE) and R^2_{Holdout}. The R^2_{Holdout} metric is a scaled version of the mean squared error that accounts for baseline performance:

$$R^2_{\text{Holdout}} = 1 - \frac{\sum_{i \in \text{Holdout}} (y_i - \hat{y}_i)^2}{\sum_{i \in \text{Holdout}} (y_i - \bar{y}_{\text{Train}})^2} \tag{8.1}$$

A score of 1 indicates a perfect prediction. A score of 0 means that the prediction is only as good as predicting the mean of the training set, and scores can be arbitrarily negative indicating worse performance.

Given a predictive probability distribution over outcomes, this metric is optimized by predicting the mean of the distribution. Thus, in binary classification problems (*Eviction*, *Job Training*, *Layoff*), the best performing models according to this evaluation metric should emit the predicted probability of the outcome rather than the class label. This motivates our choice of pipeline templates for classification problems, in which we choose final estimators that emit the predicted probability according to the learned classifier (using the `predict_proba` method).

8.3 Results

We now report the preliminary results from our collaborative modeling efforts.[2] These results represent 42 days of collaborative feature development. As of the time of writing, there were 16 data scientists collaborating on the project from 7 different institutions.

[2] These results are current as of commit `f50b2db`.

8.3.1 Feature definitions

At the time of this writing, 28 features have been accepted to the project, committed by 9 different collaborators.

Table 8.2 shows the top features ranked by estimated mutual information of the feature values with the material hardship target. Top features consume from 2–30 input columns and all produce scalar-valued features (though other features produce vector-valued features). Estimated conditional mutual information (CMI) is low after conditioning on all other feature values, indicating that no one feature is much more important than the others and that all features are somewhat correlated with each other.

	Inputs	Dimensionality	MI	CMI
name				
Income per adult ratio	20	1	1.271	0.000
HH income ratio	6	1	0.946	0.000
father_buy_stab_in_mothers_view	25	1	0.749	0.000
father_buy_stab	24	1	0.387	0.000
f5_buy_diff	18	1	0.216	0.000
t5_social	30	1	0.201	0.000
f1iwc	16	1	0.173	0.000
f2_buy_diff	12	1	0.160	0.000
normalized student-teacher ratio	2	1	0.159	0.000
f4_buy_diff	10	1	0.115	0.000

Table 8.2: The top features in the *predict-life-outcomes* feature engineering pipeline, ranked by estimated mutual information (MI) of the feature values with the material hardship target.

A fundamental difficulty in the FFC is the large number of input variables. To what extent is the collaboration able to process these variables? In Figure 8.5, we show the coverage of the variable space over time, i.e., the fraction of overall variables that are used as input to at least one feature definition. As the collaboration progresses, more input variables are used, with the distribution of input variables per feature shown in Figure 8.4.

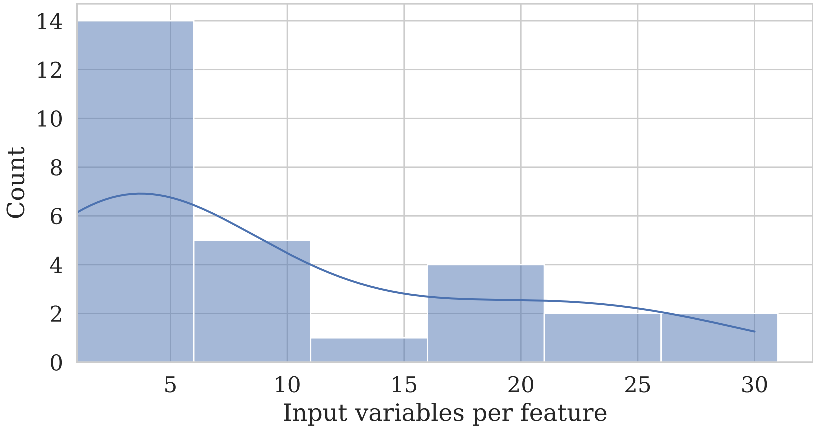


Figure 8.4: Distribution of input variables per feature with kernel density estimate.

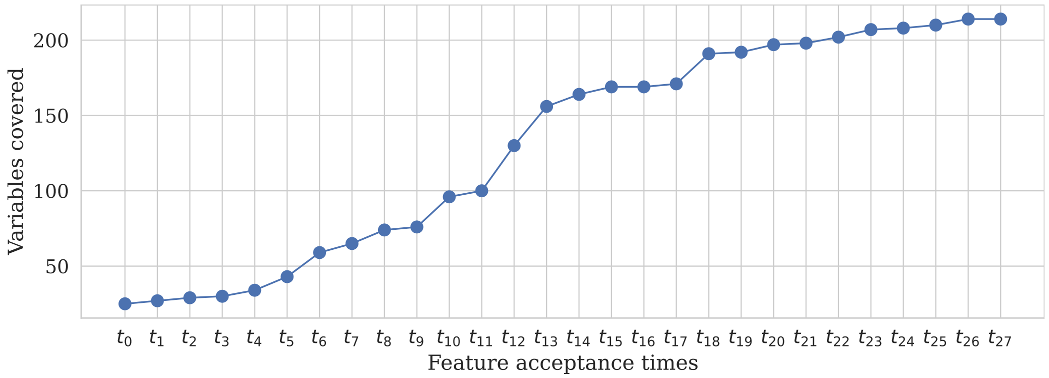


Figure 8.5: Variable coverage over time in the *predict-life-outcomes* project. As new features arrive, they increase coverage of the variable space by using as their input variables that had not previously been transformed.

8.3.2 Predictive performance

We report our predictive performance on all six prediction targets, with a focus on material hardship in some cases as this was the target on which FFC entrants performed the best and which we used for feature validation.

For the material hardship target, we show the best pipeline from each pipeline template searched during automated modeling in Table 8.3, and compare it against two baseline methods. The best-performing model in terms of test R^2_{Holdout} is the ballet feature engineering pipeline with a tuned gradient-boosted decision trees (XGB) regressor. The `train-mean` model simply predicts the mean of the train set, and scores $R^2_{\text{Holdout}} = 0.0$ by definition. The `test-mean` model "cheats" by predicting the mean of the test set, but since the sets are split using systematic sampling

(Salganik et al., 2019, Page 5), the target means are almost equal, and this model does not perform any better.

pipeline	metric	train	leaderboard	test
train-mean	R^2_{Holdout}	0.000	0.000	0.000
	MSE	0.024	0.029	0.025
test-mean	R^2_{Holdout}	0.000	0.000	0.000
	MSE	0.024	0.029	0.025
ballet-elasticnet	R^2_{Holdout}	0.087	0.051	0.085
	MSE	0.022	0.027	0.023
ballet-xgboost	R^2_{Holdout}	0.178	0.079	0.034
	MSE	0.020	0.027	0.024
ballet-knn	R^2_{Holdout}	0.061	0.050	0.060
	MSE	0.023	0.027	0.023
ballet-randomforest	R^2_{Holdout}	0.070	0.043	0.066
	MSE	0.023	0.028	0.023

Table 8.3: Performance of ML pipelines in the *predict-life-outcomes* project in predicting *Material Hardship*, in terms of mean squared error and normalized R^2.

We compare the best pipeline found in our automated modeling for each target against the models produced by FFC entrants in Table 8.4. Out of the 161 FFC entrants, the best Ballet pipeline beats over two thirds of entrants in all cases, and performs best in classification problems such as *Layoff* (96th percentile).

Target	Pipeline	R^2_{Holdout}	Wins	Percentile
Material Hardship	ballet-elasticnet	0.085	110	68.3
GPA	ballet-xgboost	0.140	122	75.8
Grit	ballet-elasticnet	0.017	124	77.0
Eviction	ballet-elasticnet	0.012	125	77.6
Layoff	ballet-elasticnet	0.021	154	95.7
Job Training	ballet-knn-proba	0.007	122	75.8

Table 8.4: Performance of the best ML pipelines in the *predict-life-outcomes* project for each target, compared to FFC entrants. *Wins* is the number of FFC entrants that the pipeline outperforms, and *Percentile* is the percent of FFC entrants that the pipeline outperforms.

One particular struggle of FFC entrants was avoiding overfitting their models to the training dataset, which partly reflects the small number of training observations. In fact, Salganik et al. (2019, Figure 7) report that there was only “modest” correlation between performance on the training set and performance on the held-out test set, ranging from -0.12 to 0.44 depending on the prediction target. We reproduce this analysis and add the generalization performance of our own ML pipelines in Figure 8.6. Our ML pipelines do not exhibit overfitting, likely for two reasons. First, the structure imposed by Ballet’s feature engineering language (Section 3.4) means that features can only be created using the development (train) set, and learn parameters from the development set only, such that no information can leak from the held-out sets. Second, due to the automated modeling facilitated by ML Bazaar, we evaluate candidate learning algorithms and hyperparameter configurations by their performance on a split that was not used for training. This leads to better estimates of generalization error, and correspondingly better performance on the unseen test set.

8.4 Discussion

In the *predict-life-outcomes* project, we set out to assess whether data scientists can fruitfully collaborate on a machine learning challenge at the scale of the FFC, and what sort of performance results from such a collaboration. In our preliminary analysis, the results are promising.

8.4.1 Private data, open-source model

In contrast to other Ballet projects like *predict-census-income*, the dataset used in *predict-life-outcomes* is private and restricted to researchers approved by the data owners. As a result, new collaborators had to onboard for one week or longer before they could begin feature development. One appeal of open-source software development is the low barrier to entry for contributing even the smallest of patches. The lengthy onboarding process of the FFC presents a high barrier to entry and may dissuade potential collaborators from joining.

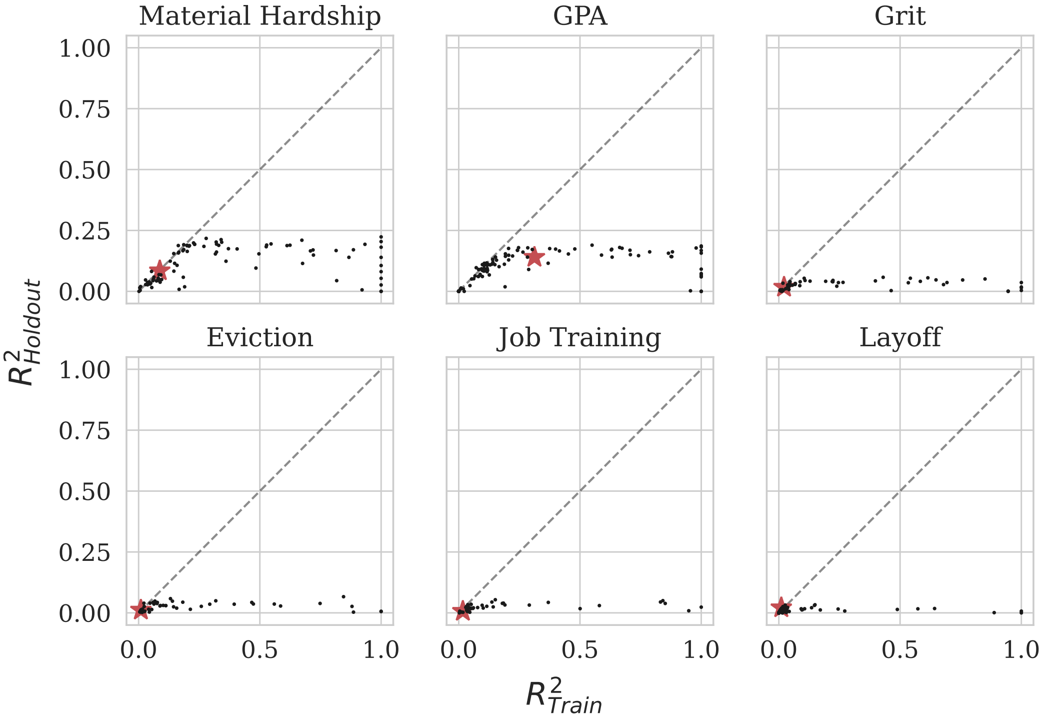


Figure 8.6: Generalization to the test set of collaborative *predict-life-outcomes* model in terms of R^2 (red stars), compared to generalization of the entrants to Fragile Families Challenge who scored above 0 (black dots). We show the relationship between R^2_{Train} and R^2_{Holdout} (on the test set). A model that generalizes perfectly would lie on the dashed 45-degree line. For the *Grit*, *Eviction*, *Job Training*, and *Layoff* targets, even the FFC winning models barely outperformed predictions of the train mean.

As considered in Section 5.4, one solution here is to generate synthetic data following the schema of the Fragile Families dataset that does not represent nor violate the privacy of any FFCWS respondents. New *predict-life-outcomes* collaborators could begin developing features immediately from the synthetic data, though the features would be validated in continuous integration using the real data. If a collaborator was inspired to fully join the project, they could then apply for the private data access.

8.4.2 Collaborative modeling without redundancy

Collaborators have been successful in submitting feature definitions to the shared project without redundancy. Most input variables are used only once, with variables being used at most twice. At one point, there were 131 variables used without any redundancy.

There are at least three possible explanations for this success. The first is that the functionalities provided by Ballet for work distribution have been successful in avoiding redundant work — namely the feature discovery and querying functionality, the feature development partitions, the visibility of existing features due to the open-source development setting, and the use of synchronous discussion rooms. The second is that the input variables are not completely "independent," but rather that a group of variables may represent the responses to one set of related questions and are likely to be used as a group by a data scientist developing features.

The third is that the lack of redundancy so far has been due to pure luck. For example, fixing the number of input variables of each existing feature, if each input variable set were chosen completely at random from the available variables, the probability of observing no duplicates among input variables is given by

$$p = \frac{n!}{(n - \sum_i \pi_i)!} \left(\prod_i \frac{n!}{(n - \pi_i)!} \right)^{-1} \tag{8.2}$$

where π_i is the number of input variables to feature i, and n is the number of variables available. The left term in the product represents the number of ways to choose the input variables with no duplicates and the right term represents the total number of ways to choose the input variables given their group structure. This is a lower bound on the probability of observing any overlap if all of the input variables were chosen with replacement one at a time, rather than in groups, because it is not possible for the variables within a single group to be duplicated.

In our preliminary analysis on the first 131 variables used, we find that $p \approx .56$; that is, the probability that there would be no duplicates if the input variable groups were chosen at random is 56%. With the full 220 variables, p falls to 21%.

To investigate this further, we compute the probability of observing no duplicates among input variables as new features arrive and consume more input variables. We estimate a kernel density of the number of variables used per feature from the existing features in the repository. We then simulate a sequence of features using those numbers of variables up to a fixed total number of variables. In Figure 8.7, we

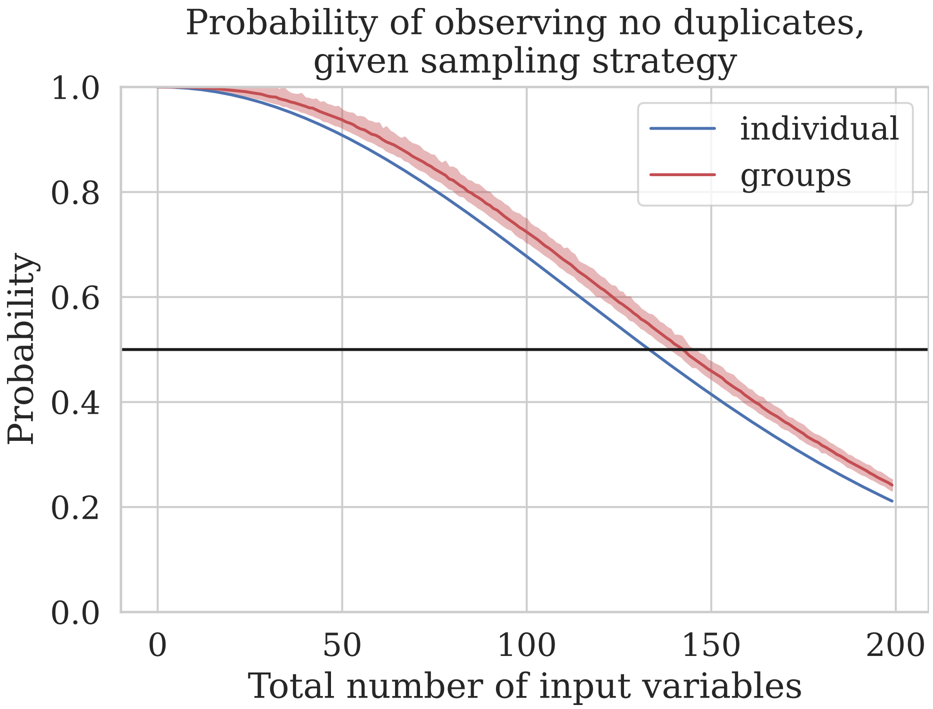


Figure 8.7: The probability of observing no duplicate input variables, given a fixed total number of input variables across features, according to Equation (8.2). The individual sampling strategy occurs if there are m features each with one input variable. The group sampling strategy occurs if there are k features with $\pi_1, \ldots, \pi_k$ input variables and $\sum_i \pi_i = m$. We simulate feature sets of this sort and show the mean and 95% interval of the computed probability over the feature sets.

compare the probability of no duplicates for this simulated data as well as a baseline of all features that consume exactly one variable. At about 140 total inputs, the probability of observing no duplicates crosses below 50%.

This all goes to show the unique challenges of scaling the distribution of work of feature development when there are on the order of tens of thousands of variables, as is the case in the FFC. Very quickly (about 1% of all variables being used), collaborators may begin to do redundant work without additional support.

Redundant features (in the statistical sense) are definitely harmful to predictive performance, but duplicate input variables are not necessarily bad. One variable might be used to construct two or more complex features that are each useful. However, given the scale of the FFC data, human effort should focus on untapped regions of the variable space.

8.4.3 Modeling performance is competitive

We describe several highlights of the modeling performance achieved by the collaborative project, including the ability for automated modeling to improve on untuned ML pipelines and the lack of overfitting. However, our performance in this preliminary analysis ranges from the 68th percentile to the 96th percentile of FFC entrants. While a strong start, this result does not yet improve upon modeling outcomes from the FFC, which were mediocre at best. As our collaborative project matures, we expect our performance to improve further. The 220 variables used so far as feature inputs represent only 1.7% of all available variables in the data, and many variables that are expected to yield useful information about the targets have not yet been processed by collaborators.

8.4.4 Models and features are interpretable

One immediate and "free" advantage from collaborative and structured development with Ballet is an interpretable model, or at least, interpretable features. Interpretability is critical for a context as sensitive as the FFC. For example, one of the pipelines we automatically tuned is an elastic net pipeline. For the prediction target of predicting a child's GPA six years into the future, we can look at the impact on the predicted outcome from changing a feature value by 1 standard deviation (Figure 8.8).

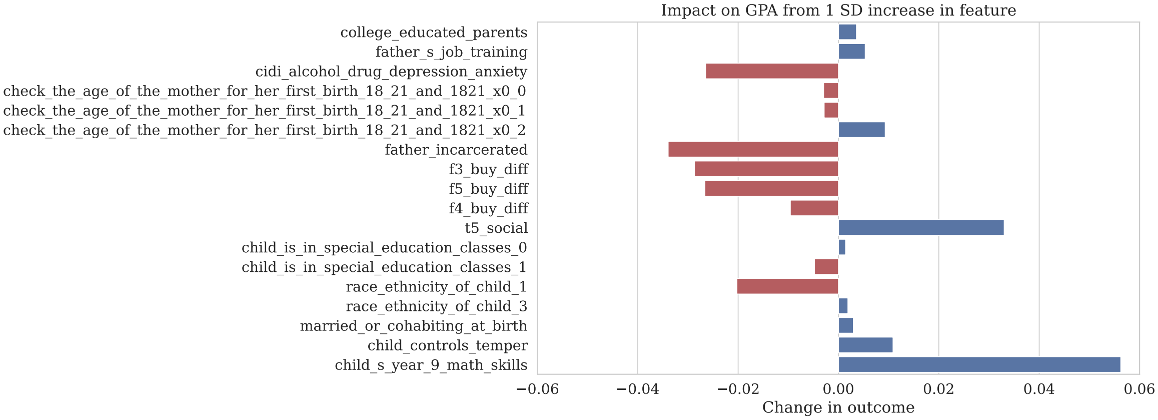


Figure 8.8: Feature importance in predicting GPA using the best performing elastic net model. Feature value names are either given by collaborators in the optional feature definition metadata fields, or are inferred automatically by Ballet.

We find that there is a natural interpretability to the feature importance analysis. For example, the feature `father_incarcerated` (whether the child's father was ever incarcerated) has a large negative impact on GPA. This is reasonable as research widely finds that incarceration has a profound negative impact not only on those who are incarcerated but also their families and loved ones. Meanwhile, the feature `child_s_year_9_math_skills` (teacher's assessment of child's math skills in year 9 compared to other students in the same grade) has a large positive impact on GPA. This too makes sense as math is one of the four subjects measured in the age 15 GPA prediction target.

Chapter 9

Future directions

9.1 Beyond feature engineering

To any reader who has made it this far, it will be quite apparent that much of the focus of this thesis has been on feature engineering, as a prominent example of collaborative workflows that can be used to create data science pipelines. Throughout the thesis, we have seen demonstrations of the importance of features in real-world data science applications, and the difficulties involved in properly specifying features and engineering those that will be the most useful for a given machine learning task.

But features are just one small part of machine learning and data science. In many applications, such as image, video, audio, and signal processing, modern deep neural networks learn a feature representation of unstructured input as part of the training process. In these applications, where handcrafted features are of little use, collaboration is still very important.

In Chapter 3, we contended that our conceptual framework can be applied to many steps in the data science process, but that we focus on feature engineering as an important manifestation of that process. In this section, we consider the application of Ballet's conceptual framework to another import step, data labeling.

While many machine learning researchers assume that supervised learning programs already contain both features and associated labels, in practice data scientists often must apply labels to observations. Sometimes this is trivial, such as obtaining the selling price of a house from public records and linking it to the house details, but sometimes human experts or crowd workers must manually label each observation.

Somewhere in the middle of this spectrum is a new approach to data labeling called *data programming* (Ratner et al., 2016), in which analysts create heuristics to automatically apply labels to subsets of the observations. Functions can apply these heuristics to the entire dataset, such that one observation may have multiple, possibly conflicting labels. A statistical model is learned that tries to recover the "true" label of an observation given the patterns of agreement and disagreement among labels. The resulting labels are *probabilistic*, leading to a paradigm called *weakly-supervised learning.*

Following Section 3.2, our goal is to define the three concepts of *data science patches*, *data science products*, and *software and statistical acceptance procedures.*

In the context of data programming, the data science patch is an individual labeling function. In the Snorkel framework (Ratner et al., 2017), a Python function can be annotated with a decorator to create a labeling function with just a few lines of code.

The data science product in this context is a labeling pipeline that can take batches of unlabeled observations and produce probabilistic labels.

The software and statistical acceptance procedures in this context are to (1) validate that the function satisfies the labeling function interface (2) validate that the function applies labels to unseen observations and (3) compare the performance of the labeling pipeline with and without the proposed labeling function on a set of held-out, gold-standard labels obtained manually or from another source.

9.2 Potential impact

What are the biggest challenges facing humans right now? According to the United Nation's Sustainable Development Goals, the top three goals are eliminating poverty, eliminating hunger, and promoting good health and well-being. These goals are just as pressing in the United States as they are in developing countries. To what extent are successes in machine learning aligned with these national and global priorities?

The most visible successes of academic machine learning concern playing games, detecting objects in images, or translating text. The progress that has been made in these areas is remarkable and reflects technical breakthroughs and enormous computational power.

We can see some areas in which machine learning successes are contributing toward development goals:

- Advances in computer vision and image recognition are leading to smart farming equipment that could improve output while reducing reliance on pesticides.
- Machine learning on satellite images can lead to detailed, real-time maps of soil and crop conditions for smallholder farmers.
- Machine learning on electronic health records, medical imaging, and genomes can lead to better and more personalized medical treatments.

While these directions are laudable, most of the current machine learning research only helps the richest producers or consumers in the world's developed countries. Even within the United States, many observers think that the current direction of machine learning progress is likely to perpetuate inequalities in what is largely a winner-take-all system, rather than lifting the living standards and well-being of the less well-off.

Meanwhile, there is an urgent need for machine learning and artificial intelligence technologies that can supplement policy efforts and activism in addressing the most critical problems like poverty, hunger, and health. As described in this thesis, survey data is an important data modality that is widely used in better understanding and intervening in situations affecting humans.

The research introduced in this thesis, including Ballet and ML Bazaar, serves to improve the ability of data scientists and machine learning researchers to use survey data in prediction policy problems. However, much work remains in creating better developer tools and statistical methods for processing such data.

The following are important future directions for machine learning on survey data:

- Building better tools for automatically detecting and processing survey metadata. This includes detecting column data types, column relationships (i.e., responses to multiple choice questions coded across several columns), and making inferences about columns through processing question descriptions and labels.

- Developing algorithms for detecting and imputing missing values due to the complex skip patterns in survey responses.

Chapter 10

Conclusion

This thesis describes our research in collaborative, open, and automated data science, and our contributions in designing and implementing frameworks for data scientists to use and better understand collaborations in practice. As machine learning and data science continue to grow in influence, the ability of data scientists and other stakeholders with varying experience, skills, roles, and responsibilities to work together on impactful projects will be increasingly important. I expect that continued research in this area will enhance the ability of close-knit data science teams and wide-ranging open collaborations alike to deliver models and analyses.

Bibliography

Martín Abadi, Ashish Agarwal, Paul Barham, Eugene Brevdo, Zhifeng Chen, Craig Citro, Greg S. Corrado, Andy Davis, Jeffrey Dean, Matthieu Devin, Sanjay Ghemawat, Ian Goodfellow, Andrew Harp, Geoffrey Irving, Michael Isard, Yangqing Jia, Rafal Jozefowicz, Lukasz Kaiser, Manjunath Kudlur, Josh Levenberg, Dandelion Mané, Rajat Monga, Sherry Moore, Derek Murray, Chris Olah, Mike Schuster, Jonathon Shlens, Benoit Steiner, Ilya Sutskever, Kunal Talwar, Paul Tucker, Vincent Vanhoucke, Vijay Vasudevan, Fernanda Viégas, Oriol Vinyals, Pete Warden, Martin Wattenberg, Martin Wicke, Yuan Yu, and Xiaoqiang Zheng. TensorFlow: Large-scale machine learning on heterogeneous systems, 2015. URL `https://www.tensorflow.org/`. Software available from tensorflow.org.

John M. Abowd, Gary L. Benedetto, Simson L. Garfinkel, Scot A. Dahl, Aref N. Dajani, Matthew Graham, Michael B. Hawes, Vishesh Karwa, Daniel Kifer, Hang Kim, Philip Leclerc, Ashwin Machanavajjhala, Jerome P. Reiter, Rolando Rodriguez, Ian M. Schmutte, William N. Sexton, Phyllis E. Singer, and Lars Vilhuber. The modernization of statistical disclosure limitation at the U.S. Census Bureau. Working Paper, U.S. Census Bureau, August 2020.

Sarah Alnegheimish, Najat Alrashed, Faisal Aleissa, Shahad Althobaiti, Dongyu Liu, Mansour Alsaleh, and Kalyan Veeramachaneni. Cardea: An Open Automated Machine Learning Framework for Electronic Health Records. In *2020 IEEE 7th International Conference on Data Science and Advanced Analytics (DSAA)*, pages 536–545, October 2020. doi: 10.1109/DSAA49011.2020.00068.

American Community Survey Office. American community survey 2018 ACS 1-year PUMS files readme. `https://www2.census.gov/programs-surveys/acs/tech_docs/pums/ACS2018_PUMS_README.pdf`, November 2019. Accessed 2021-08-21.

Michael Anderson, Dolan Antenucci, Victor Bittorf, Matthew Burgess, Michael Cafarella, Arun Kumar, Feng Niu, Yongjoo Park, Christopher Ré, and Ce Zhang. Brainwash: A Data System for Feature Engineering. In *6th Biennial Conference on Innovative Data Systems Research*, pages 1–4, 2013.

Peter Auer, Nicolò Cesa-Bianchi, and Paul Fischer. Finite-time Analysis of the Multiarmed Bandit Problem. *Machine Learning*, 47(2):235–256, May 2002. ISSN 1573-0565. doi: 10.1023/A:1013689704352.

Peter Bailis. Humans, not machines, are the main bottleneck in modern analytics. `https://sisudata.com/blog/humans-not-machines-are-the-bottleneck-in-modern-analytics`, December 2020.

Adam Baldwin. Details about the event-stream incident — the npm blog. `https://blog.npmjs.org/post/180565383195/details-about-the-event-stream-incident`, 2018. Accessed 2018-11-30.

Flore Barcellini, Françoise Détienne, and Jean-Marie Burkhardt. A situated approach of roles and participation in open source software communities. *Human–Computer Interaction*, 29(3):205–255, 2014.

Guillaume Baudart, Martin Hirzel, Kiran Kate, Parikshit Ram, and Avraham Shinnar. Lale: Consistent Automated Machine Learning. *arXiv:2007.01977 [cs]*, July 2020.

Denis Baylor, Eric Breck, Heng-Tze Cheng, Noah Fiedel, Chuan Yu Foo, Zakaria Haque, Salem Haykal, Mustafa Ispir, Vihan Jain, Levent Koc, Chiu Yuen Koo, Lukasz Lew, Clemens Mewald, Akshay Naresh Modi, Neoklis Polyzotis, Sukriti Ramesh, Sudip Roy, Steven Euijong Whang, Martin Wicke, Jarek Wilkiewicz, Xin Zhang, and Martin Zinkevich. TFX: A TensorFlow-Based Production-Scale Machine Learning Platform. In *Proceedings of the 23rd ACM SIGKDD International Conference on Knowledge Discovery and Data Mining*, KDD '17, pages 1387–1395, New York, NY, USA, 2017. ACM. ISBN 978-1-4503-4887-4. doi: 10.1145/3097983.3098021.

Emily M. Bender, Timnit Gebru, Angelina McMillan-Major, and Shmargaret Shmitchell. On the dangers of stochastic parrots: Can language models be too big? In *Proceedings of the 2021 ACM Conference on Fairness, Accountability, and Transparency*, FAccT '21, pages 610–623, New York, NY, USA, 2021. Association for Computing Machinery. ISBN 9781450383097. doi: 10.1145/3442188.3445922.

James Bennett and Stan Lanning. The Netflix prize. In *Proceedings of KDD Cup and Workshop 2007*, pages 1–4, 2007.

Evangelia Berdou. *Organization in open source communities: At the crossroads of the gift and market economies.* Routledge, 2010.

James Bergstra and Yoshua Bengio. Random Search for Hyper-Parameter Optimization. *Journal of Machine Learning Research*, 13:281–305, 2012. ISSN 1532-4435. doi: 10.1162/153244303322533223.

James Bergstra, Rémi Bardenet, Yoshua Bengio, and Balázs Kégl. Algorithms for hyper-parameter optimization. In *Proceedings of the 24th International Conference on Neural Information Processing Systems*, NIPS'11, pages 2546–2554, Red Hook, NY, USA, December 2011. Curran Associates Inc. ISBN 978-1-61839-599-3.

Anant Bhardwaj, Amol Deshpande, Aaron J. Elmore, David Karger, Sam Madden, Aditya Parameswaran, Harihar Subramanyam, Eugene Wu, and Rebecca Zhang. Collaborative data analytics with DataHub. *Proceedings of the VLDB Endowment*, 8(12):1916–1919, August 2015. ISSN 21508097. doi: 10.14778/2824032.2824100.

Steven Bird, Ewan Klein, and Edward Loper. *Natural language processing with Python: analyzing text with the natural language toolkit.* O'Reilly Media, Inc., 2009.

Bernd Bischl, Giuseppe Casalicchio, Matthias Feurer, Frank Hutter, Michel Lang, Rafael G. Mantovani, Jan N. van Rijn, and Joaquin Vanschoren. OpenML Benchmarking Suites. *arXiv:1708.03731 [cs, stat]*, September 2019.

Matthias Boehm, Michael Dusenberry, Deron Eriksson, Alexandre V. Evfimievski, Faraz Makari Manshadi, Niketan Pansare, Berthold Reinwald, Frederick R. Reiss, Prithviraj Sen, Arvind C. Surve, and Shirish Tatikonda. SystemML: Declarative Machine Learning on Spark. *Proceedings of the VLDB Endowment*, 9(13):1425–1436, 2016. ISSN 21508097. doi: 10.14778/3007263.3007279.

Andreas Böhm. Theoretical coding: Text analysis in. *A companion to qualitative research*, 1, 2004.

Tolga Bolukbasi, Kai-Wei Chang, James Y. Zou, Venkatesh Saligrama, and A. Kalai. Man is to computer programmer as woman is to homemaker? debiasing word embeddings. In *NIPS*, 2016.

Nathan Bos, Ann Zimmerman, Judith Olson, Jude Yew, Jason Yerkie, Erik Dahl, and Gary Olson. From shared databases to communities of practice: A taxonomy of collaboratories. *Journal of Computer-Mediated Communication*, 12(2):318–338, 2007.

G. Bradski. The OpenCV Library. *Dr. Dobb's Journal of Software Tools*, 2000.

Eric Breck, Neoklis Polyzotis, Sudip Roy, Steven Euijong Whang, and Martin Zinkevich. Data Validation for Machine Learning. In *Proceedings of the 2nd SysML Conference*, pages 1–14, 2019.

Leo Breiman. Statistical Modeling: The Two Cultures. *Statistical Science*, 16(3): 199–231, 2001. ISSN 08834237. doi: 10.2307/2676681.

Frederick P. Brooks Jr. *The mythical man-month: essays on software engineering.* Pearson Education, 1995.

Eli Brumbaugh, Atul Kale, Alfredo Luque, Bahador Nooraei, John Park, Krishna Puttaswamy, Kyle Schiller, Evgeny Shapiro, Conglei Shi, Aaron Siegel, Nikhil Simha, Mani Bhushan, Marie Sbrocca, Shi-Jing Yao, Patrick Yoon, Varant Zanoyan, Xiao-Han T. Zeng, Qiang Zhu, Andrew Cheong, Michelle Gu-Qian Du, Jeff Feng, Nick Handel, Andrew Hoh, Jack Hone, and Brad Hunter. Bighead: A Framework-Agnostic, End-to-End Machine Learning Platform. In *2019 IEEE International*

Conference on Data Science and Advanced Analytics (DSAA), pages 551–560, Washington, DC, USA, October 2019. IEEE. ISBN 978-1-72814-493-1. doi: 10.1109/DSAA.2019.00070.

Lars Buitinck, Gilles Louppe, Mathieu Blondel, Fabian Pedregosa, Andreas Mueller, Olivier Grisel, Vlad Niculae, Peter Prettenhofer, Alexandre Gramfort, Jaques Grobler, Robert Layton, Jake VanderPlas, Arnaud Joly, Brian Holt, and Gaël Varoquaux. API design for machine learning software: experiences from the scikit-learn project. In *ECML PKDD Workshop: Languages for Data Mining and Machine Learning*, pages 108–122, 2013.

José P. Cambronero, Jürgen Cito, and Martin C. Rinard. AMS: Generating AutoML search spaces from weak specifications. In *Proceedings of the 28th ACM Joint Meeting on European Software Engineering Conference and Symposium on the Foundations of Software Engineering*, pages 763–774, Virtual Event USA, November 2020. ACM. ISBN 978-1-4503-7043-1. doi: 10.1145/3368089.3409700.

Souti Chattopadhyay, Ishita Prasad, Austin Z. Henley, Anita Sarma, and Titus Barik. What's wrong with computational notebooks? pain points, needs, and design opportunities. In *Proceedings of the 2020 CHI Conference on Human Factors in Computing Systems*, pages 1–12. ACM, Apr 2020. ISBN 978-1-4503-6708-0. doi: 10.1145/3313831.3376729.

Vincent Chen, Sen Wu, Alexander J. Ratner, Jen Weng, and Christopher Ré. Slice-based learning: A programming model for residual learning in critical data slices. In *33rd Conference on Neural Information Processing Systems*, pages 1–11, 2019.

Justin Cheng and Michael S. Bernstein. Flock: Hybrid Crowd-Machine Learning Classifiers. *Proceedings of the 18th ACM Conference on Computer Supported Cooperative Work & Social Computing - CSCW '15*, pages 600–611, 2015.

Joohee Choi and Yla Tausczik. Characteristics of Collaboration in the Emerging Practice of Open Data Analysis. In *Proceedings of the 2017 ACM Conference on Computer Supported Cooperative Work and Social Computing - CSCW '17*, pages 835–846, Portland, Oregon, USA, 2017. ACM Press. ISBN 978-1-4503-4335-0. doi: 10.1145/2998181.2998265.

Alexandra Chouldechova, Emily Putnam-Hornstein, Suzanne Dworak-Peck, Diana Benavides-Prado, Oleksandr Fialko, Rhema Vaithianathan, Sorelle A. Friedler, and Christo Wilson. A case study of algorithm-assisted decision making in child maltreatment hotline screening decisions. In *Proceedings of Machine Learning Research*, volume 81, pages 1–15, 2018.

Maximilian Christ, Nils Braun, Julius Neuffer, and Andreas W. Kempa-Liehr. Time series feature extraction on basis of scalable hypothesis tests (tsfresh–a python package). *Neurocomputing*, 307:72–77, 2018.

Drew Conway. The Data Science Venn Diagram. `http://drewconway.com/zia/2013/3/26/the-data-science-venn-diagram`, March 2013.

Carl Cook, Warwick Irwin, and Neville Churcher. A user evaluation of synchronous collaborative software engineering tools. In *12th Asia-Pacific Software Engineering Conference (APSEC'05)*, pages 1–6, December 2005. doi: 10.1109/APSEC.2005.22.

Daniel Crankshaw, Peter Bailis, Joseph E. Gonzalez, Haoyuan Li, Zhao Zhang, Michael J. Franklin, Ali Ghodsi, and Michael I. Jordan. The Missing Piece in Complex Analytics: Low Latency, Scalable Model Management and Serving with Velox. In *7th Biennial Conference on Innovative Data Systems Research (CIDR '15)*, Asilomar, California, USA, 2015.

Andrew Crotty, Alex Galakatos, Emanuel Zgraggen, Carsten Binnig, and Tim Kraska. Vizdom: Interactive analytics through pen and touch. *Proceedings of the VLDB Endowment*, 8(12):2024–2027, August 2015. ISSN 21508097. doi: 10.14778/2824032.2824127.

Kevin Crowston, Jeff S. Saltz, Amira Rezgui, Yatish Hegde, and Sangseok You. Socio-technical Affordances for Stigmergic Coordination Implemented in MIDST, a Tool for Data-Science Teams. *Proceedings of the ACM on Human-Computer Interaction*, 3(CSCW):1–25, November 2019. ISSN 2573-0142, 2573-0142. doi: 10.1145/3359219.

Dean De Cock. Ames, iowa: Alternative to the boston housing data as an end of semester regression project. *Journal of Statistics Education*, 19(3), 2011.

Alexandre Decan, Tom Mens, and Maelick Claes. On the topology of package dependency networks: A comparison of three programming language ecosystems. In *Proccedings of the 10th European Conference on Software Architecture Workshops*, ECSAW '16, pages 21:1–21:4, New York, NY, USA, 2016. ACM.

Dong Deng, Raul Castro Fernandez, Ziawasch Abedjan, Sibo Wang, Michael Stonebraker, Ahmed Elmagarmid, Ihab F. Ilyas, Samuel Madden, Mourad Ouzzani, and Nan Tang. The Data Civilizer System. In *8th Biennial Conference on Innovative Data Systems Research (CIDR '17)*, pages 1–7, Chaminade, California, USA, 2017.

Ian Dewancker, Michael McCourt, Scott Clark, Patrick Hayes, Alexandra Johnson, and George Ke. A Strategy for Ranking Optimization Methods using Multiple Criteria. In *Workshop on Automatic Machine Learning*, pages 11–20. PMLR, December 2016.

Pedro Domingos. A few useful things to know about machine learning. *Communications of the ACM*, 55(10):78–87, October 2012. ISSN 00010782. doi: 10.1145/2347736.2347755.

Iddo Drori, Yamuna Krishnamurthy, Remi Rampin, Raoni de Paula Lourenco, Jorge Piazentin Ono, Kyunghyun Cho, Claudio Silva, and Juliana Freire. AlphaD3M: Machine Learning Pipeline Synthesis. *JMLR: Workshop and Conference Proceedings*, 1:1–8, 2018.

Cynthia Dwork. Differential privacy: A survey of results. In *International conference on theory and applications of models of computation*, pages 1–19. Springer, 2008.

Epidemic Prediction Initiative. Dengue forecasting project. `https://web.archive.org/web/20190916180225/https://predict.phiresearchlab.org/post/5a4fcc3e2c1b1669c22aa261`. Accessed 2018-04-30.

Nick Erickson, Jonas Mueller, Alexander Shirkov, Hang Zhang, Pedro Larroy, Mu Li, and Alexander Smola. AutoGluon-Tabular: Robust and Accurate AutoML for Structured Data. *arXiv:2003.06505 [cs, stat]*, March 2020.

Stefan Falkner, Aaron Klein, and Frank Hutter. BOHB: Robust and Efficient Hyperparameter Optimization at Scale. In *Proceedings of the 35th International Conference on Machine Learning*, Stockholm, Sweden, 2018. ISBN 978-1-5108-6796-3.

Ethan Fast and Michael S. Bernstein. Meta: Enabling programming languages to learn from the crowd. In *Proceedings of the 29th Annual Symposium on User Interface Software and Technology - UIST '16*, pages 259–270. ACM Press, 2016. ISBN 978-1-4503-4189-9. doi: 10.1145/2984511.2984532.

Matthias Feurer, Aaron Klein, Katharina Eggensperger, Jost Springenberg, Manuel Blum, and Frank Hutter. Efficient and Robust Automated Machine Learning. *Advances in Neural Information Processing Systems 28*, pages 2944–2952, 2015. ISSN 10495258.

Utsav Garg, Viraj Prabhu, Deshraj Yadav, Ram Ramrakhya, Harsh Agrawal, and Dhruv Batra. Fabrik: An online collaborative neural network editor. *arXiv e-prints*, art. arXiv:1810.11649, 2018.

Alexander Geiger, Dongyu Liu, Sarah Alnegheimish, Alfredo Cuesta-Infante, and Kalyan Veeramachaneni. TadGAN: Time Series Anomaly Detection Using Generative Adversarial Networks. In *2020 IEEE International Conference on Big Data (Big Data)*, pages 33–43, December 2020. doi: 10.1109/BigData50022.2020.9378139.

Pieter Gijsbers, Erin Ledell, Janek Thomas, Sébastien Poirier, Bernd Bischl, and Joaquin Vanschoren. An Open Source AutoML Benchmark. *6th ICML Workshop on Automated Machine Learning*, pages 1–8, 2019.

GitHub. About github - where the world builds software. `https://web.archive.org/web/20210609020420/https://github.com/about`, June 2021. Accessed 2021-06-08.

Leonid Glanz, Patrick Müller, Lars Baumgärtner, Michael Reif, Sven Amann, Pauline Anthonysamy, and Mira Mezini. Hidden in plain sight: Obfuscated strings threatening your privacy. In *Proceedings of the 15th ACM Asia Conference on Computer and Communications Security*, pages 694–707, 2020.

GNU. The gnu operating system. `https://www.gnu.org`.

Daniel Golovin, Benjamin Solnik, Subhodeep Moitra, Greg Kochanski, John 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*, KDD '17, pages 1487–1495, New York, NY, USA, August 2017. Association for Computing Machinery. ISBN 978-1-4503-4887-4. doi: 10.1145/3097983.3098043.

Taciana A.F. Gomes, Ricardo B.C. Prudêncio, Carlos Soares, André L.D. Rossi, and André Carvalho. Combining meta-learning and search techniques to select parameters for support vector machines. *Neurocomputing*, 75(1):3–13, January 2012. ISSN 09252312. doi: 10.1016/j.neucom.2011.07.005.

Ming Gong, Linjun Shou, Wutao Lin, Zhijie Sang, Quanjia Yan, Ze Yang, Feixiang Cheng, and Daxin Jiang. NeuronBlocks: Building Your NLP DNN Models Like Playing Lego. In *Proceedings of the 2019 Conference on Empirical Methods in Natural Language Processing and the 9th International Joint Conference on Natural Language Processing (EMNLP-IJCNLP): System Demonstrations*, pages 163–168, Hong Kong, China, 2019. Association for Computational Linguistics. doi: 10.18653/v1/D19-3028.

Georgios Gousios, Martin Pinzger, and Arie van Deursen. An exploratory study of the pull-based software development model. In *Proceedings of the 36th International Conference on Software Engineering - ICSE 2014*, pages 345–355, Hyderabad, India, 2014. ACM Press. ISBN 978-1-4503-2756-5. doi: 10.1145/2568225.2568260.

Georgios Gousios, Andy Zaidman, Margaret-Anne Storey, and Arie van Deursen. Work Practices and Challenges in Pull-Based Development: The Integrator's Perspective. In *2015 IEEE/ACM 37th IEEE International Conference on Software Engineering*, volume 1, pages 358–368, May 2015. doi: 10.1109/ICSE.2015.55.

Georgios Gousios, Margaret-Anne Storey, and Alberto Bacchelli. Work Practices and Challenges in Pull-Based Development: The Contributor's Perspective. In *2016 IEEE/ACM 38th International Conference on Software Engineering (ICSE)*, pages 285–296, May 2016. doi: 10.1145/2884781.2884826.

Roger B. Grosse and David K. Duvenaud. Testing MCMC code. In *2014 NIPS Workshop on Software Engineering for Machine Learning*, pages 1–8, 2014.

Isabelle Guyon and André Elisseeff. An Introduction to Variable and Feature Selection. *Journal of Machine Learning Research (JMLR)*, 3(3):1157–1182, 2003.

Isabelle Guyon, Kristin Bennett, Gavin Cawley, Hugo Jair Escalante, Sergio Escalera, Tin Kam Ho, Nuria Macia, Bisakha Ray, Mehreen Saeed, Alexander Statnikov, and Evelyne Viegas. Design of the 2015 ChaLearn AutoML challenge. In *2015 International Joint Conference on Neural Networks (IJCNN)*, pages 1–8, Killarney, Ireland, July 2015. IEEE. ISBN 978-1-4799-1960-4. doi: 10.1109/IJCNN.2015.7280767.

Aric A. Hagberg, Daniel A. Schult, and Pieter J. Swart. Exploring network structure, dynamics, and function using networkx. In Gaël Varoquaux, Travis Vaught, and Jarrod Millman, editors, *SciPy*, pages 11–15, 2008.

Sandra G. Hart and Lowell E. Staveland. *Development of NASA-TLX (Task Load Index): Results of Empirical and Theoretical Research*, volume 52, pages 139–183. Elsevier, 1988. ISBN 978-0-444-70388-0. doi: 10.1016/s0166-4115(08)62386-9.

Øyvind Hauge, Claudia Ayala, and Reidar Conradi. Adoption of open source software in software-intensive organizations–a systematic literature review. *Information and Software Technology*, 52(11):1133–1154, 2010.

Andrew Head, Fred Hohman, Titus Barik, Steven M. Drucker, and Robert DeLine. Managing messes in computational notebooks. In *Proceedings of the 2019 CHI Conference on Human Factors in Computing Systems*, CHI '19, pages 270:1–270:12, New York, NY, USA, 2019. ACM.

Jeremy Hermann and Mike Del Balso. Meet michelangelo: Uber's machine learning platform. `https://eng.uber.com/michelangelo-machine-learning-platform/`, 2017. Accessed 2019-07-01.

Youyang Hou and Dakuo Wang. Hacking with NPOs: Collaborative Analytics and Broker Roles in Civic Data Hackathons. *Proceedings of the ACM on Human-Computer Interaction*, 1(CSCW):1–16, December 2017. ISSN 2573-0142. doi: 10.1145/3134688.

Jez Humble and David Farley. *Continuous delivery: reliable software releases through build, test, and deployment automation.* Pearson Education, 2010.

Kyle Hundman, Valentino Constantinou, Christopher Laporte, Ian Colwell, and Tom Soderstrom. Detecting Spacecraft Anomalies Using LSTMs and Nonparametric Dynamic Thresholding. In *Proceedings of the 24th ACM SIGKDD International Conference on Knowledge Discovery & Data Mining - KDD '18*, pages 387–395, London, United Kingdom, 2018. ACM Press. ISBN 978-1-4503-5552-0. doi: 10.1145/3219819.3219845.

Nick Hynes, D Sculley, and Michael Terry. The Data Linter: Lightweight, Automated Sanity Checking for ML Data Sets. *Workshop on ML Systems at NIPS 2017*, 2017.

Insight Lane. Crash model. `https://github.com/insight-lane/crash-model`, 2019.

Kevin Jamieson and Ameet Talwalkar. Non-stochastic Best Arm Identification and Hyperparameter Optimization. In *Artificial Intelligence and Statistics*, pages 240–248. PMLR, May 2016.

Justin P. Johnson. Collaboration, peer review and open source software. *Information Economics and Policy*, 18(4):477–497, November 2006. ISSN 01676245. doi: 10.1016/j.infoecopol.2006.07.001.

Daniel Kang, Deepti Raghavan, Peter Bailis, and Matei Zaharia. Model Assertions for Monitoring and Improving ML Models. *arXiv:2003.01668 [cs]*, March 2020.

James Max Kanter and Kalyan Veeramachaneni. Deep Feature Synthesis: Towards Automating Data Science Endeavors. In *2015 IEEE International Conference on Data Science and Advanced Analytics (DSAA)*, pages 1–10, 2015. ISBN 978-1-4673-8273-1. doi: 10.1109/DSAA.2015.7344858.

James Max Kanter, Owen Gillespie, and Kalyan Veeramachaneni. Label, segment, featurize: A cross domain framework for prediction engineering. *Proceedings - 3rd IEEE International Conference on Data Science and Advanced Analytics, DSAA 2016*, pages 430–439, 2016.

Bojan Karlaš, Matteo Interlandi, Cedric Renggli, Wentao Wu, Ce Zhang, Deepak Mukunthu Iyappan Babu, Jordan Edwards, Chris Lauren, Andy Xu, and Markus Weimer. Building Continuous Integration Services for Machine Learning. In *Proceedings of the 26th ACM SIGKDD International Conference on Knowledge Discovery & Data Mining*, pages 2407–2415, Virtual Event CA USA, August 2020. ACM. ISBN 978-1-4503-7998-4. doi: 10.1145/3394486.3403290.

Gilad Katz, Eui Chul Richard Shin, and Dawn Song. ExploreKit: Automatic Feature Generation and Selection. In *2016 IEEE 16th International Conference on Data Mining (ICDM)*, pages 979–984, Barcelona, Spain, December 2016. IEEE. ISBN 978-1-5090-5473-2. doi: 10.1109/ICDM.2016.0123.

Mary Beth Kery, Marissa Radensky, Mahima Arya, Bonnie E. John, and Brad A. Myers. The Story in the Notebook: Exploratory Data Science using a Literate Programming Tool. In *Proceedings of the 2018 CHI Conference on Human Factors in Computing Systems*, CHI '18, pages 1–11, New York, NY, USA, April 2018. Association for Computing Machinery. ISBN 978-1-4503-5620-6. doi: 10.1145/3173574.3173748.

Udayan Khurana, Deepak Turaga, Horst Samulowitz, and Srinivasan Parthasrathy. Cognito: Automated feature engineering for supervised learning. In *2016 IEEE 16th International Conference on Data Mining Workshops (ICDMW)*, pages 1304–1307. IEEE, 2016.

Jon Kleinberg, Jens Ludwig, Sendhil Mullainathan, and Ziad Obermeyer. Prediction Policy Problems. *American Economic Review*, 105(5):491–495, May 2015. ISSN 0002-8282. doi: 10.1257/aer.p20151023.

Jon Kleinberg, Jens Ludwig, and Sendhil Mullainathan. A Guide to Solving Social Problems with Machine Learning. *Harvard Business Review*, December 2016. ISSN 0017-8012.

Thomas Kluyver, Benjamin Ragan-Kelley, Fernando Pérez, Brian Granger, Matthias Bussonnier, Jonathan Frederic, Kyle Kelley, Jessica Hamrick, Jason Grout, Sylvain Corlay, Paul Ivanov, Damián Avila, Safia Abdalla, and Carol Willing. Jupyter notebooks – a publishing format for reproducible computational workflows. In F. Loizides and B. Schmidt, editors, *Positioning and Power in Academic Publishing: Players, Agents and Agendas*, pages 87–90. IOS Press, 2016.

Ron Kohavi. Scaling up the accuracy of naive-bayes classifiers: a decision-tree hybrid. In *KDD*, pages 1–6, 1996.

Alexander Kraskov, Harald Stögbauer, and Peter Grassberger. Estimating mutual information. *Physical Review E - Statistical Physics, Plasmas, Fluids, and Related Interdisciplinary Topics*, 69(6):1–16, 2004.

Max Kuhn. Building Predictive Models in R Using the caret Package. *Journal of Statistical Software*, 28(5):159–160, 2008.

Maciej Kula. Metadata embeddings for user and item cold-start recommendations. In *Proceedings of the 2nd Workshop on New Trends on Content-Based Recommender Systems*, volume 1448, pages 14–21, 2015.

Thomas D. Latoza and André Van Der Hoek. Crowdsourcing in Software Engineering: Models, Opportunities, and Challenges. *IEEE Software*, pages 1–13, 2016.

Haiguang Li, Xindong Wu, Zhao Li, and Wei Ding. Group feature selection with streaming features. *Proceedings - IEEE International Conference on Data Mining, ICDM*, pages 1109–1114, 2013.

Liam Li, Kevin Jamieson, Afshin Rostamizadeh, Ekaterina Gonina, Jonathan Bentzur, Moritz Hardt, Benjamin Recht, and Ameet Talwalkar. A System for Massively Parallel Hyperparameter Tuning. *Proceedings of Machine Learning and Systems*, 2:230–246, March 2020.

Lisha Li, Kevin Jamieson, Giulia DeSalvo, Afshin Rostamizadeh, and Ameet Talwalkar. Hyperband: A novel bandit-based approach to hyperparameter optimization. *The Journal of Machine Learning Research*, 18(1):6765–6816, January 2017. ISSN 1532-4435.

Linux. The Linux kernel organization. `https://www.kernel.org`.

Richard Lippmann, William Campbell, and Joseph Campbell. An Overview of the DARPA Data Driven Discovery of Models (D3M) Program. In *NIPS Workshop on Artificial Intelligence for Data Science*, pages 1–2, 2016.

Zachary C. Lipton and Jacob Steinhardt. Troubling Trends in Machine Learning Scholarship: Some ML papers suffer from flaws that could mislead the public and stymie future research. *Queue*, 17(1):45–77, February 2019. ISSN 1542-7730, 1542-7749. doi: 10.1145/3317287.3328534.

David M. Liu and Matthew J. Salganik. Successes and Struggles with Computational Reproducibility: Lessons from the Fragile Families Challenge. *Socius: Sociological Research for a Dynamic World*, 5:1–21, 2019. doi: 10.1177/2378023119849803.

Ilya Loshchilov and Frank Hutter. CMA-ES for Hyperparameter Optimization of Deep Neural Networks. *arXiv:1604.07269 [cs]*, April 2016.

Kelvin Lu. Feature engineering and evaluation in lightweight systems. M.eng. thesis, Massachusetts Institute of Technology, 2019.

Yaoli Mao, Dakuo Wang, Michael Muller, Kush R. Varshney, Ioana Baldini, Casey Dugan, and Aleksandra Mojsilović. How Data Scientists Work Together With Domain Experts in Scientific Collaborations: To Find The Right Answer Or To Ask The Right Question? *Proceedings of the ACM on Human-Computer Interaction*, 3 (GROUP):1–23, December 2019. ISSN 2573-0142. doi: 10.1145/3361118.

Leslie Marsh and Christian Onof. Stigmergic epistemology, stigmergic cognition. *Cognitive Systems Research*, 9(1):136–149, March 2008. ISSN 1389-0417. doi: 10.1016/j.cogsys.2007.06.009.

Michael Meli, Matthew R. McNiece, and Bradley Reaves. How Bad Can It Git? Characterizing Secret Leakage in Public GitHub Repositories. In *Network and Distributed Systems Security (NDSS) Symposium*, pages 1–15, San Diego, CA, USA, 2019. doi: 10.14722/ndss.2019.23418.

Meta Kaggle. Meta Kaggle: Kaggle's public data on competitions, users, submission scores, and kernels. `https://www.kaggle.com/kaggle/meta-kaggle`, August 2021. Version 539.

Hui Miao, Ang Li, Larry S. Davis, and Amol Deshpande. Towards Unified Data and Lifecycle Management for Deep Learning. In *2017 IEEE 33rd International Conference on Data Engineering (ICDE)*, pages 571–582, April 2017. doi: 10.1109/ICDE.2017.112.

Justin Middleton, Emerson Murphy-Hill, and Kathryn T. Stolee. Data Analysts and Their Software Practices: A Profile of the Sabermetrics Community and Beyond. *Proceedings of the ACM on Human-Computer Interaction*, 4(CSCW1):1–27, May 2020. ISSN 2573-0142, 2573-0142. doi: 10.1145/3392859.

Michael Muller, Ingrid Lange, Dakuo Wang, David Piorkowski, Jason Tsay, Q. Vera Liao, Casey Dugan, and Thomas Erickson. How Data Science Workers Work with Data: Discovery, Capture, Curation, Design, Creation. In *Proceedings of the 2019 CHI Conference on Human Factors in Computing Systems*, CHI '19, pages 1–15, New York, NY, USA, May 2019. Association for Computing Machinery. ISBN 978-1-4503-5970-2. doi: 10.1145/3290605.3300356.

OAuth Working Group. The OAuth 2.0 authorization framework. RFC 6749, RFC Editor, October 2012. URL `https://www.rfc-editor.org/rfc/rfc6749`.

ChangYong Oh, Efstratios Gavves, and Max Welling. BOCK : Bayesian Optimization with Cylindrical Kernels. In *International Conference on Machine Learning*, pages 3868–3877. PMLR, July 2018.

Randal S. Olson, Nathan Bartley, Ryan J. Urbanowicz, and Jason H. Moore. Evaluation of a Tree-based Pipeline Optimization Tool for Automating Data Science. In *Proceedings of the Genetic and Evolutionary Computation Conference 2016*, pages 485–492, Denver Colorado USA, July 2016. ACM. ISBN 978-1-4503-4206-3. doi: 10.1145/2908812.2908918.

William G. Ouchi. A conceptual framework for the design of organizational control mechanisms. *Management science*, 25(9):833–848, 1979.

Shoumik Palkar, James Thomas, Deepak Narayanan, Pratiksha Thaker, Rahul Palamuttam, Parimajan Negi, Anil Shanbhag, Malte Schwarzkopf, Holger Pirk, Saman Amarasinghe, Samuel Madden, and Matei Zaharia. Evaluating end-to-end optimization for data analytics applications in weld. *Proceedings of the VLDB Endowment*, 11(9):1002–1015, May 2018. ISSN 2150-8097. doi: 10.14778/3213880.3213890.

Neha Patki, Roy Wedge, and Kalyan Veeramachaneni. The Synthetic Data Vault. In *2016 IEEE International Conference on Data Science and Advanced Analytics (DSAA)*, pages 399–410, October 2016. doi: 10.1109/DSAA.2016.49.

Christian Payne. On the security of open source software. *Information systems journal*, 12(1):61–78, 2002.

Zhenhui Peng, Jeehoon Yoo, Meng Xia, Sunghun Kim, and Xiaojuan Ma. Exploring how software developers work with mention bot in github. In *Proceedings of the Sixth International Symposium of Chinese CHI on – ChineseCHI '18*, pages 152–155. ACM Press, 2018. ISBN 978-1-4503-6508-6. doi: 10.1145/3202667.3202694.

Project Jupyter Contributors. jupyterlab-google-drive. `https://github.com/jupyterlab/jupyterlab-google-drive`, a. Accessed on 2021-01-10 (commit ab727c4).

Project Jupyter Contributors. Jupyterlab github. `https://github.com/jupyterlab/jupyterlab-github`, b. Accessed on 2021-01-10 (commit 065aa44).

Alexander Ratner, Christopher De Sa, Sen Wu, Daniel Selsam, and Christopher Ré. Data programming: Creating large training sets, quickly. *Advances in neural information processing systems*, 29:3567–3575, 2016.

Alexander Ratner, Stephen H. Bach, Henry Ehrenberg, Jason Fries, Sen Wu, and Christopher Ré. Snorkel: Rapid Training Data Creation with Weak Supervision. *Proceedings of the VLDB Endowment*, 11(3):269–282, November 2017. ISSN 21508097. doi: 10.14778/3157794.3157797.

Eric Raymond. The cathedral and the bazaar. *Knowledge, Technology & Policy*, 12 (3):23–49, 1999.

Nancy E. Reichman, Julien O. Teitler, Irwin Garfinkel, and Sara S. McLanahan. Fragile Families: Sample and design. *Children and Youth Services Review*, 23(4-5): 303–326, 2001. ISSN 01907409. doi: 10.1016/S0190-7409(01)00141-4.

Cedric Renggli, Bojan Karlaš, Bolin Ding, Feng Liu, Kevin Schawinski, Wentao Wu, and Ce Zhang. Continuous Integration of Machine Learning Models With ease.ml/ci: Towards a Rigorous Yet Practical Treatment. In *Proceedings of the 2nd SysML Conference*, pages 1–12, 2019.

Jeffrey A. Roberts, Il-Horn Hann, and Sandra A. Slaughter. Understanding the motivations, participation, and performance of open source software developers: A longitudinal study of the apache projects. *Management science*, 52(7):984–999, 2006.

Matthew Rocklin. Dask: Parallel Computation with Blocked algorithms and Task Scheduling. In *Python in Science Conference*, pages 126–132, Austin, Texas, 2015. doi: 10.25080/Majora-7b98e3ed-013.

Andrew Slavin Ross and Jessica Zosa Forde. Refactoring Machine Learning. In *Workshop on Critiquing and Correcting Trends in Machine Learning at NeuRIPS 2018*, pages 1–6, 2018.

Adam Rule, Aurélien Tabard, and James D. Hollan. Exploration and Explanation in Computational Notebooks. In *Proceedings of the 2018 CHI Conference on Human Factors in Computing Systems*, pages 1–12, Montreal QC Canada, April 2018. ACM. ISBN 978-1-4503-5620-6. doi: 10.1145/3173574.3173606.

Per Runeson and Martin Höst. Guidelines for conducting and reporting case study research in software engineering. *Empirical Software Engineering*, 14(2):131–164, Apr 2009. ISSN 1382-3256, 1573-7616. doi: 10.1007/s10664-008-9102-8.

Adam Sadilek, Stephanie Caty, Lauren DiPrete, Raed Mansour, Tom Schenk, Mark Bergtholdt, Ashish Jha, Prem Ramaswami, and Evgeniy Gabrilovich. Machine-learned epidemiology: Real-time detection of foodborne illness at scale. *npj Digital Medicine*, pages 1–7, December 2018. ISSN 2398-6352. doi: 10.1038/s41746-018-0045-1.

Matthew J. Salganik, Ian Lundberg, Alexander T. Kindel, and Sara McLanahan. Introduction to the Special Collection on the Fragile Families Challenge. *Socius: Sociological Research for a Dynamic World*, 5:1–21, January 2019. ISSN 2378-0231, 2378-0231. doi: 10.1177/2378023119871580.

Matthew J. Salganik, Ian Lundberg, Alexander T. Kindel, et al. Measuring the predictability of life outcomes with a scientific mass collaboration. *Proceedings of the National Academy of Sciences*, 117(15):8398–8403, April 2020. ISSN 0027-8424, 1091-6490. doi: 10.1073/pnas.1915006117.

Iflaah Salman and Burak Turhan. Effect of time-pressure on perceived and actual performance in functional software testing. In *Proceedings of the 2018 International Conference on Software and System Process - ICSSP '18*, pages 130–139. ACM Press, 2018. ISBN 978-1-4503-6459-1. doi: 10.1145/3202710.3203148.

Shubhra Kanti Karmaker Santu, Md Mahadi Hassan, Micah J. Smith, Lei Xu, ChengXiang Zhai, and Kalyan Veeramachaneni. AutoML to Date and Beyond: Challenges and Opportunities. *arXiv:2010.10777 [cs]*, May 2021.

Gerald Schermann, Jürgen Cito, Philipp Leitner, and Harald Gall. Towards quality gates in continuous delivery and deployment. In *2016 IEEE 24th International Conference on Program Comprehension (ICPC)*, pages 1–4, May 2016. doi: 10.1109/ICPC.2016.7503737.

D. Sculley, Gary Holt, Daniel Golovin, Eugene Davydov, Todd Phillips, Dietmar Ebner, Vinay Chaudhary, Michael Young, Jean-François Crespo, and Dan Dennison. Hidden technical debt in machine learning systems. *Advances in Neural Information Processing Systems*, pages 2494–2502, 2015.

Zeyuan Shang, Emanuel Zgraggen, Benedetto Buratti, Ferdinand Kossmann, Philipp Eichmann, Yeounoh Chung, Carsten Binnig, Eli Upfal, and Tim Kraska. Democratizing Data Science through Interactive Curation of ML Pipelines. In *Proceedings of the 2019 International Conference on Management of Data - SIGMOD '19*, pages 1171–1188, Amsterdam, Netherlands, 2019. ACM Press. ISBN 978-1-4503-5643-5. doi: 10.1145/3299869.3319863.

Ben Shneiderman, Catherine Plaisant, Maxine Cohen, Steven Jacobs, Niklas Elmqvist, and Nicholas Diakopoulos. *Designing the user interface: strategies for effective human-computer interaction.* Pearson, 2016.

Micah J. Smith. Scaling collaborative open data science. S.M. Thesis, Massachusetts Institute of Technology, 2018.

Micah J. Smith, Roy Wedge, and Kalyan Veeramachaneni. FeatureHub: Towards collaborative data science. In *2017 IEEE International Conference on Data Science and Advanced Analytics (DSAA)*, pages 590–600, October 2017.

Micah J. Smith, Carles Sala, James Max Kanter, and Kalyan Veeramachaneni. The Machine Learning Bazaar: Harnessing the ML Ecosystem for Effective System Development. In *Proceedings of the 2020 ACM SIGMOD International Conference on Management of Data*, SIGMOD '20, pages 785–800, Portland, OR, USA, 2020. Association for Computing Machinery. ISBN 978-1-4503-6735-6. doi: 10.1145/3318464.3386146.

Micah J. Smith, Jürgen Cito, Kelvin Lu, and Kalyan Veeramachaneni. Enabling collaborative data science development with the Ballet framework. *Proceedings of the ACM on Human-Computer Interaction*, 5(CSCW2):1–39, October 2021a. doi: 10.1145/3479575.

Micah J. Smith, Jürgen Cito, and Kalyan Veeramachaneni. Meeting in the notebook: A notebook-based environment for micro-submissions in data science collaborations. *arXiv:2103.15787 [cs]*, March 2021b.

Jasper Snoek, Hugo Larochelle, and Ryan P. Adams. Practical Bayesian optimization of machine learning algorithms. In *Proceedings of the 25th International Conference on Neural Information Processing Systems - Volume 2*, NIPS'12, pages 2951–2959, Red Hook, NY, USA, December 2012. Curran Associates Inc.

Julian Spector. Chicago Is Using Data to Predict Food Safety Violations. So Why Aren't Other Cities? *Bloomberg.com*, January 2016.

Kate Stewart, Shuah Khan, Daniel M. German, Greg Kroah-Hartman, Jon Corbet, Konstantin Ryabitsev, David A. Wheeler, Jason Perlow, Steve Winslow, Mike Dolan, Craig Ross, and Alison Rowan. 2020 Linux Kernel History Report. Technical report, The Linux Foundation, August 2020.

Stockfish. Stockfish: A strong open source chess engine. `https://stockfishchess.org`. Accessed 2019-09-05.

Emma Strubell, Ananya Ganesh, and Andrew McCallum. Energy and Policy Considerations for Deep Learning in NLP. In *Proceedings of the 57th Annual Meeting of the Association for Computational Linguistics*, pages 3645–3650, Florence, Italy, 2019. Association for Computational Linguistics. doi: 10.18653/v1/P19-1355.

Krishna Subramanian, Nur Hamdan, and Jan Borchers. Casual notebooks and rigid scripts: Understanding data science programming. In *2020 IEEE Symposium on Visual Languages and Human-Centric Computing (VL/HCC)*, pages 1–5, Aug 2020. doi: 10.1109/VL/HCC50065.2020.9127207.

Thomas Swearingen, Will Drevo, Bennett Cyphers, Alfredo Cuesta-Infante, Arun Ross, and Kalyan Veeramachaneni. ATM: A distributed, collaborative, scalable system for automated machine learning. In *2017 IEEE International Conference on Big Data (Big Data)*, pages 151–162, Boston, MA, December 2017. IEEE. ISBN 978-1-5386-2715-0. doi: 10.1109/BigData.2017.8257923.

Chris Thornton, Frank Hutter, Holger H. Hoos, and Kevin Leyton-Brown. Auto-WEKA: Combined selection and hyperparameter optimization of classification algorithms. In *Proceedings of the 19th ACM SIGKDD International Conference on Knowledge Discovery and Data Mining*, KDD '13, pages 847–855, New York, NY, USA, August 2013. Association for Computing Machinery. ISBN 978-1-4503-2174-7. doi: 10.1145/2487575.2487629.

Tom van der Weide, Dimitris Papadopoulos, Oleg Smirnov, Michal Zielinski, and Tim van Kasteren. Versioning for End-to-End Machine Learning Pipelines. In *Proceedings of the 1st Workshop on Data Management for End-to-End Machine Learning - DEEM'17*, pages 1–9, Chicago, IL, USA, 2017. ACM Press. ISBN 978-1-4503-5026-6. doi: 10.1145/3076246.3076248.

Jan N. van Rijn, Salisu Mamman Abdulrahman, Pavel Brazdil, and Joaquin Vanschoren. Fast Algorithm Selection Using Learning Curves. In Elisa Fromont, Tijl De Bie, and Matthijs van Leeuwen, editors, *Advances in Intelligent Data Analysis XIV*, volume 9385, pages 298–309. Springer International Publishing, Cham, 2015. ISBN 978-3-319-24464-8 978-3-319-24465-5. doi: 10.1007/978-3-319-24465-5_26.

Joaquin Vanschoren, Jan N. van Rijn, Bernd Bischl, and Luís Torgo. OpenML: Networked science in machine learning. *SIGKDD Explorations*, 15:49–60, 2013.

Bogdan Vasilescu, Stef van Schuylenburg, Jules Wulms, Aerebrenik Serebrenik, and Mark. G. J. van den Brand. Continuous Integration in a Social-Coding World: Empirical Evidence from GitHub. In *2014 IEEE International Conference on Software Maintenance and Evolution*, pages 401–405, September 2014. doi: 10.1109/ICSME.2014.62.

Bogdan Vasilescu, Yue Yu, Huaimin Wang, Premkumar Devanbu, and Vladimir Filkov. Quality and productivity outcomes relating to continuous integration in GitHub. *Proceedings of the 2015 10th Joint Meeting on Foundations of Software Engineering - ESEC/FSE 2015*, pages 805–816, 2015.

Kalyan Veeramachaneni, Una-May O'Reilly, and Colin Taylor. Towards Feature Engineering at Scale for Data from Massive Open Online Courses. *arXiv:1407.5238 [cs]*, 2014.

Kiri L. Wagstaff. Machine Learning that Matters. In *Proceedings of the 29th International Conference on Machine Learning*, pages 1–6, Edinburgh, Scotland, UK, 2012.

April Yi Wang, Anant Mittal, Christopher Brooks, and Steve Oney. How Data Scientists Use Computational Notebooks for Real-Time Collaboration. *Proceedings of the ACM on Human-Computer Interaction*, 3(CSCW):1–30, November 2019a. ISSN 2573-0142. doi: 10.1145/3359141.

Dakuo Wang, Justin D. Weisz, Michael Muller, Parikshit Ram, Werner Geyer, Casey Dugan, Yla Tausczik, Horst Samulowitz, and Alexander Gray. Human-AI Collaboration in Data Science: Exploring Data Scientists' Perceptions of Automated AI. *Proceedings of the ACM on Human-Computer Interaction*, 3(CSCW):1–24, November 2019b. ISSN 2573-0142, 2573-0142. doi: 10.1145/3359313.

Dakuo Wang, Q. Vera Liao, Yunfeng Zhang, Udayan Khurana, Horst Samulowitz, Soya Park, Michael Muller, and Lisa Amini. How Much Automation Does a Data Scientist Want? *arXiv:2101.03970 [cs]*, January 2021.

Hao Wang, Bas van Stein, Michael Emmerich, and Thomas 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)*, pages 507–512, October 2017. doi: 10.1109/SMC.2017.8122656.

Jing Wang, Meng Wang, Peipei Li, Luoqi Liu, Zhongqiu Zhao, Xuegang Hu, and Xindong Wu. Online Feature Selection with Group Structure Analysis. *IEEE Transactions on Knowledge and Data Engineering*, 27(11):3029–3041, 2015.

Qianwen Wang, Yao Ming, Zhihua Jin, Qiaomu Shen, Dongyu Liu, Micah J. Smith, Kalyan Veeramachaneni, and Huamin Qu. ATMSeer: Increasing Transparency and Controllability in Automated Machine Learning. In *Proceedings of the 2019 CHI Conference on Human Factors in Computing Systems*, pages 1–12, Glasgow Scotland Uk, May 2019c. ACM. ISBN 978-1-4503-5970-2. doi: 10.1145/3290605.3300911.

Wei Wang, Jinyang Gao, Meihui Zhang, Sheng Wang, Gang Chen, Teck Khim Ng, Beng Chin Ooi, Jie Shao, and Moaz Reyad. Rafiki: Machine learning as an analytics service system. *Proceedings of the VLDB Endowment*, 12(2):128–140, October 2018. ISSN 21508097. doi: 10.14778/3282495.3282499.

Sarah Wooders, Peter Schafhalter, and Joseph E. Gonzalez. Feature Stores: The Data Side of ML Pipelines. `https://medium.com/riselab/feature-stores-the-data-side-of-ml-pipelines-7083d69bff1c`, April 2021.

Xindong Wu, Kui Yu, Wei Ding, Hao Wang, and Xingquan Zhu. Online feature selection with streaming features. *IEEE Transactions on Pattern Analysis and Machine Intelligence*, 35(5):1178–1192, 2013.

Doris Xin, Eva Yiwei Wu, Doris Jung-Lin Lee, Niloufar Salehi, and Aditya Parameswaran. Whither AutoML? Understanding the Role of Automation in Machine Learning Workflows. *arXiv:2101.04834 [cs]*, January 2021.

Lei Xu, Maria Skoularidou, Alfredo Cuesta-Infante, and Kalyan Veeramachaneni. Modeling tabular data using conditional gan. In *NeurIPS*, 2019.

Qian Yang, Jina Suh, Nan-Chen Chen, and Gonzalo Ramos. Grounding interactive machine learning tool design in how non-experts actually build models. *Proceedings of the 2018 on Designing Interactive Systems Conference 2018 - DIS '18*, pages 573–584, 2018. doi: 10.1145/3196709.3196729.

Quanming Yao, Mengshuo Wang, Yuqiang Chen, Wenyuan Dai, Yu-Feng Li, Wei-Wei Tu, Qiang Yang, and Yang Yu. Taking Human out of Learning Applications: A Survey on Automated Machine Learning. *arXiv:1810.13306 [cs, stat]*, December 2019.

Kui Yu, Xindong Wu, Wei Ding, and Jian Pei. Scalable and accurate online feature selection for big data. *TKDD*, 11:16:1–16:39, 2016.

Liguo Yu and Srini Ramaswamy. Mining CVS repositories to understand open-source project developer roles. In *Fourth International Workshop on Mining Software Repositories (MSR'07: ICSE Workshops 2007)*, pages 1–8. IEEE, 2007.

Matei Zaharia, Reynold S. Xin, Patrick Wendell, Tathagata Das, Michael Armbrust, Ankur Dave, Xiangrui Meng, Josh Rosen, Shivaram Venkataraman, Michael J. Franklin, Ali Ghodsi, Joseph Gonzalez, Scott Shenker, and Ion Stoica. Apache Spark: A unified engine for big data processing. *Communications of the ACM*, 59 (11):56–65, October 2016. ISSN 0001-0782, 1557-7317. doi: 10.1145/2934664.

Amy X. Zhang, Michael Muller, and Dakuo Wang. How do Data Science Workers Collaborate? Roles, Workflows, and Tools. *Proceedings of the ACM on Human-Computer Interaction*, 4(CSCW1):1–23, May 2020. ISSN 2573-0142, 2573-0142. doi: 10.1145/3392826.

Yangyang Zhao, Alexander Serebrenik, Yuming Zhou, Vladimir Filkov, and Bogdan Vasilescu. The impact of continuous integration on other software development practices: A large-scale empirical study. In *2017 32nd IEEE/ACM International Conference on Automated Software Engineering (ASE)*, pages 60–71, October 2017. doi: 10.1109/ASE.2017.8115619.

Jing Zhou, Dean Foster, Robert Stine, and Lyle Ungar. Streaming feature selection using alpha-investing. *Proceeding of the eleventh ACM SIGKDD international conference on Knowledge discovery in data mining - KDD '05*, pages 384–393, 2005.