CSCE 585: Machine Learning Systems

Lecture 6: Designing Machine Learning Systems

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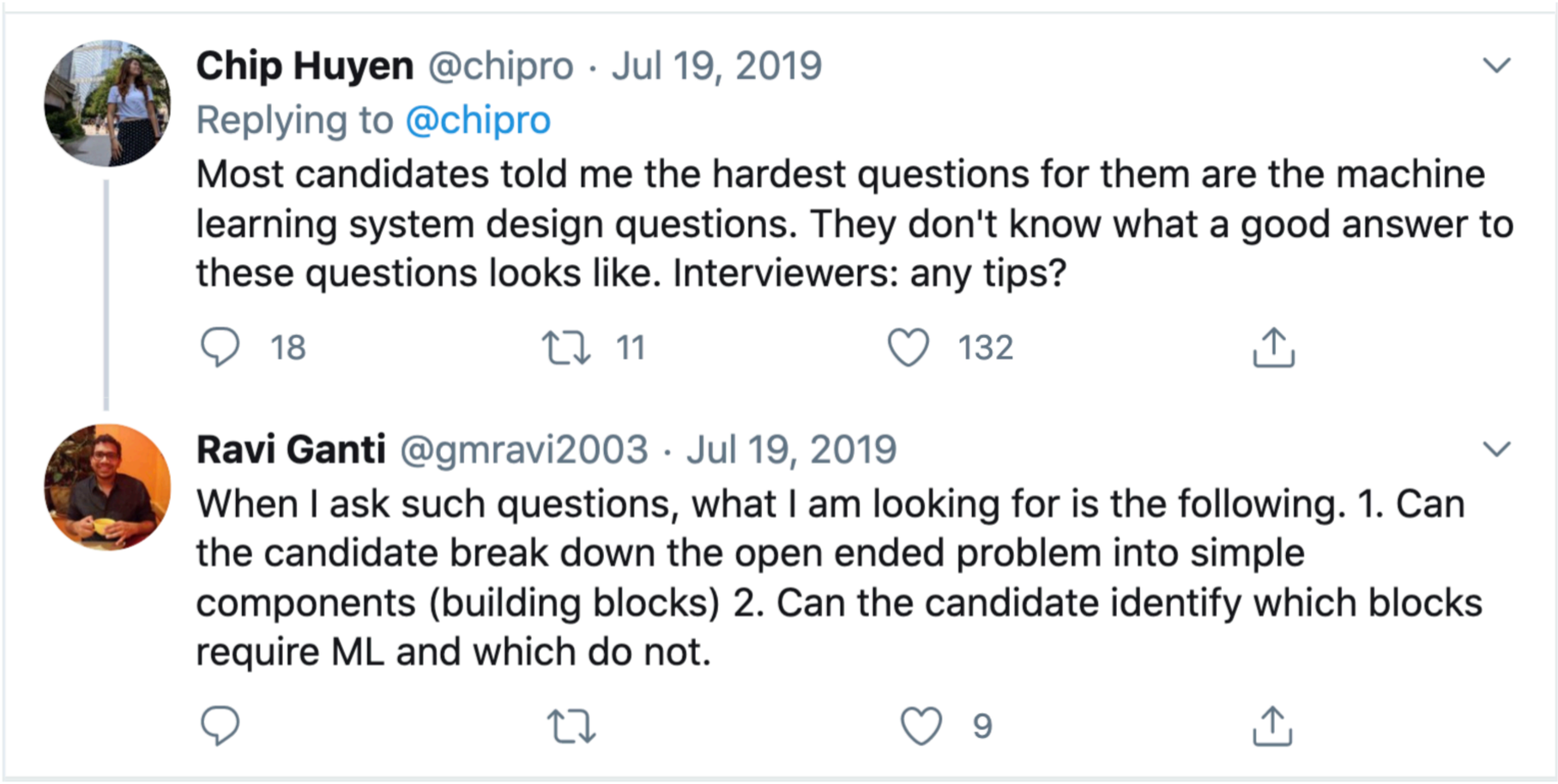
Fall 2024 | Course Website: https://pooyanjamshidi.github.io/mls/

UNIVERSITY OF South Carolina

What is missing?

The gap between ML Research and Production



Chip Huyen @chipro · Jul 19, 2019

Replying to @chipro

Most candidates told me the hardest questions for them are the machine learning system design questions. They don't know what a good answer to these questions looks like. Interviewers: any tips?

18 11 132

Ravi Ganti @gmravi2003 · Jul 19, 2019

When I ask such questions, what I am looking for is the following. 1. Can the candidate break down the open ended problem into simple components (building blocks) 2. Can the candidate identify which blocks require ML and which do not.

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What is missing?

The gap between ML Research and Production

Dmitry Kislyuk @dkislyuk · Jul 19, 2019

Replying to @lishali88 and @chipro

Most candidates know the model classes (linear, decision trees, lstms, convnets) and memorize the relevant info, so for me the interesting bits in ML systems interviews are data cleaning, data prep, logging, eval metrics, scalable inference, feature stores (recommenders/rankers)

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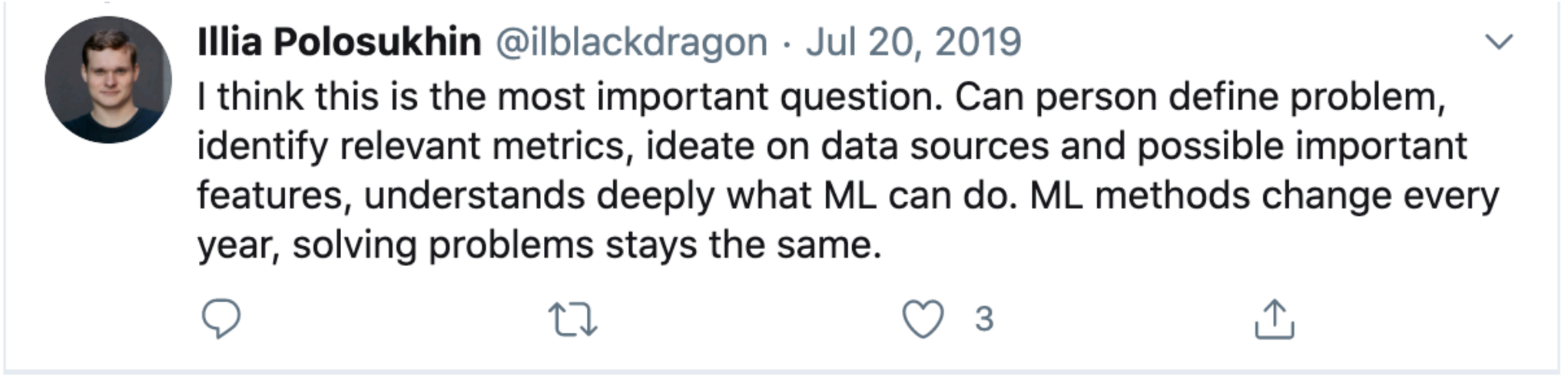
What is missing?

The gap between ML Research and Production



In ML Systems, only a small fraction is comprised of actual ML code

Hidden Technical Debt in Machine Learning Systems

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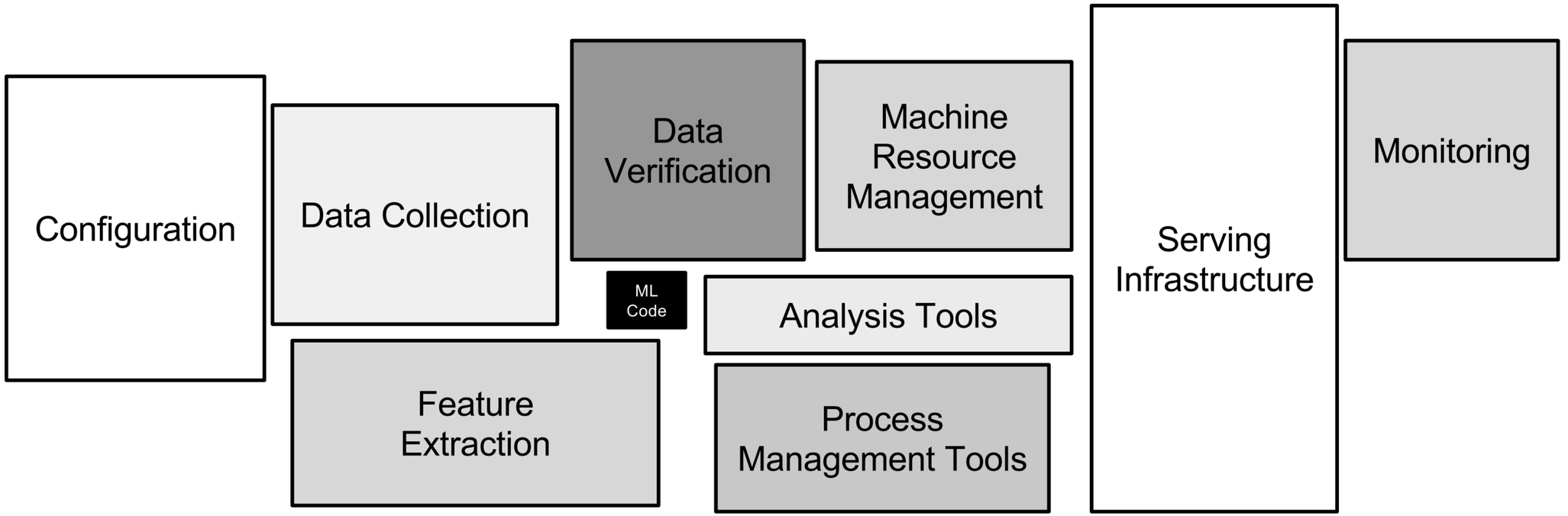
Abstract

Machine learning offers a fantastically powerful toolkit for building useful complex prediction systems quickly. This paper argues it is dangerous to think of these quick wins as coming for free. Using the software engineering framework of *technical debt*, we find it is common to incur massive ongoing maintenance costs in real-world ML systems. We explore several ML-specific risk factors to account for in system design. These include boundary erosion, entanglement, hidden feedback loops, undeclared consumers, data dependencies, configuration issues, changes in the external world, and a variety of system-level anti-patterns.

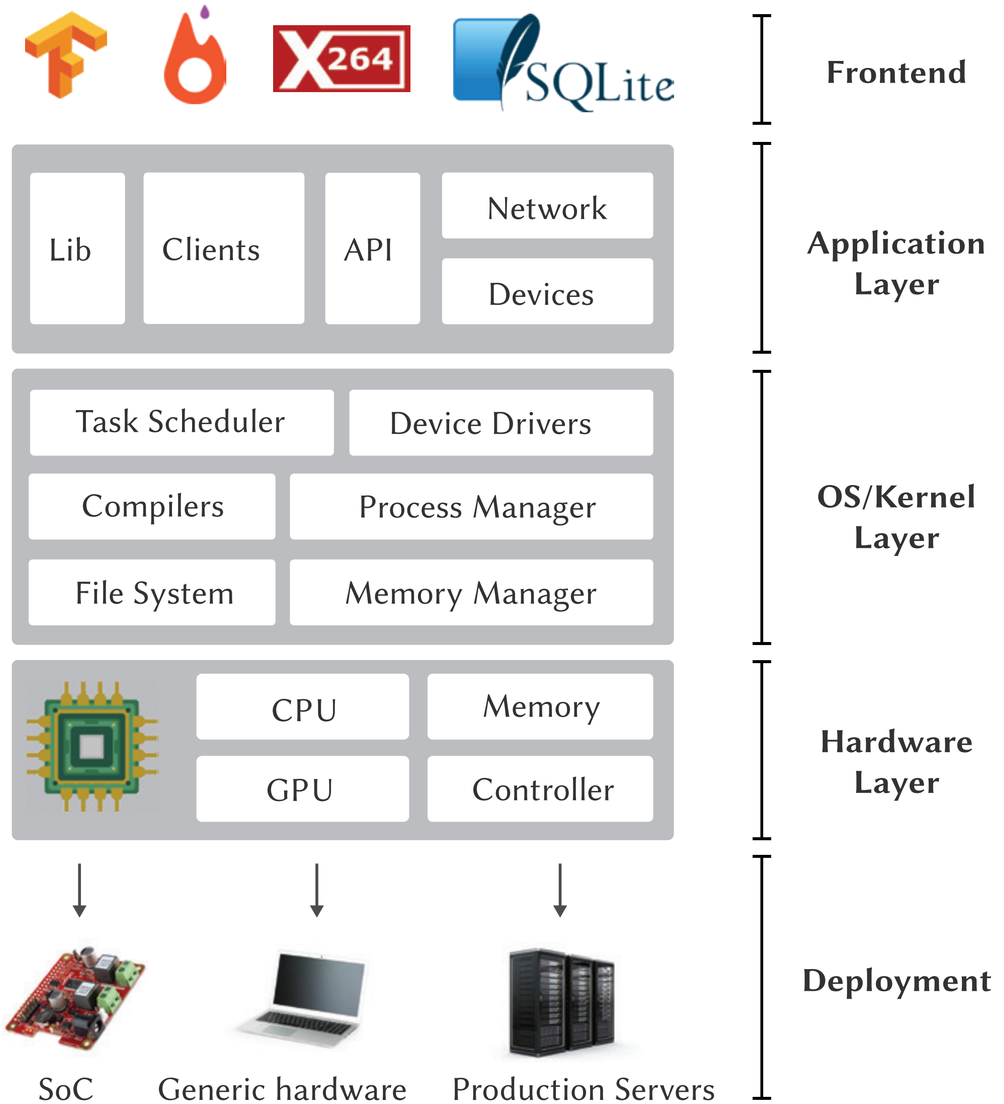
A vast array of surrounding infrastructure and processes is needed to support evolution of ML systems



Technical debt that can accumulate in ML systems

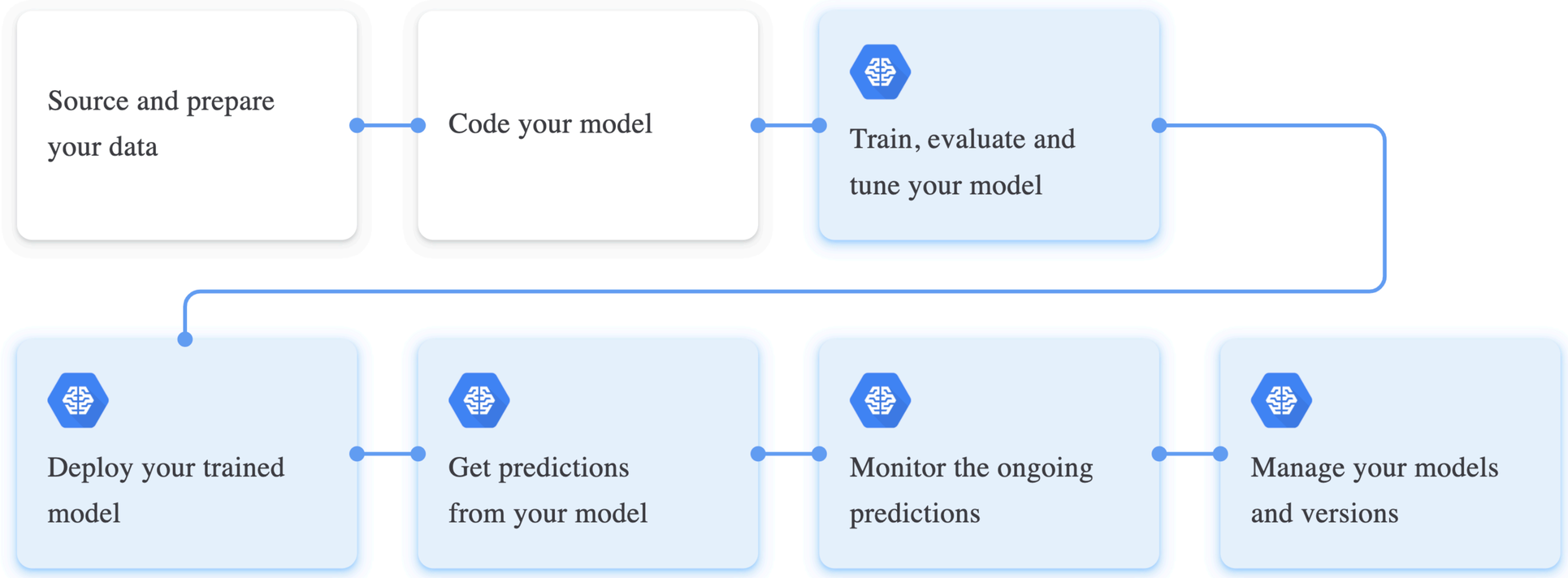
- Data dependencies
- Model complexity
- Reproducibility
- Testing
- Monitoring
- Configuration issues
- External changes

System = Software + Middleware + Hardware



The Building Process of ML Systems

Continuous Delivery for ML Systems



A Machine Learning System is more than just a model

The 3 axes of change in a ML System — data, model, and code — and a few reasons for them to change

Data	Model	Code
Schema	Algorithms	Business Needs
Sampling over Time	More Training	Bug Fixes
Volume	Experiments	Configuration

Continuous Delivery for Machine Learning Systems

***Continuous Delivery for Machine Learning* (CD4ML)** *is a software engineering approach in which a cross-functional team produces machine learning applications based on code, data, and models in small and safe increments that can be reproduced and reliably released at any time, in short adaptation cycles.*

A Machine Learning Application for Sales Forecasting

Corporación Favorita Grocery Sales Forecasting

Can you accurately predict sales for a large grocery chain?

Overview | Data | Code | Models | Discussion | Leaderboard | Rules

Overview

Start
Oct 19, 2017

Close
Jan 15, 2018

Merger & Entry

Description

Brick-and-mortar grocery stores are always in a delicate dance with purchasing and sales forecasting. Predict a little over, and grocers are stuck with overstocked, perishable goods. Guess a little under, and popular items quickly sell out, leaving money on the table and customers fuming.

The problem becomes more complex as retailers add new locations with unique needs, new products, ever transitioning seasonal tastes, and unpredictable product marketing. Corporación Favorita, a large Ecuadorian-based grocery retailer, knows this all too well. They operate hundreds of supermarkets, with over 200,000 different products on their shelves.

Corporación Favorita has challenged the Kaggle community to build a model that more accurately forecasts product sales. They currently rely on subjective forecasting methods with very little data to back them up and very little automation to execute plans. They're excited to see how machine learning could better ensure they please customers by having just enough of the right products at the right time.

Competition Host
Corporación Favorita

Prizes & Awards
$30,000
Awards Points & Medals

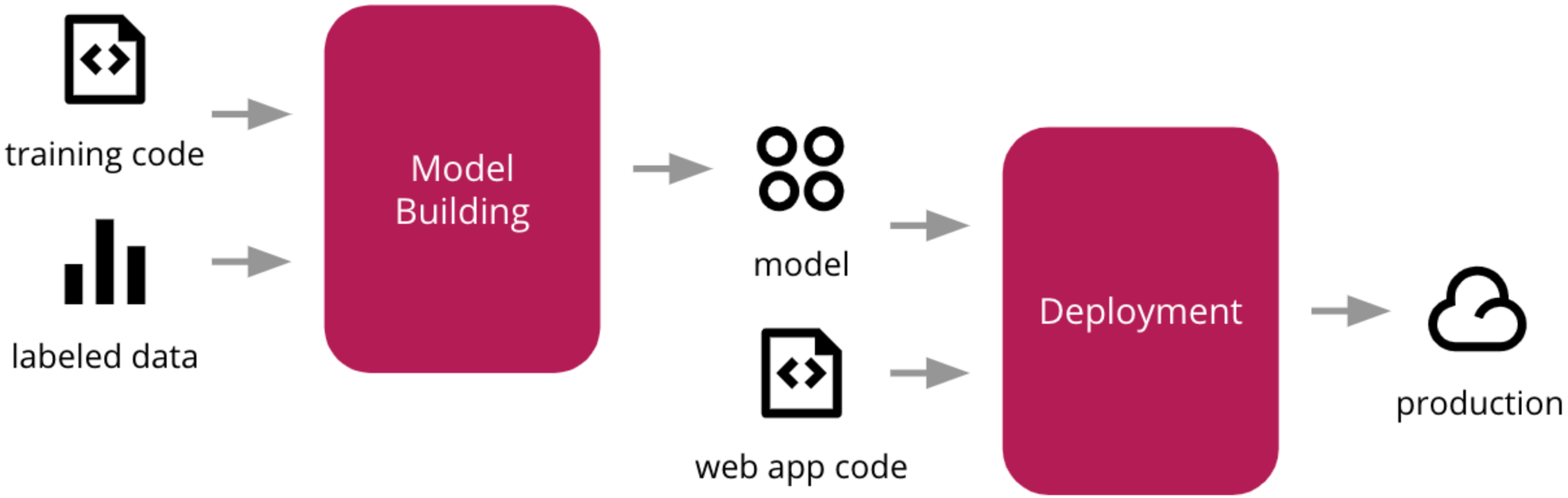
Participation
9,832 Entrants
1,868 Participants
1,671 Teams
31,241 Submissions

Tags

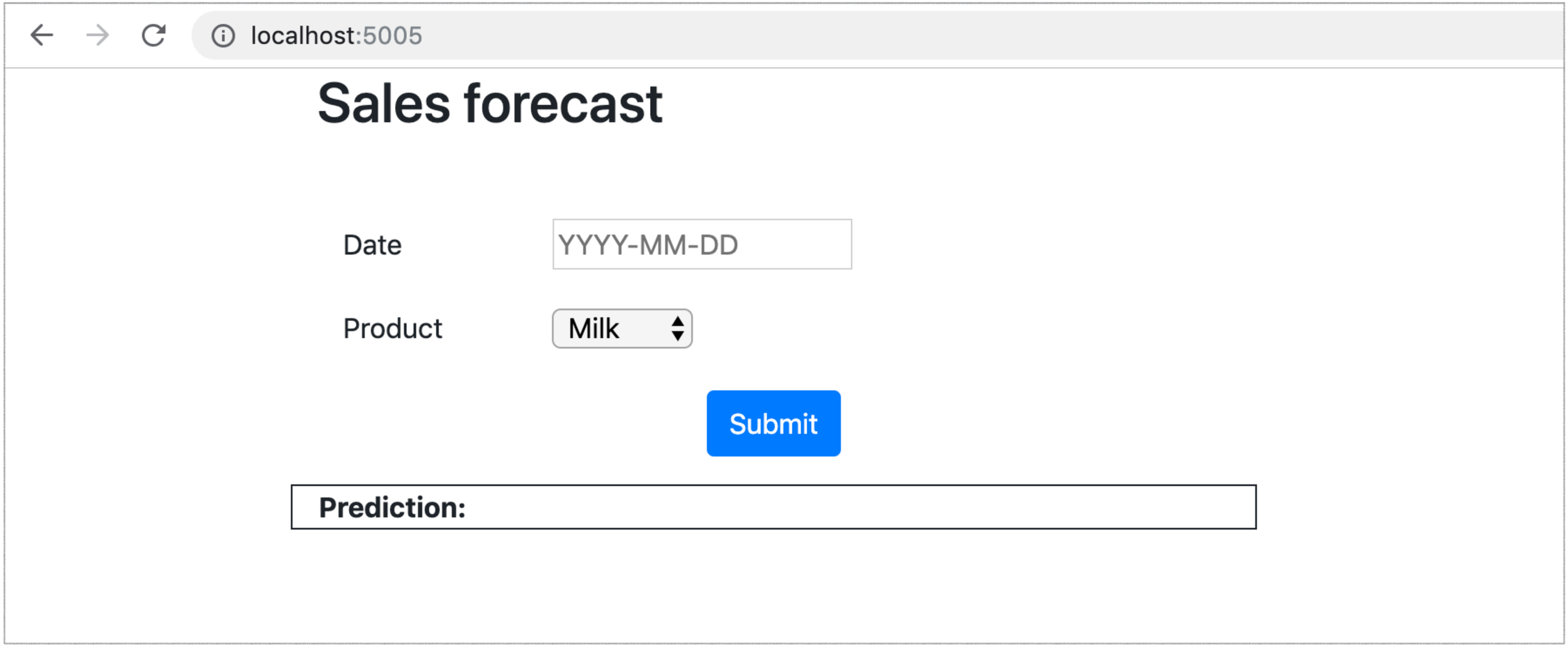
Regression | Food | Tabular | Custom Metric

Table of Contents

Train ML model, integrate it with an application, and deploy into production

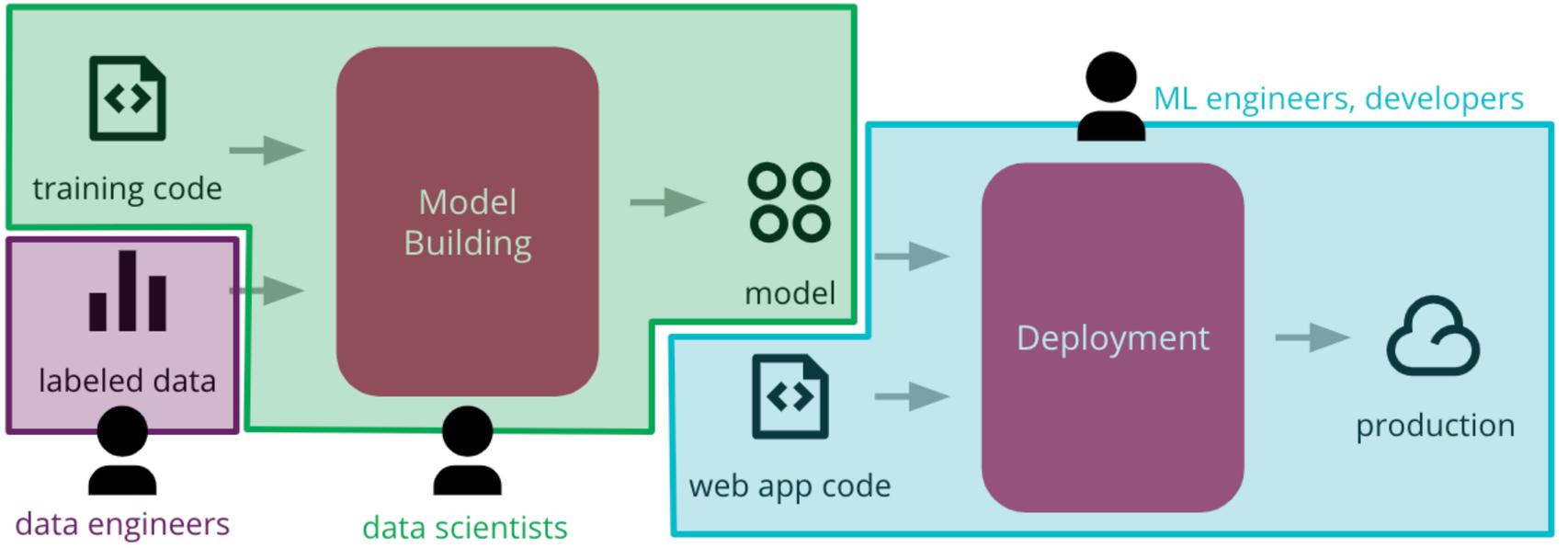


ML model behind a web application



Common Challenges

1. **Organizational** challenge:
   - Throw over the wall
   - Models that only work in a lab environment
   - Even if make it to production, they become stale and hard to update
2. **Technical** challenge: How to make the process
   - Reproducible
   - Auditable



Technical Components of CD for ML Systems

The first step was to understand the data set:

- **Products**, like their categorization and whether they are perishable or not
- **Stores**, like their location and how they are clustered together
- **Events**, like public holidays, seasonal events, or a 7.8 magnitude earthquake that struck Ecuador in 2016
- **Sales transactions**, including the number of units sold for a given product, date, and location

Discoverable and Accessible Data

- It is important that the data is easily discoverable and accessible.
- The harder it is for Data Scientists to find the data they need, the longer it will take for them to build useful models.
- We should also consider they will want to engineer new features on top of the input data that might help improve their model's performance.

Let’s see what we need to do in our example scenario

Initial Exploratory Data Analysis

- To **de-normalize** multiple files into a single CSV file.
- To **cleanup** the data points that were not relevant or that could introduce unwanted noise into the model (like the negative sales).
- We then **store** the output in a cloud storage system like Amazon S3, Google Cloud Storage, or Azure Storage Account.
- Using this file to represent a snapshot of the input training data, we are able to devise a simple approach to **version our dataset** based on the folder structure and file naming conventions. Data versioning is an extensive topic, as it can change in two different axis:
  - Structural **changes** to its schema, and
  - The actual **sampling** of data over time.

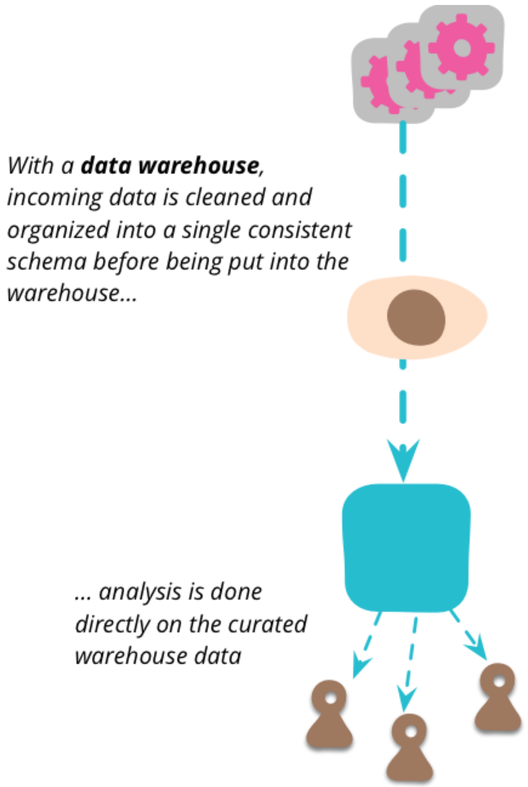
Discoverable and Accessible Data

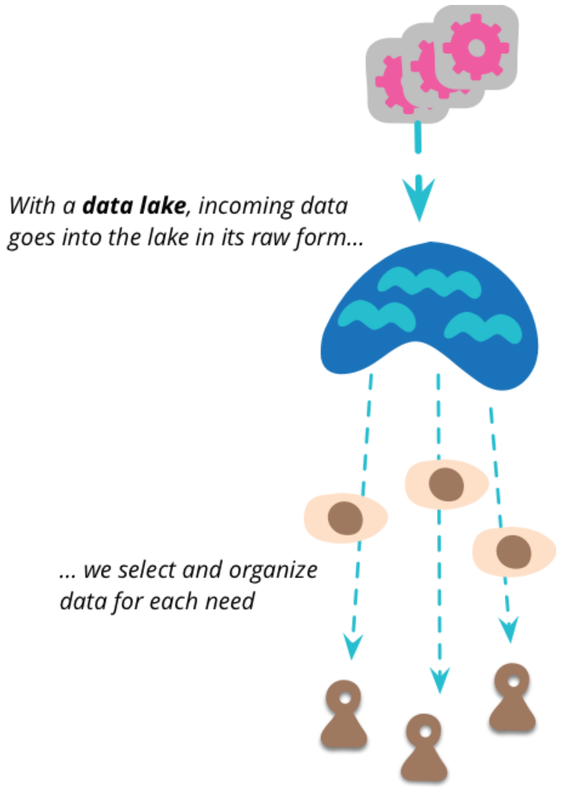
In the real world, you will likely have more complex data pipelines to move data from multiple sources into a place where it can be accessed and used by Data Scientists.

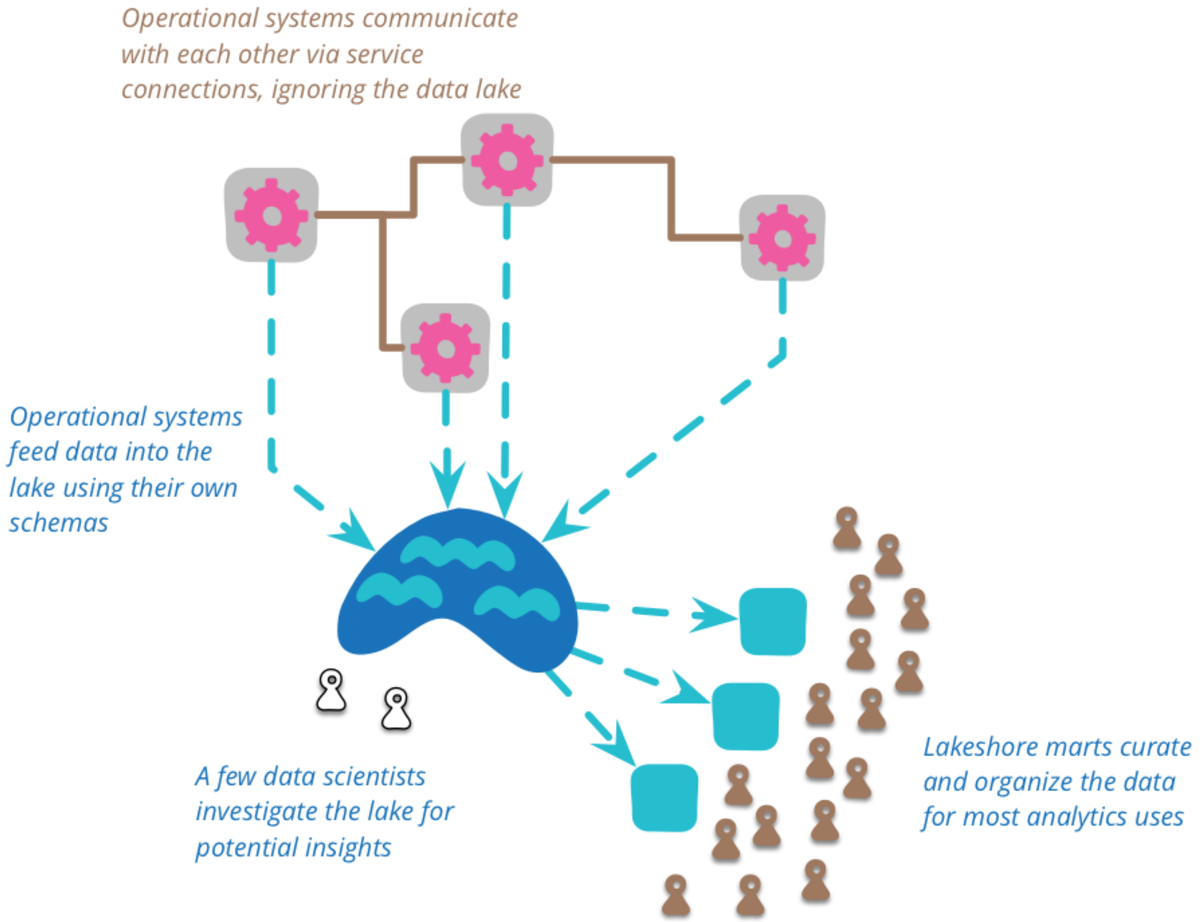
- The most common **source of data** will be your core transactional systems.
- However, there is also value in bringing other data sources from **outside your organization**.
- A few common patterns for collecting and making data available:
  - **Data Lake** architecture: a traditional data warehouse
  - **Data Mesh** architecture: decentralized

From Data Warehouse to Data Lake

The idea is to have a single store for all of the raw data that anyone in an organization might need to analyze.

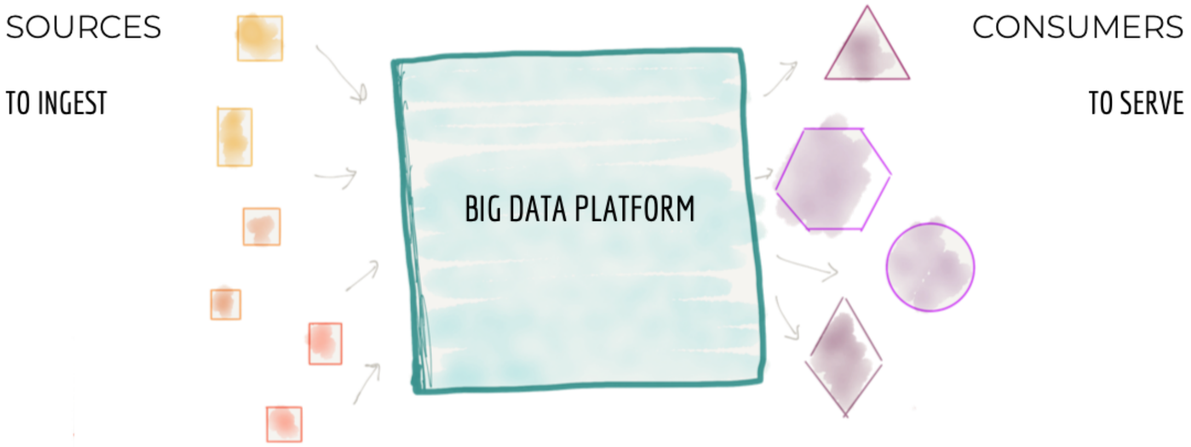


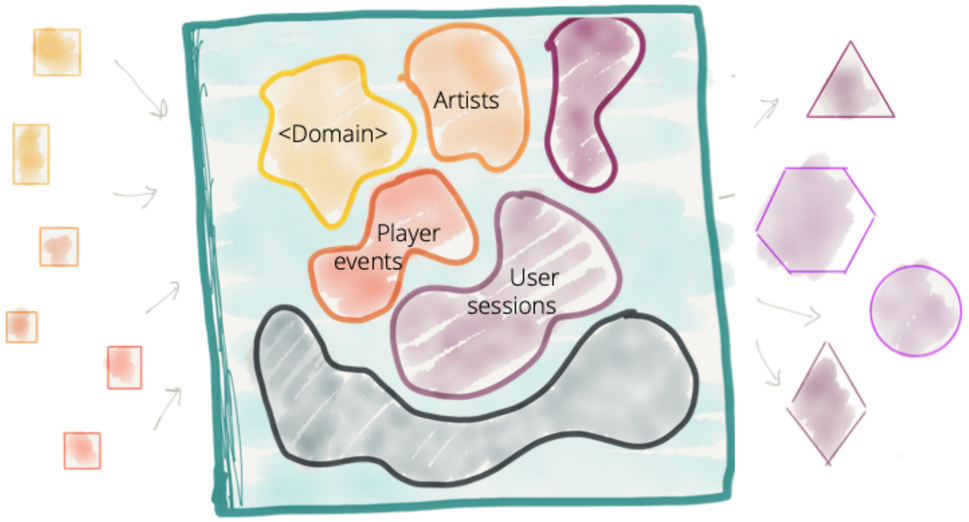




Architectural failure modes

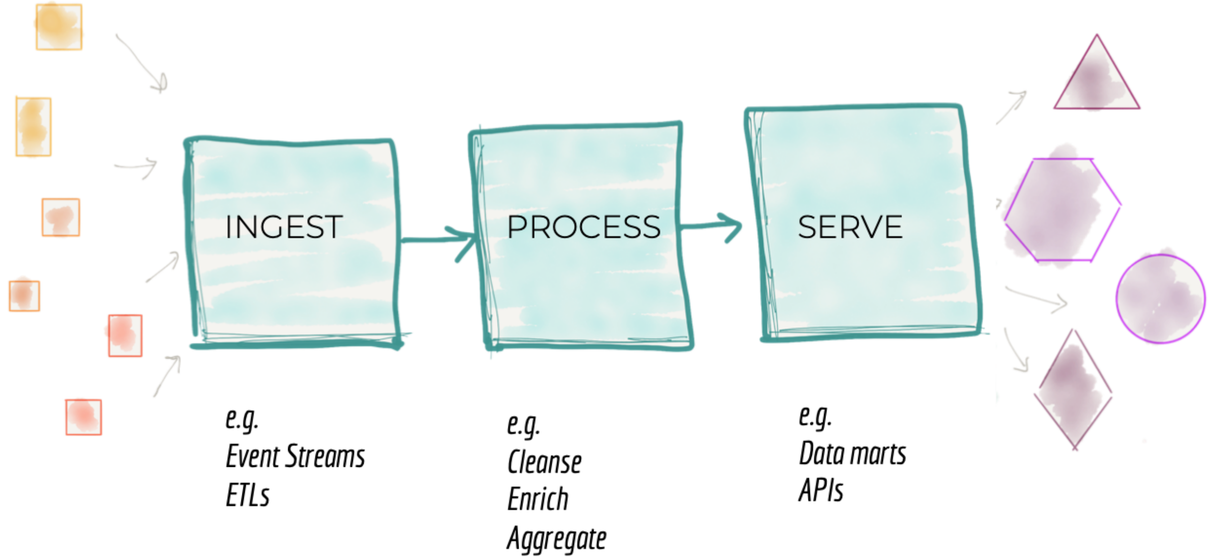
Centralized data platform with no clear data domain boundaries and ownership of domain-oriented data



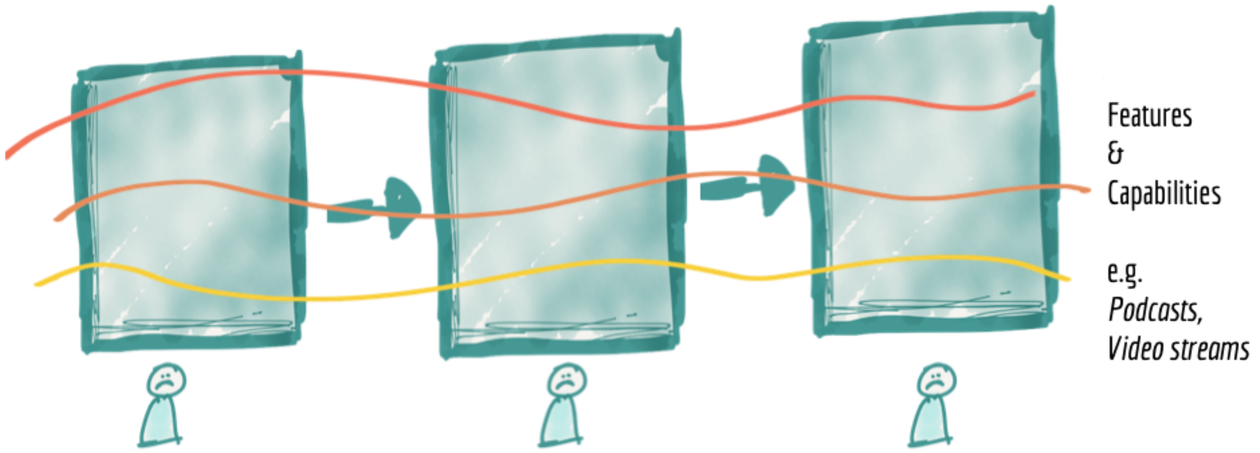


Architectural failure modes

Coupled pipeline decomposition

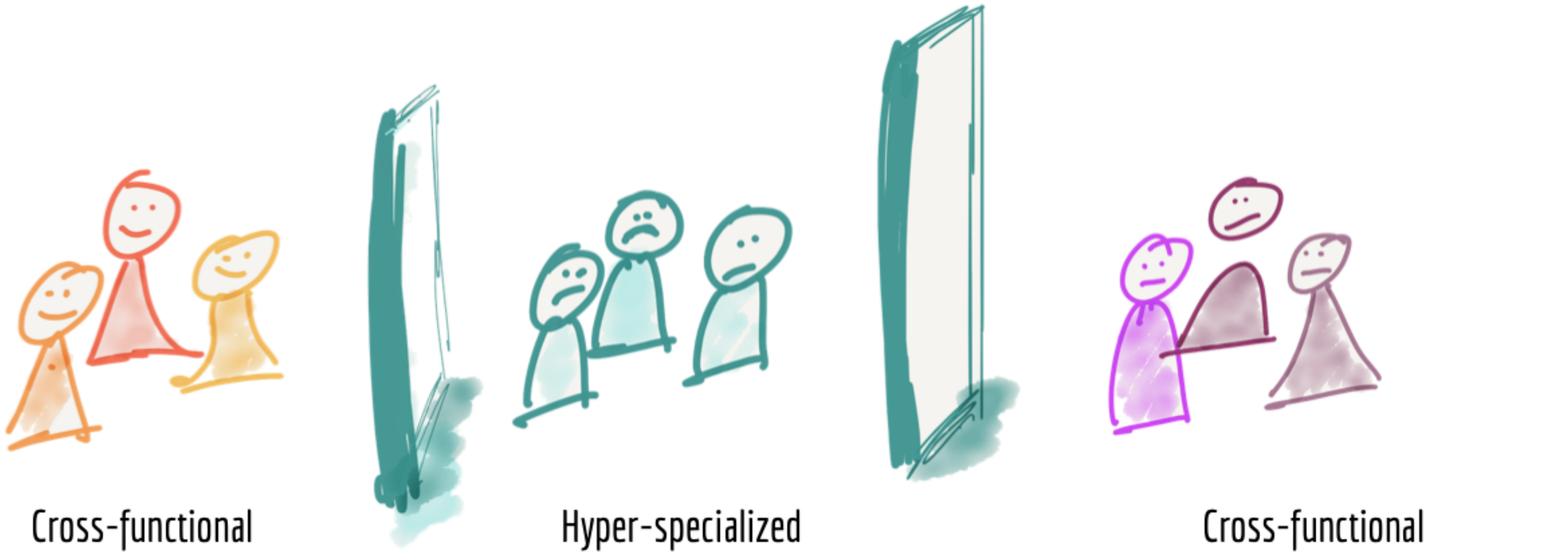


Architecture decomposition is orthogonal to the axis of change when introducing or enhancing features, leading to coupling and slower delivery



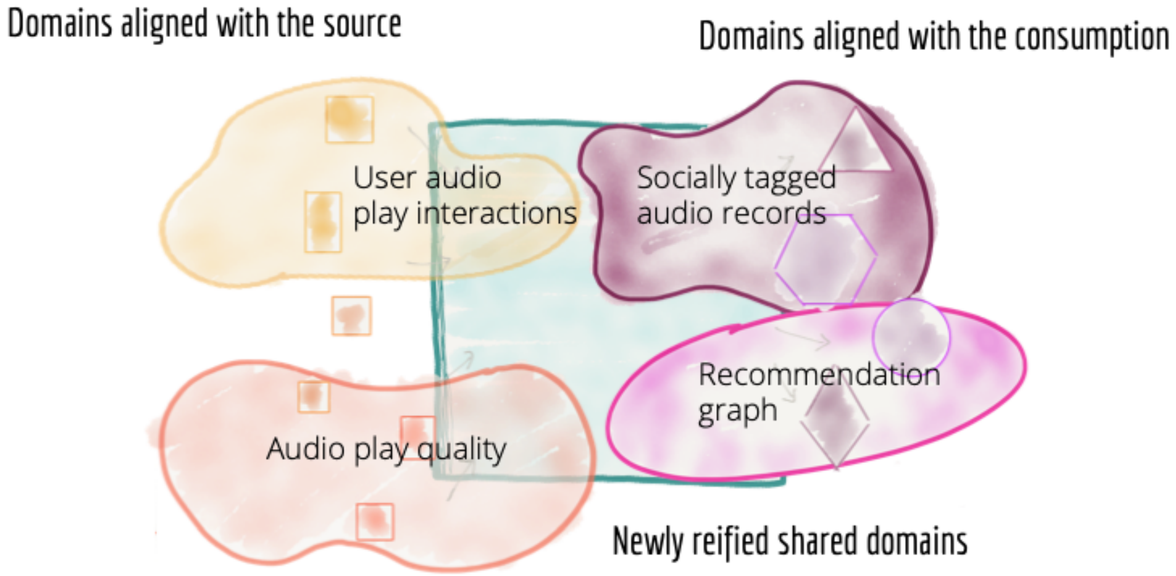
Architectural failure modes

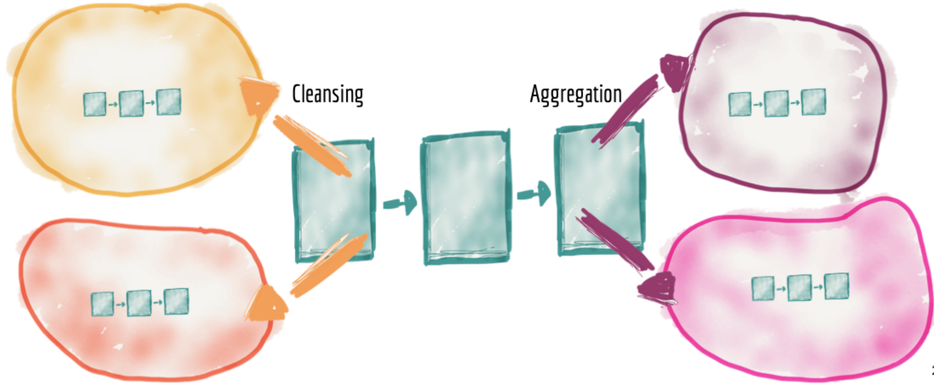
Siloed and hyper-specialized ownership



Data mesh

Decomposing the architecture and teams owning the data based on domains - source, consumer, and newly created shared domains





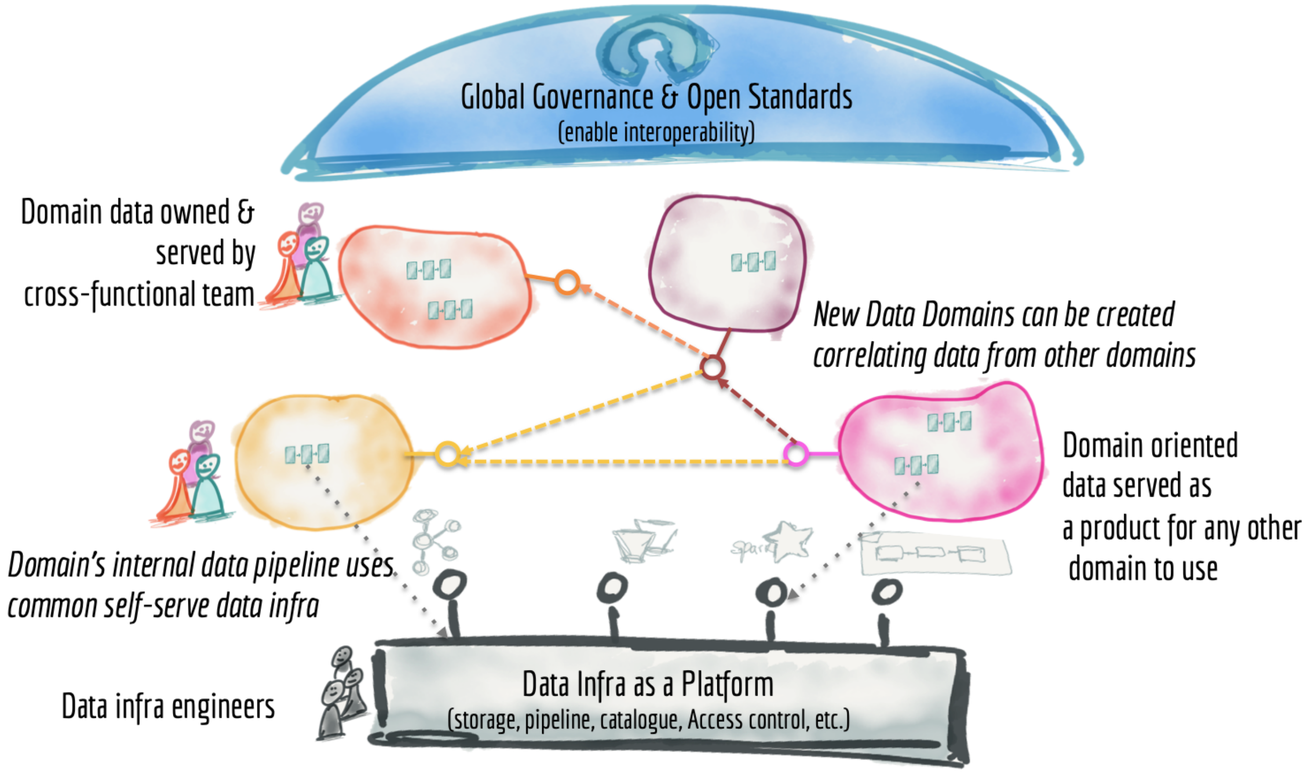
Data mesh

The third and current generation data platforms are more or less similar to the previous generation

A. Streaming for real-time data availability with architectures such as Kappa,

B. Unifying the batch and stream processing for data transformation with frameworks such as Apache Beam, as well as

C. Fully embracing cloud-based managed services for storage, data pipeline execution engines, and machine learning platforms



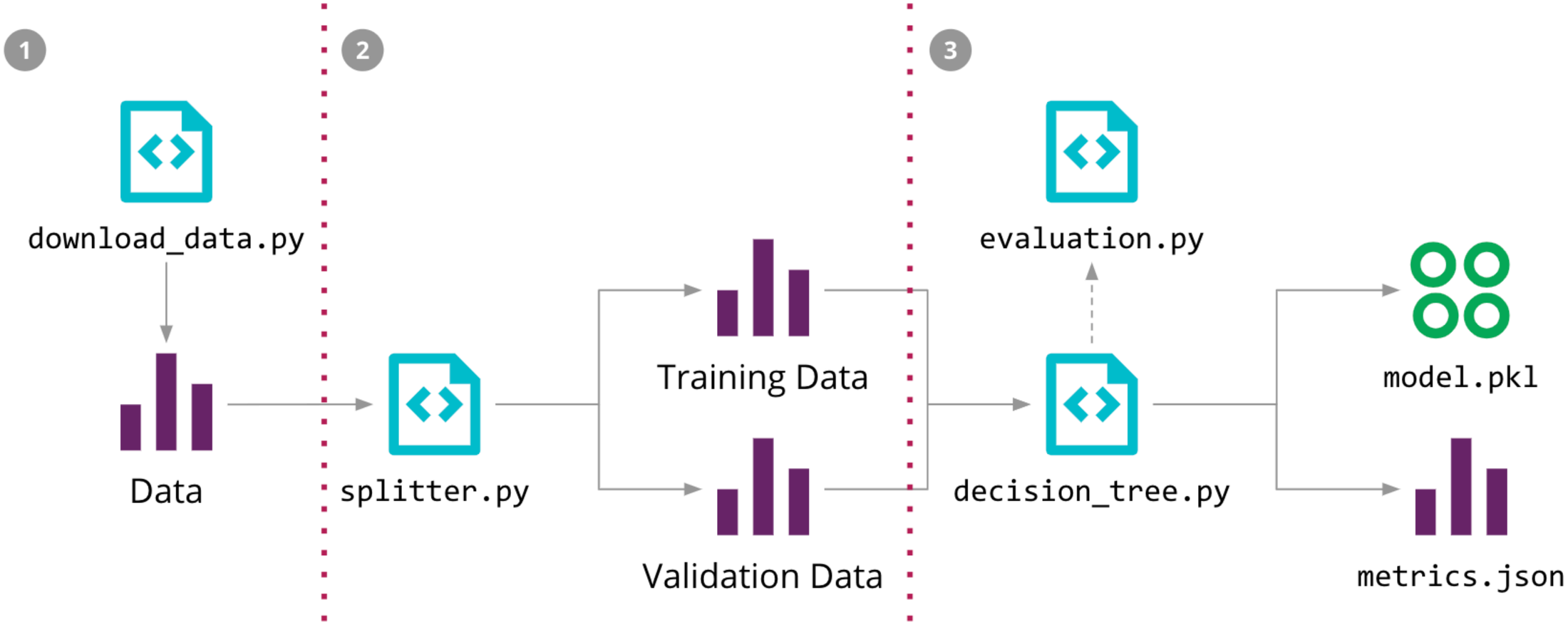
Discoverable Data

- A data product must be easily discoverable.
- A common implementation is to have a registry, a data catalogue, of all available data products with their meta information such as their owners, source of origin, lineage, sample datasets, etc.
- This centralized discoverability service allows data consumers, engineers and scientists in an organization, to find a dataset of their interest easily.
- Each domain data product must register itself with this centralized data catalogue for easy discoverability.

Addressable Data

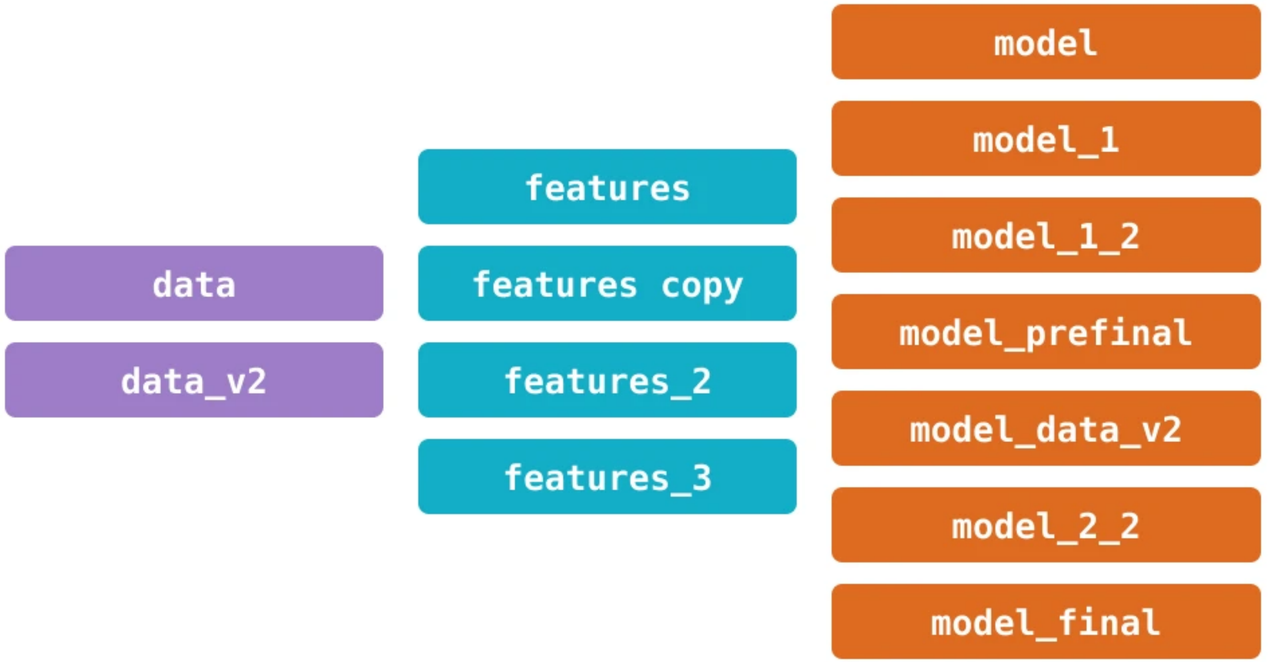
- A data product, once discovered, should have a unique address following a global convention that helps its users to programmatically access it.
- Organizations may adopt different naming conventions for their data, depending on the underlying storage and format of the data.
- Considering the ease of use as an objective, in a decentralized architecture, it is necessary for common conventions to be developed.
- Different domains might store and serve their datasets in different formats, events might be stored and accessed through streams such as Kafka topics, columnar datasets might use CSV files, or AWS S3 buckets of serialized Parquet files.
- A standard for addressability of datasets in a polyglot environment removes friction when finding and accessing information.

ML pipeline


1
2
3
download_data.py
Data
splitter.py
Training Data
Validation Data
evaluation.py
decision_tree.py
model.pkl
metrics.json

Versioning Data and Models

- How do we **keep track of changes** in data, source code, and ML models together?
- What's the best way to organize and store **variations** of these files and directories?

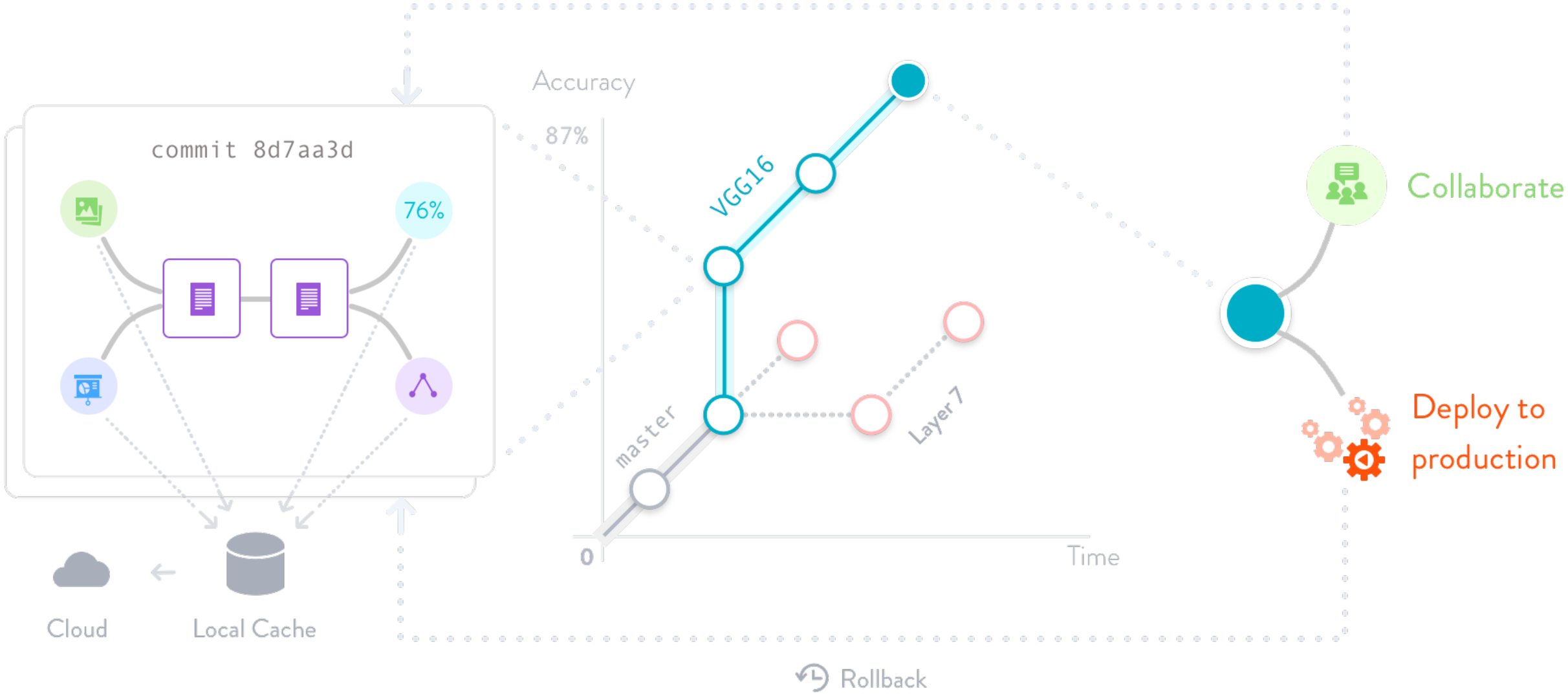


How about bookkeeping?

Another problem in the field has to do with bookkeeping

- being able to identify past data inputs and processes to understand their results, for knowledge sharing, or for debugging.

Configure ML pipeline: DVC tracks ML models and data sets



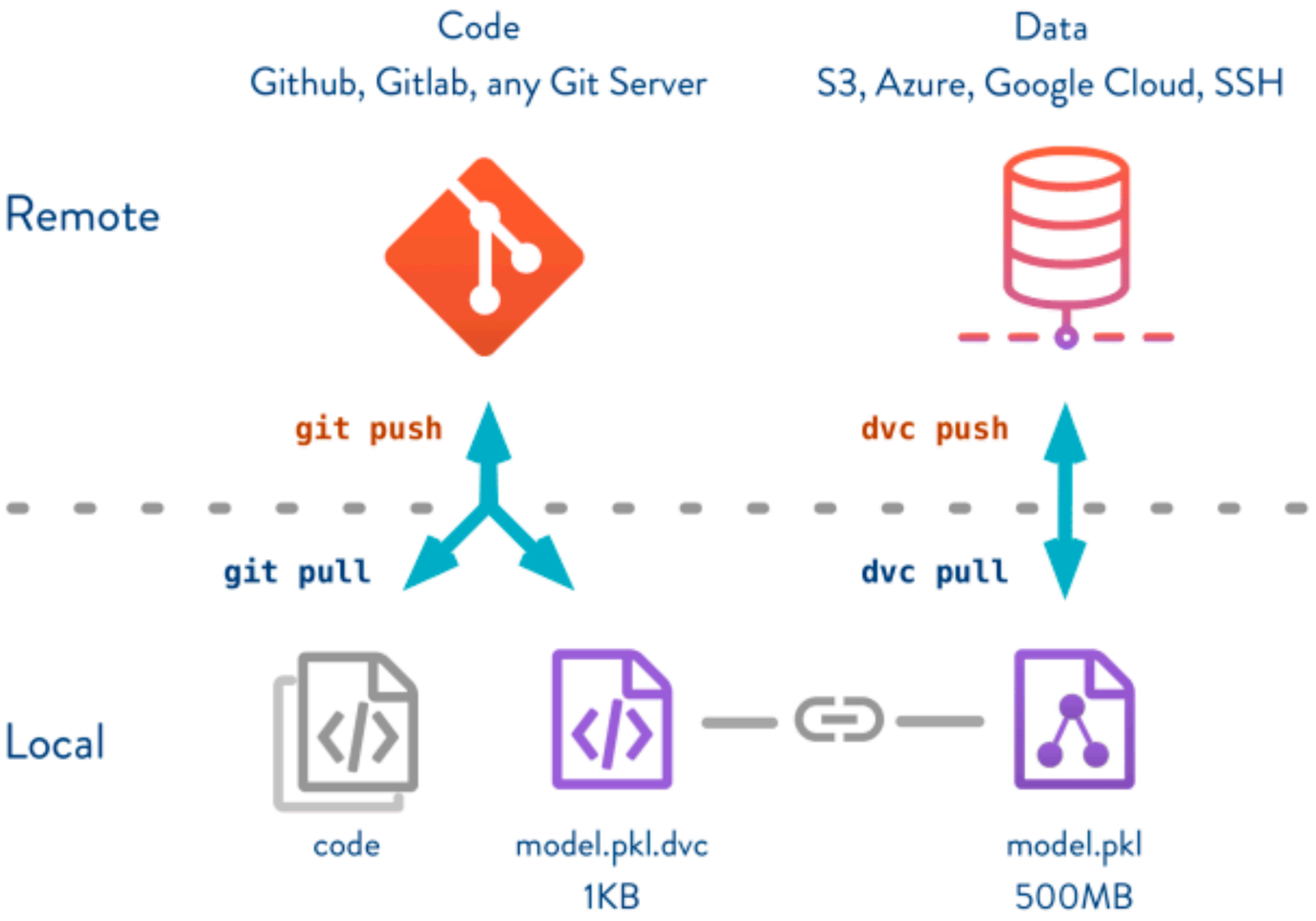
Configure ML pipeline: DVC tracks ML models and data sets

```
dvc run -f input.dvc \ ❶
  -d src/download_data.py -o data/raw/store47-2016.csv python src/download_data.py
dvc run -f split.dvc \ ❷
  -d data/raw/store47-2016.csv -d src/splitter.py \
  -o data/splitter/train.csv -o data/splitter/validation.csv python src/splitter.py
dvc run ❸
  -d data/splitter/train.csv -d data/splitter/validation.csv -d src/decision_tree.py \
  -o data/decision_tree/model.pkl -M results/metrics.json python src/decision_tree.py
```

Configure ML pipeline: DVC tracks ML models and data sets

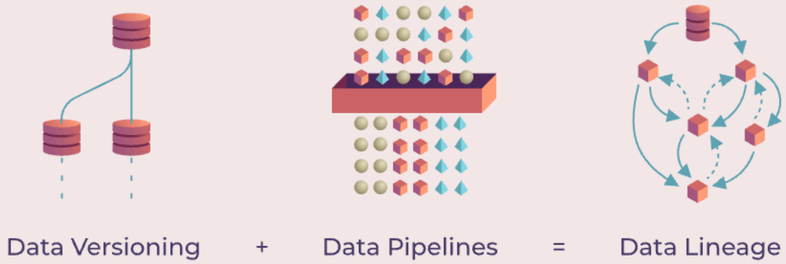
- Each run will create a file, that can be committed to version control
- DVC allows other people to reproduce the entire ML pipeline, by executing the *dvc repro* command.
- Once we find a suitable model, we will treat it as an artifact that needs to be *versioned* and *deployed* to production.
- With DVC, we can use the *dvc push* and *dvc pull* commands to publish and fetch it from *external storage*.

Configure ML pipeline: DVC tracks ML models and data sets



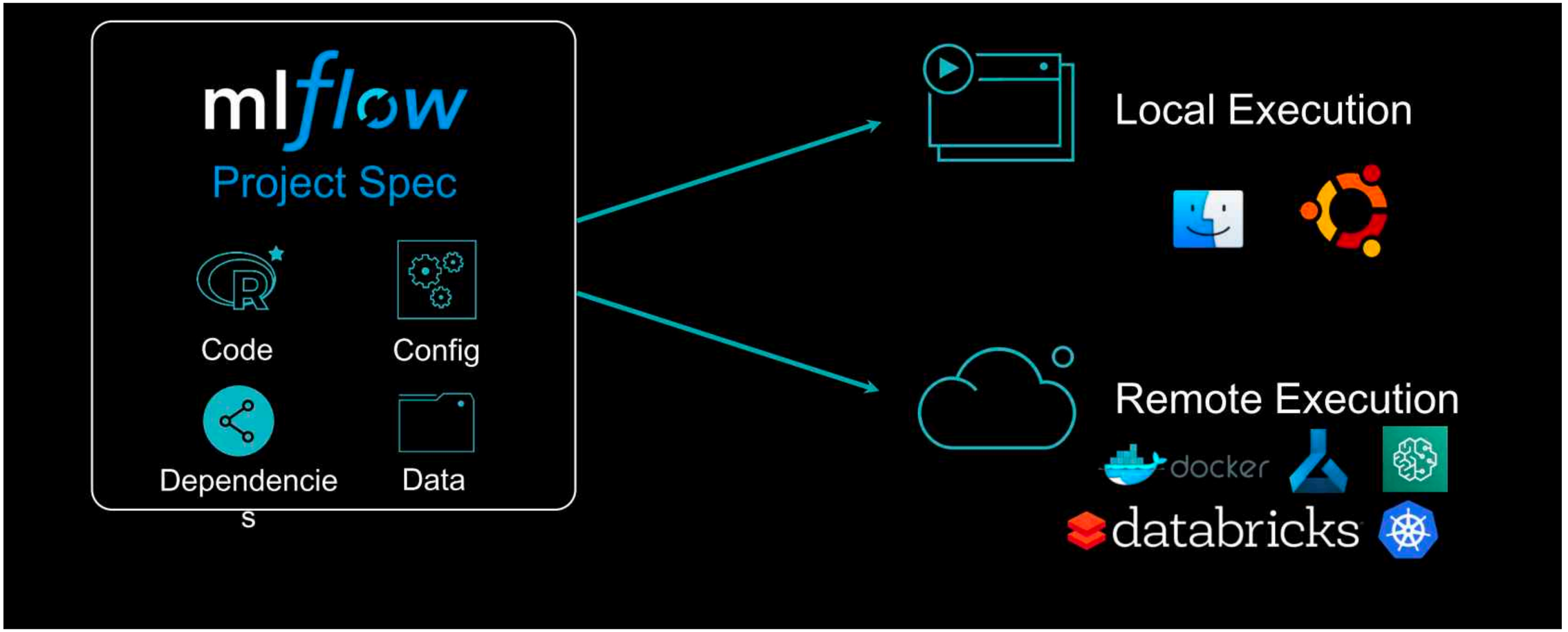
There are other open source tools for versioning

Pachyderm



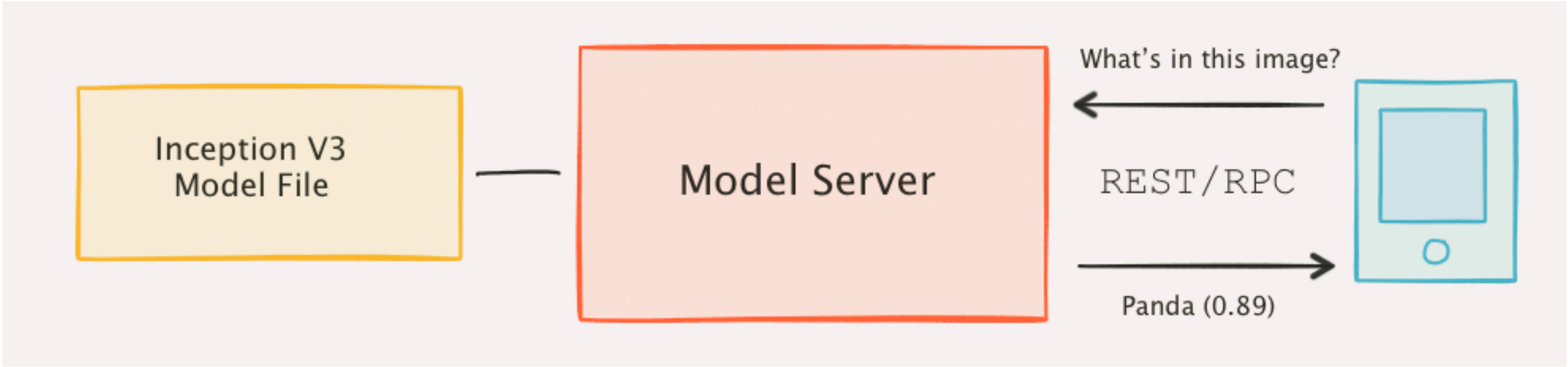
There are other open source tools for versioning

MLflow



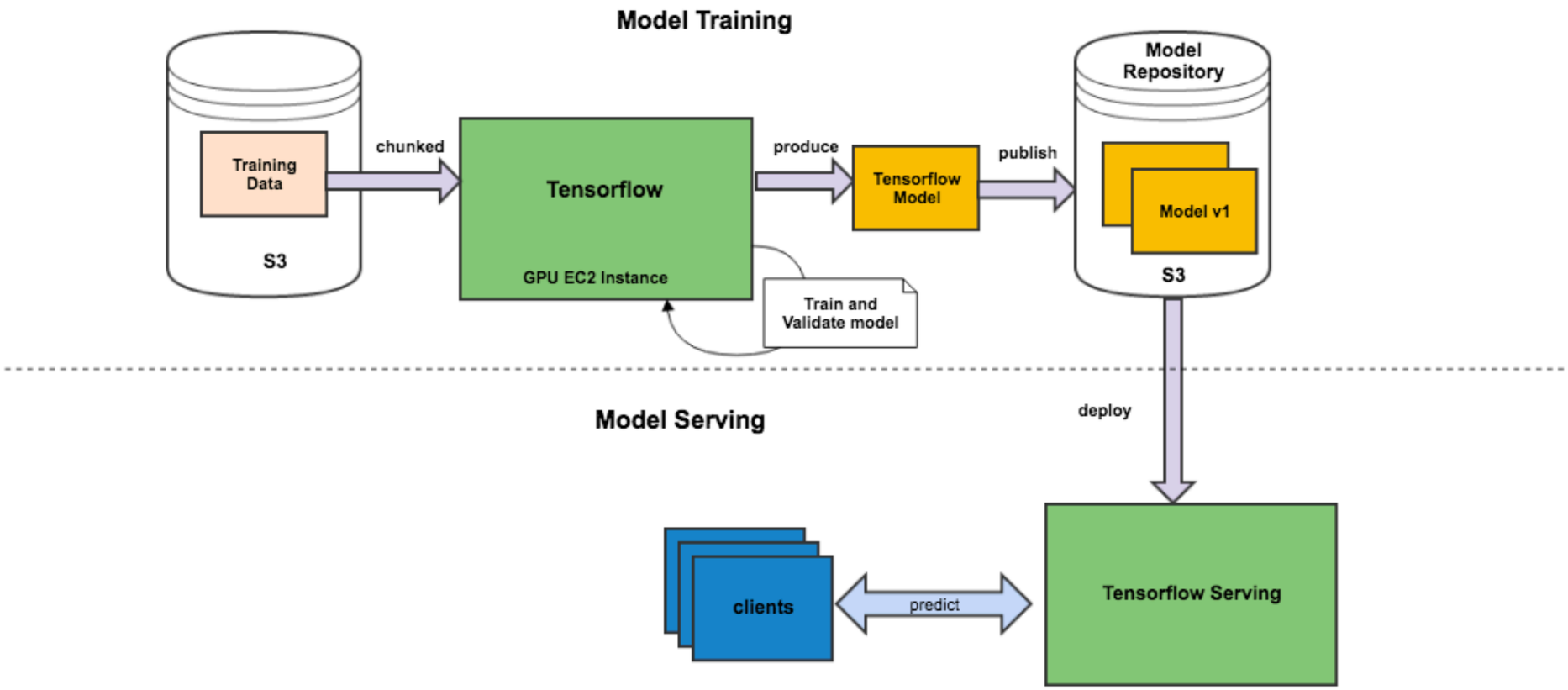
Model Serving

Abstract level



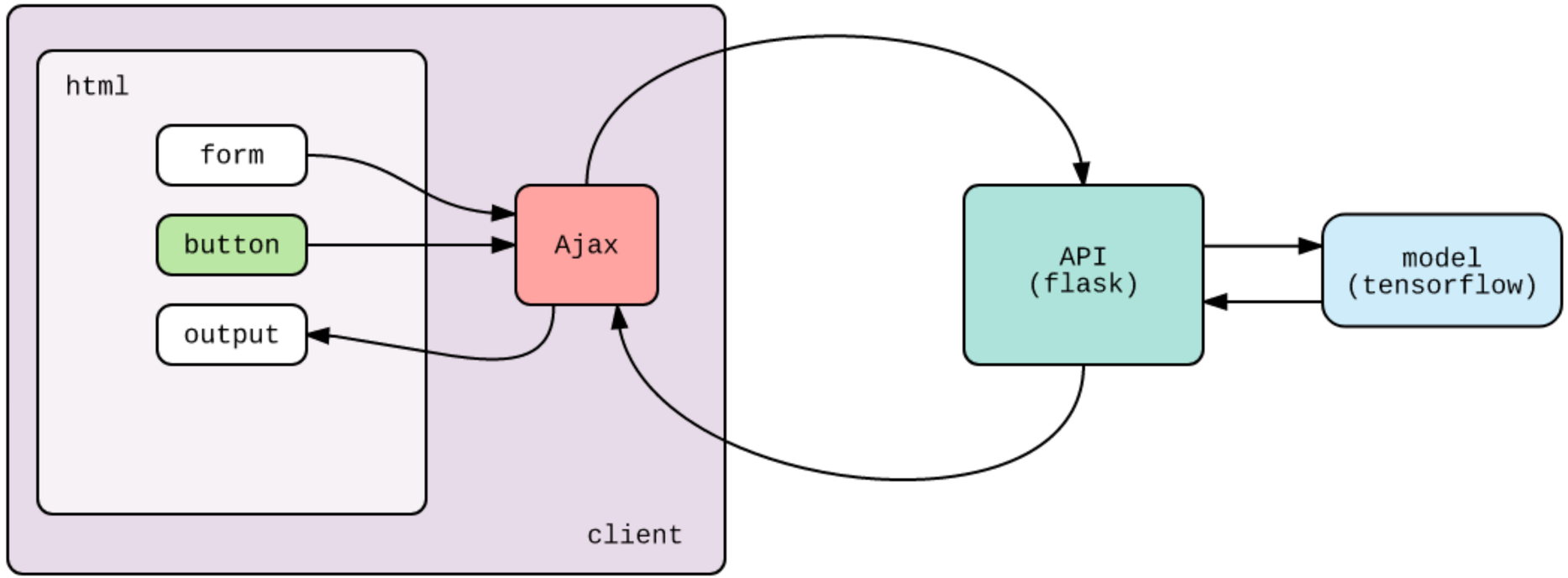
Model Serving

TF Serving



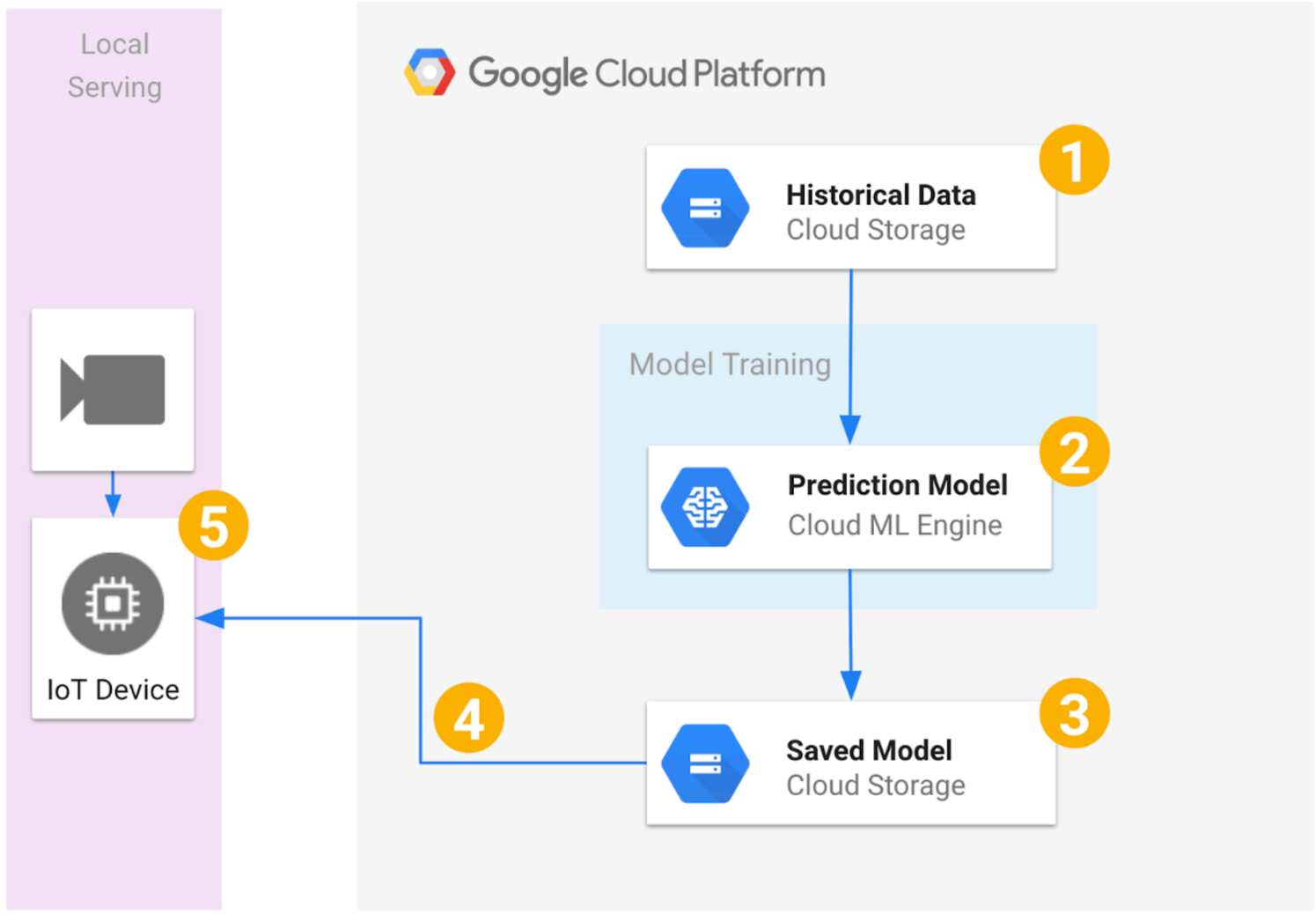
Model Serving

Web app



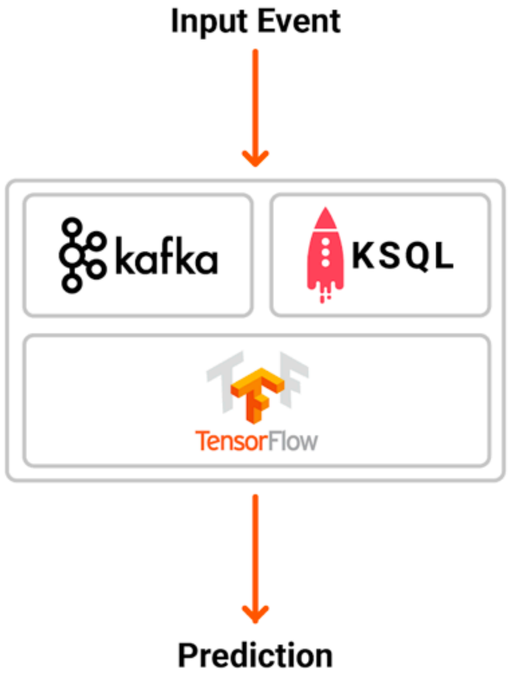
Model Serving

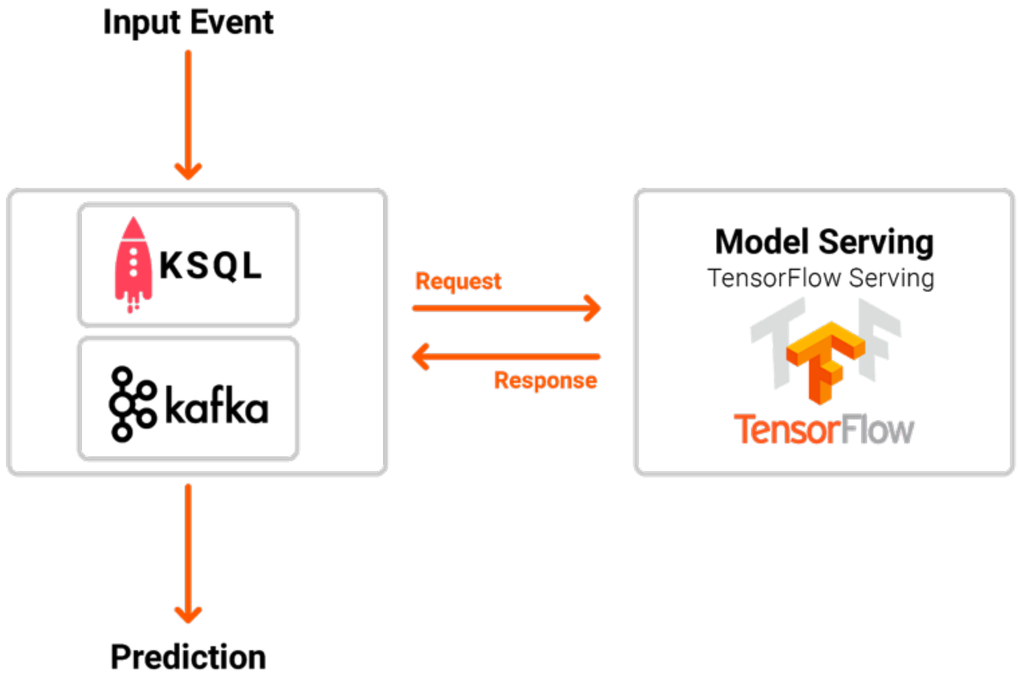
Internet of Thing



Model Serving

Stream Processing System





Model Serving

Embedded model

- Simple approach
- You treat the model artifact as a dependency that is built and packaged within the consuming application.
- You can treat the application artifact and version as being a combination of the application code and the chosen model.

Model Serving

Model deployed as a separate service

- The model is wrapped in a service that can be deployed independently of the consuming applications.
- This allows updates to the model to be released independently, but it can also introduce latency at inference time
- There will be some sort of remote invocation required for each prediction.

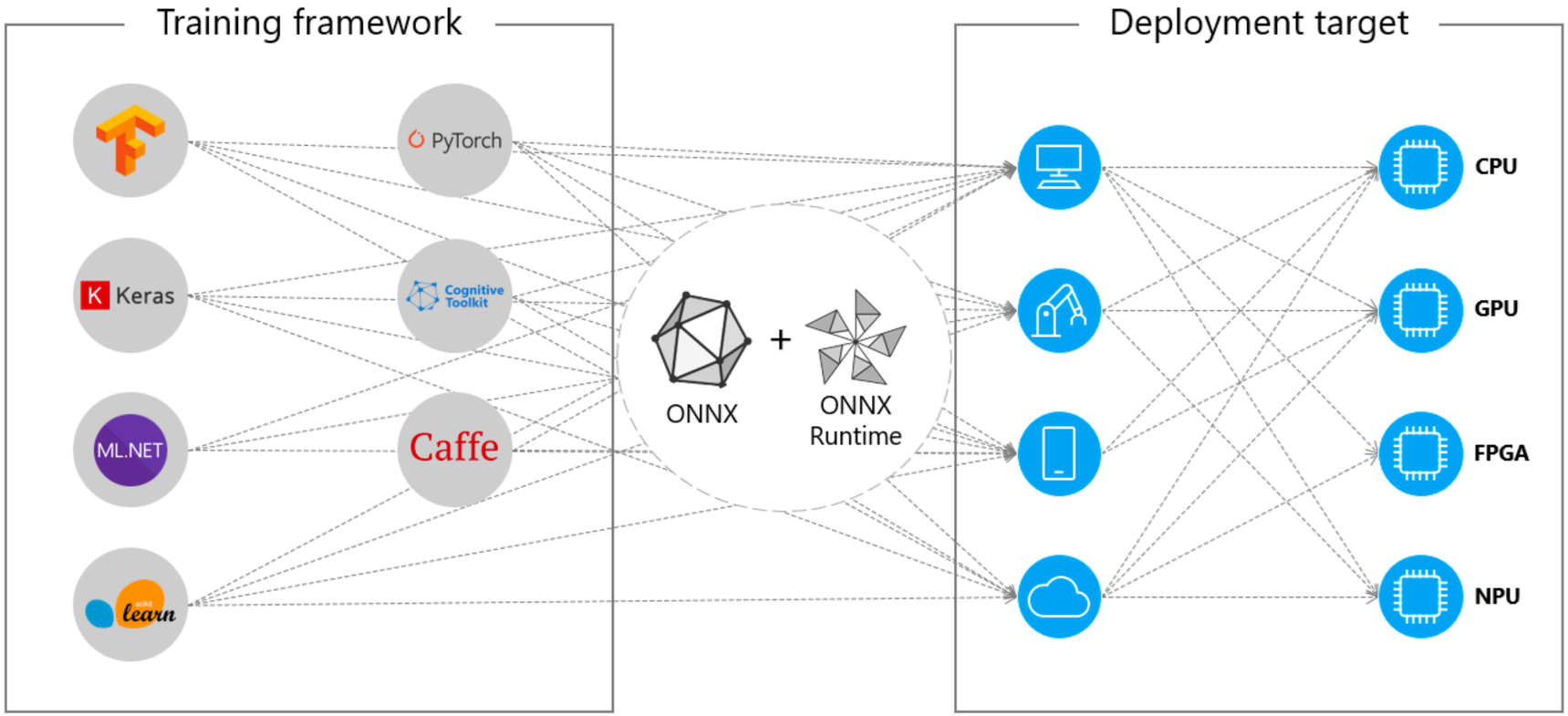
Model Serving

Model published as data

- The model is also treated and published independently,
- But the consuming application will ingest it as data at runtime.
- We have seen this used in streaming/real-time scenarios where the application can subscribe to events that are published whenever a new model version is released, and ingest them into memory while continuing to predict using the previous version.
- Software release patterns such as Canary Releases can also be applied in this scenario.

Export ML models to production environment

Open Neural Network Exchange

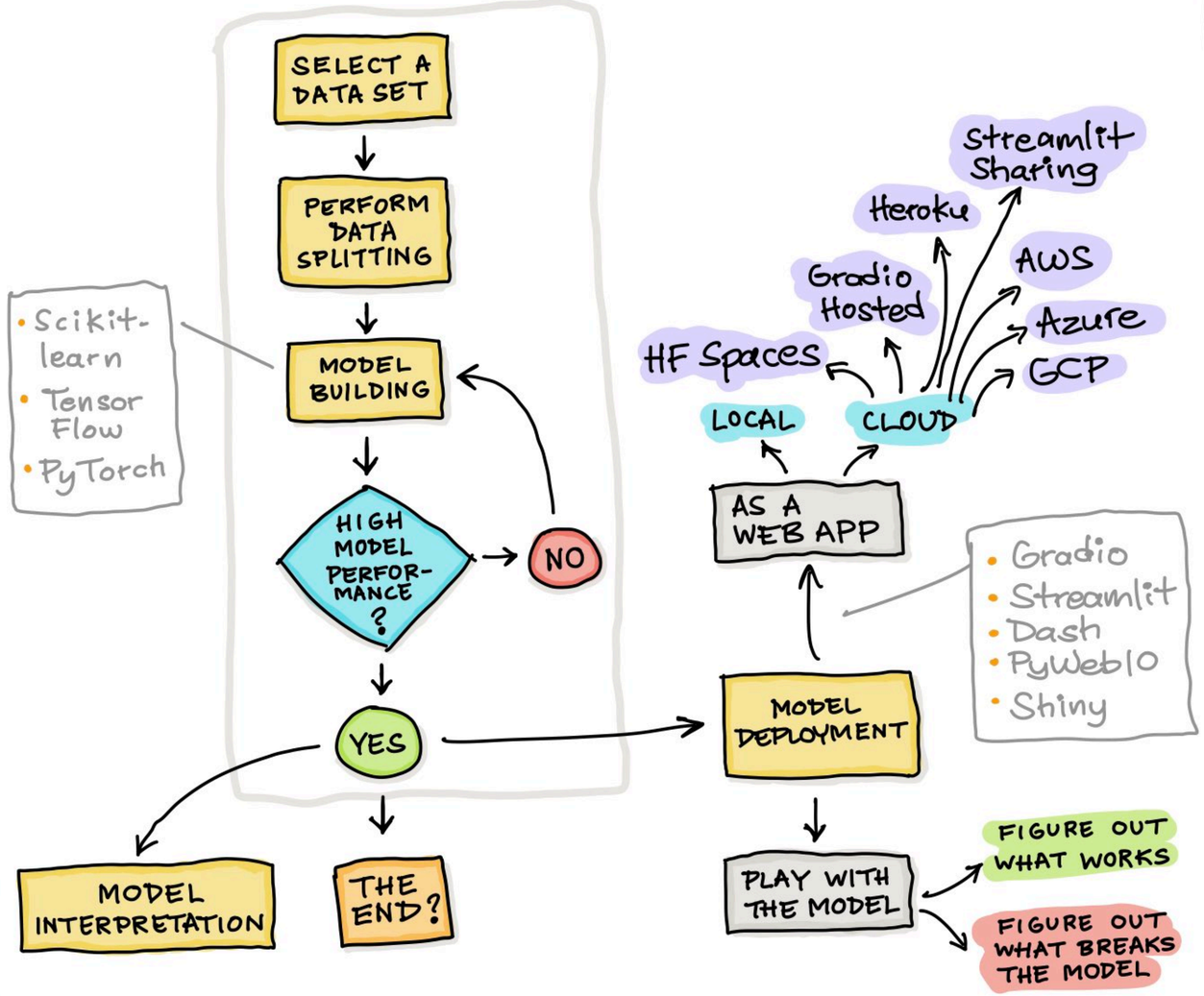


Testing and Quality in Machine Learning

- Regardless of which pattern you decide to use, there is always an implicit contract between the model and its consumers.
- The model will usually expect input data in a certain shape, and if Data Scientists change that contract to require new input or add new features, you can cause integration issues and break the applications using it.
- So testing becomes important.

Continuous Delivery for Machine Learning

QUICKLY DEPLOY MACHINE LEARNING MODELS



DRAWN BY CHANIN NANTASENAMAT

DATA PROFESSOR http://youtube.com/dataprofessor

Gradio powering clinical trials of machine learning models

4 Model's mistakes collected

1 Interdisciplinary team build/improve skin cancer classification model

2 They deploy it easily using Gradio

3 Model undergoes clinical validation at multiple sites

Testing Machine Learning Systems

Validating data

- Tests to **validate input data** against the expected schema, or to validate our **assumptions** about its valid values:
  - Values fall within expected ranges
  - Values are not null
- Unit tests to check **features** are calculated correctly:
  - Numeric features are scaled or normalized,
  - One-hot encoded vectors contain all zeroes and a single 1
  - Missing values are replaced appropriately

Testing Machine Learning Systems

Validating component integration

- Test the **integration** between different services:
  - Contract Tests to validate that the expected model interface is compatible with the consuming application.
- Test that the **exported model** still produces the same results:
  - Running the original and the productionized models against the same validation dataset, and comparing the results are the same.

Testing Machine Learning Systems

Validating the model quality

- ML **model performance** is non-deterministic.
- Collect and monitor **metrics** to evaluate a model's performance,
  - Error rates, accuracy
  - Precision, recall
  - AUC, ROC, confusion matrix
- **Threshold Tests** in our pipeline, to ensure that new models don't degrade against a known performance baseline.

Testing Machine Learning Systems

Validating model bias and fairness

- Check how the model performs against **baselines** for specific **data slices**:
  - Inherent bias in the training data where there are many more data points for a given value of a feature (e.g. race, gender, or region) compared to the actual distribution in the real world.
- A tool like **Facets** can help you visualize those slices and the distribution of values across the features in your datasets.

Testing Machine Learning Systems

Integration Test

- When models are **distributed or exported** to be used by a different application, the engineered features are **calculated differently** between training and serving time.
- Distribute a **holdout dataset** along with the model artifact, and allow the consuming application team to reassess the model's performance against the holdout dataset after it is integrated.
- This would be the equivalent of a broad **Integration Test** in traditional software development.

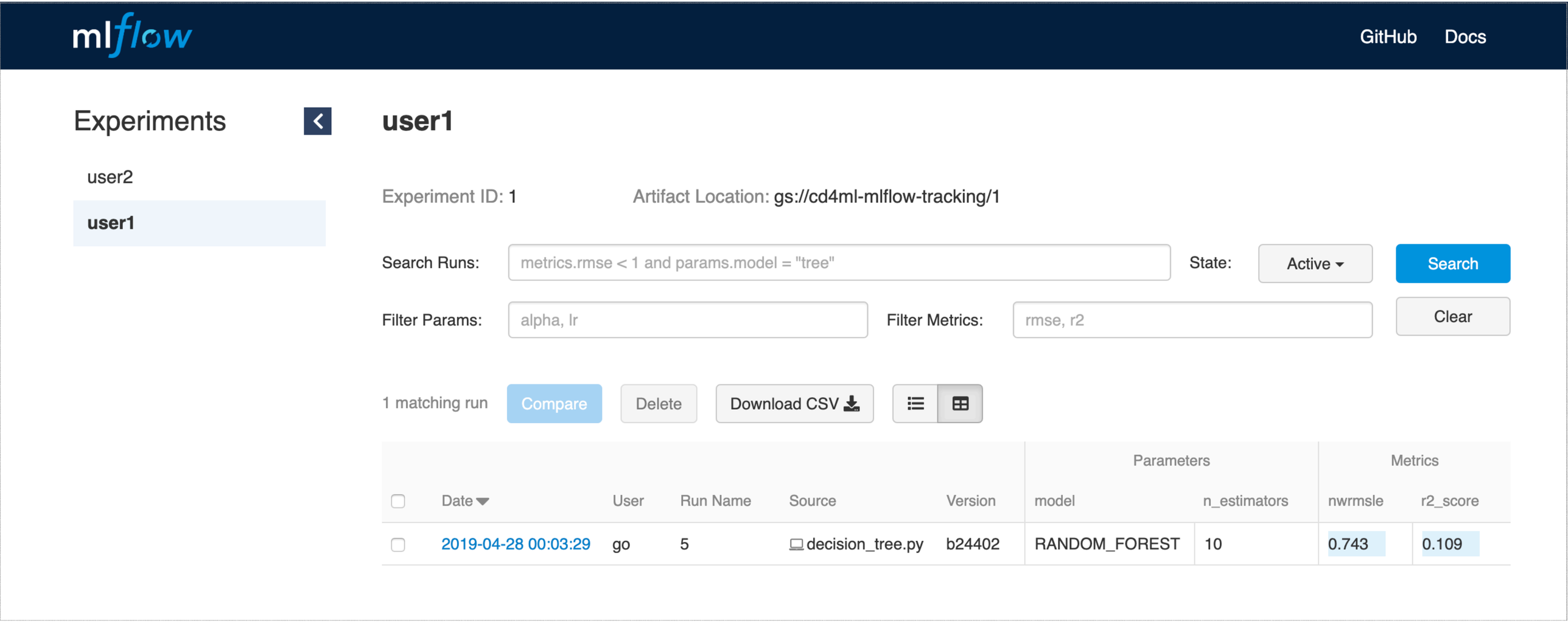
Governance process for ML Systems

Experiments Tracking

- To capture and display information that will allow humans to decide if and which model should be promoted to production.
- It is common that you will have multiple experiments being tried in parallel, and many of them might not ever make it to production.
- The code for many of these experiments will be thrown away, and only a few of them will be deemed worthy of making it to production.
- Different Git branches to track the different experiments in source control.
- Tools such as DVC can fetch and display metrics from experiments running in different branches or tags, making it easy to navigate between them.

Governance process for ML Systems

MLflow Tracking web UI



Model Deployment

Multiple models

- More than one model performing the same task.
  - Train a model to predict demand for each product.
- Deploying the models as a separate service might be better for consuming applications to get predictions with a single API call.
- You can later evolve how many models are needed behind that Published Interface.

Model Deployment

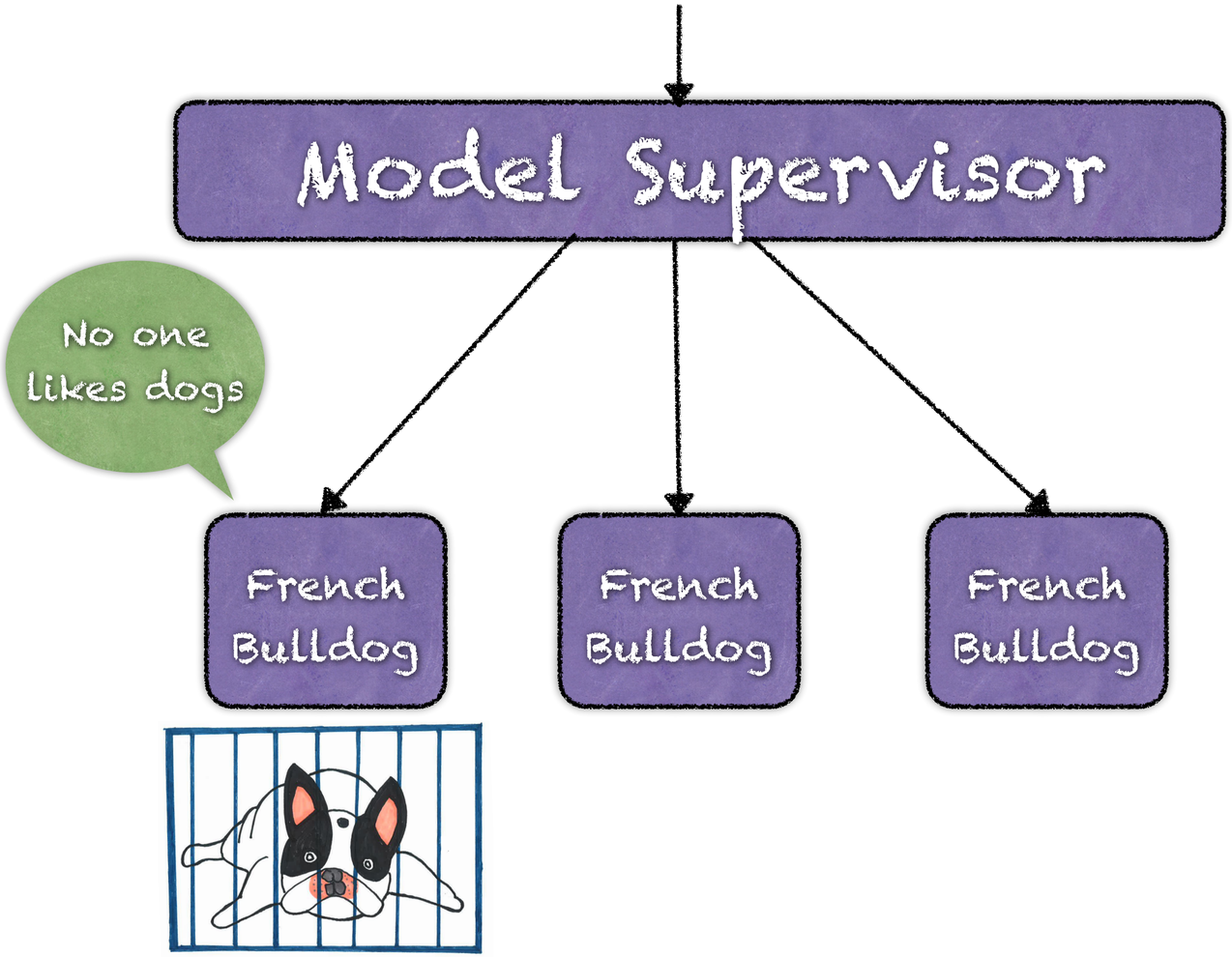
Shadow models

- Deploy the new model side-by-side with the current one, as a shadow model
- Send the same production traffic to gather data on how the shadow model performs before promoting it into the production.

Model Deployment

Competing models

- Multiple versions of the model in production — like an A/B test
  - Infrastructure and routing rules required to ensure the traffic is being redirected to the right models.
  - To gather enough data to make statistically significant decisions, which can take some time.
- Evaluating multiple competing models is Multi-Armed Bandits,
  - To define a way to calculate and monitor the reward associated with using each model.


Model Supervisor
No one likes dogs
French Bulldog
French Bulldog
French Bulldog

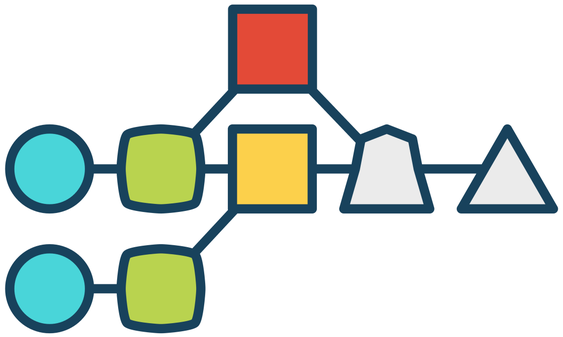
Model Deployment

Online learning models

- To use algorithms and techniques that can continuously improve its performance with the arrival of new data.
- Constantly learning in production.
- Extra complexities, as versioning the model as a static artifact won't yield the same results if it is not fed the same data.
- You will need to version not only the training data, but also the production data that will impact the model's performance.

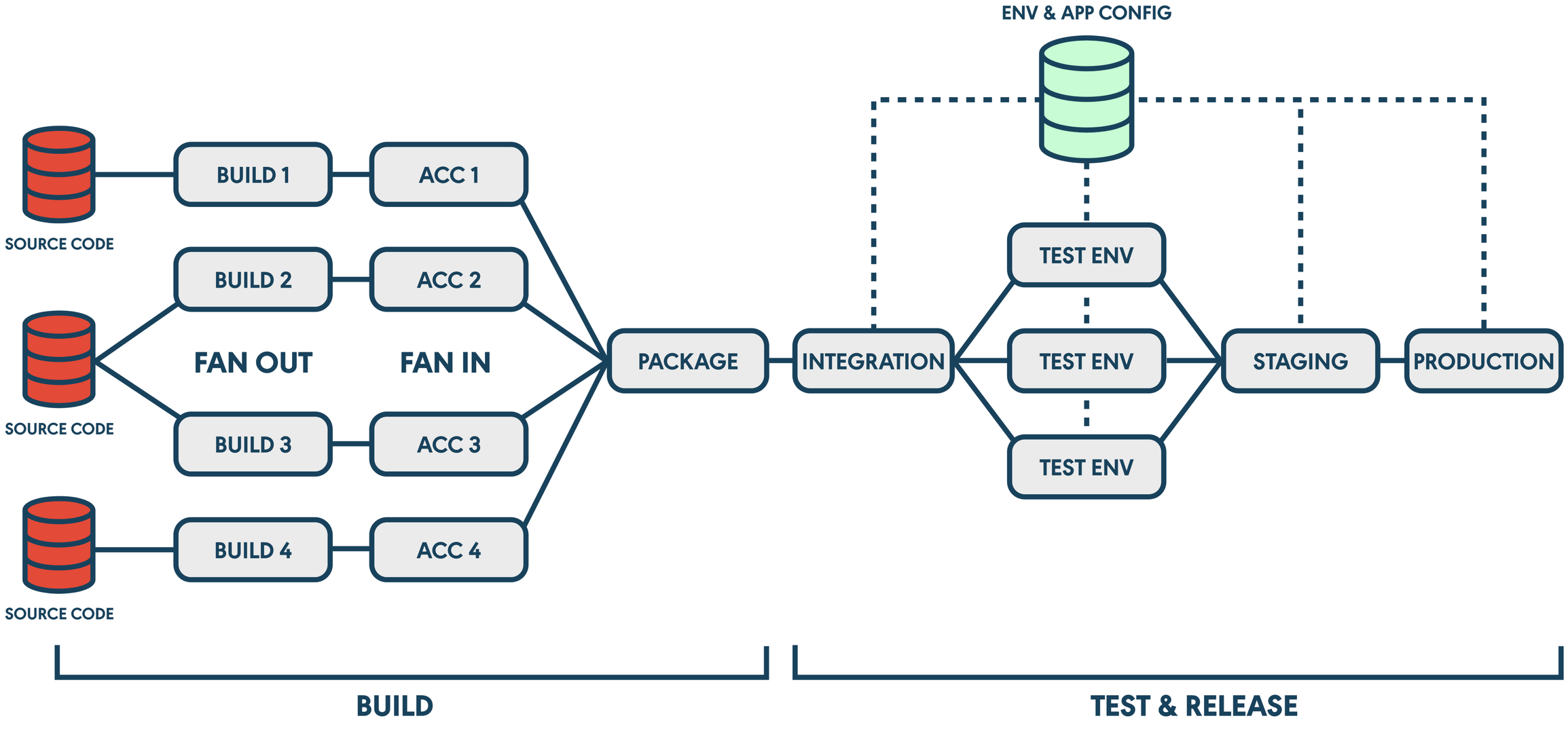
Orchestration in ML Pipelines

- Provisioning of infrastructure and the execution of the ML Pipelines to train and capture metrics from multiple model experiments
- Building, testing, and deploying Data Pipelines
- Testing and validation to decide which models to promote
- Provisioning of infrastructure and deployment of models to production



Continuous Integration and Delivery

GoCD

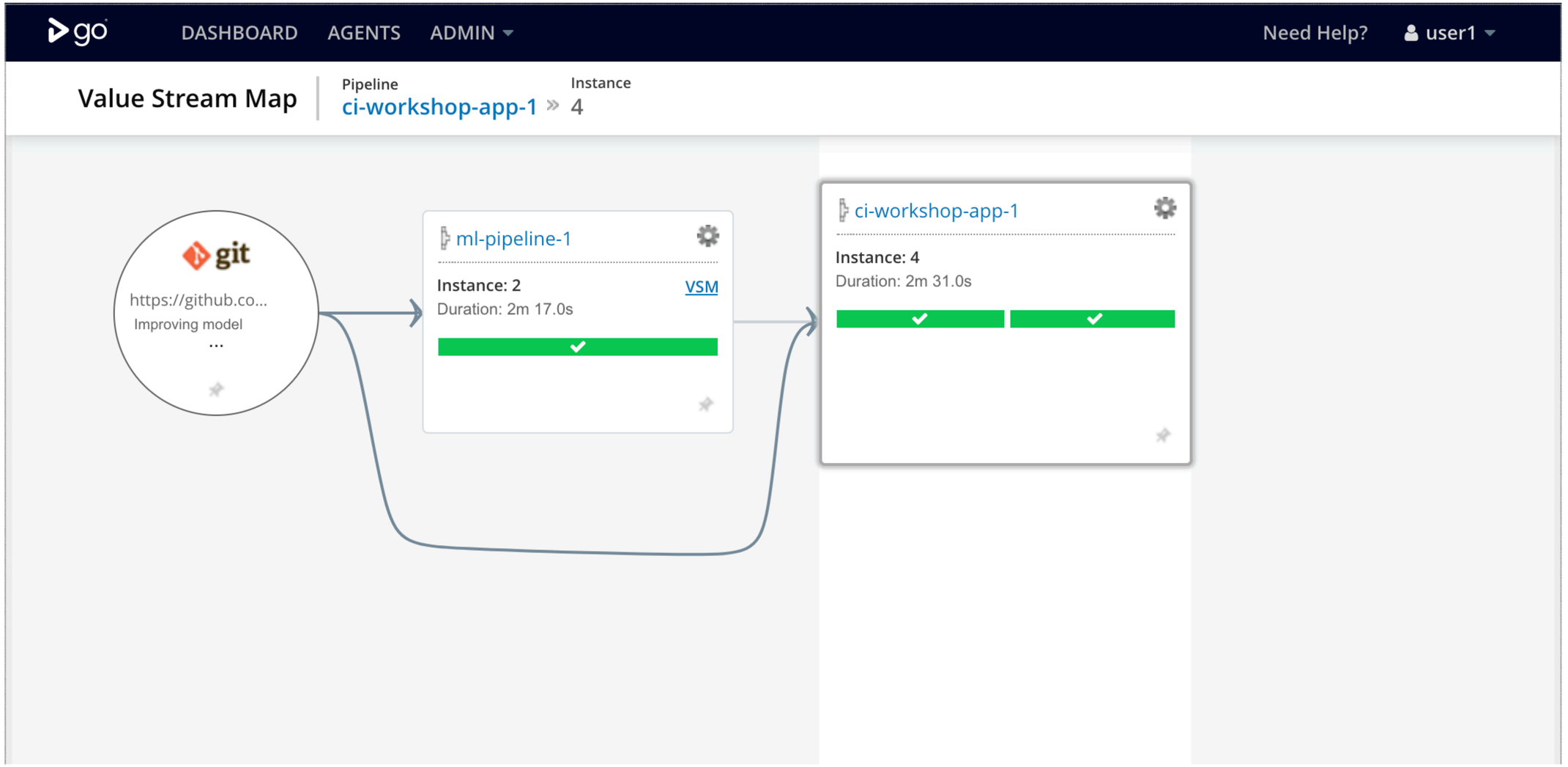


A Continuous Delivery Scenario for ML

1. **Machine Learning Pipeline**:
   - To train and evaluate ML models
   - To execute threshold test to decide if the model can be promoted or not
   - *dvc push* to publish it as an artifact
2. **Application Deployment Pipeline**:
   - To build and test the application code
   - To fetch the promoted model from the upstream pipeline using *dvc pull*
   - To package a new combined artifact that contains the model and the application as a Docker image
   - To deploy them to a production cluster

Continuous Delivery for Machine Learning

Combining Machine Learning Pipeline and Application Deployment Pipeline



ML Model Monitoring

How models perform in production and rollback mechanisms

- **Model inputs**:
  - What data is being fed to the models, identifying training-serving skew.
- **Model outputs**:
  - What predictions and recommendations are the models making from these inputs, to understand how the model is performing with real data.

ML Model Monitoring

How models perform in production and rollback mechanisms

- **Model interpretability outputs**:
  - Metrics such as model coefficients, ELI5, or LIME outputs that allow further investigation to understand how the models are making predictions to identify potential overfit or bias that was not found during training.

hi there, i am here looking for some help. my friend is a interic
graphics software on pc. any suggestion on which software to
sophisticated software(the more features it has,the better)

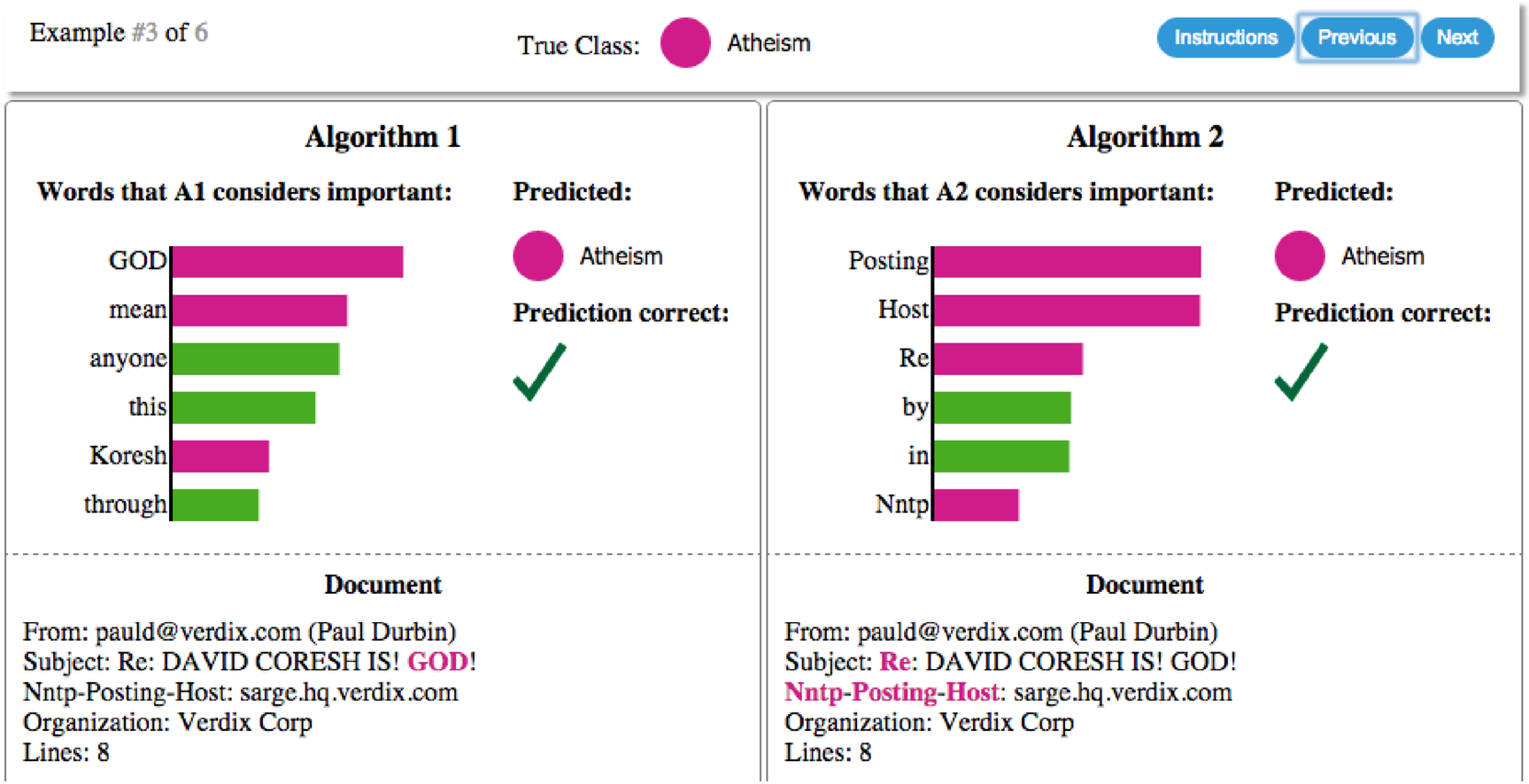
y=0 (probability **0.000**) top features		
Contribution[?]	Feature	Value
+0.301	<BIAS>	1.000
+0.064	color_intensity	8.500
+0.004	malic_acid	4.600
-0.018	alcalinity_of_ash	25.000
-0.044	total_phenols	1.980
-0.055	flavanoids	0.960
-0.100	proline	630.000
-0.153	hue	0.670

y=1 (probability **0.100**) top features		
Contribution[?]	Feature	Value
+0.427	<BIAS>	1.000
+0.033	proline	630.000
+0.022	od280/od315_of_diluted_wines	1.920
+0.009	alcalinity_of_ash	25.000
+0.006	total_phenols	1.980
-0.003	proanthocyanins	1.110
-0.010	alcohol	13.400
-0.028	flavanoids	0.960
-0.060	malic_acid	4.600
-0.137	hue	0.670
-0.160	color_intensity	8.500

y=2 (probability **0.900**) top features		
Contribution[?]	Feature	Value
+0.289	hue	0.670
+0.272	<BIAS>	1.000
+0.095	color_intensity	8.500
+0.083	flavanoids	0.960
+0.067	proline	630.000
+0.056	malic_acid	4.600
+0.038	total_phenols	1.980
+0.010	alcohol	13.400
+0.009	alcalinity_of_ash	25.000
+0.003	proanthocyanins	1.110
-0.022	od280/od315_of_diluted_wines	1.920

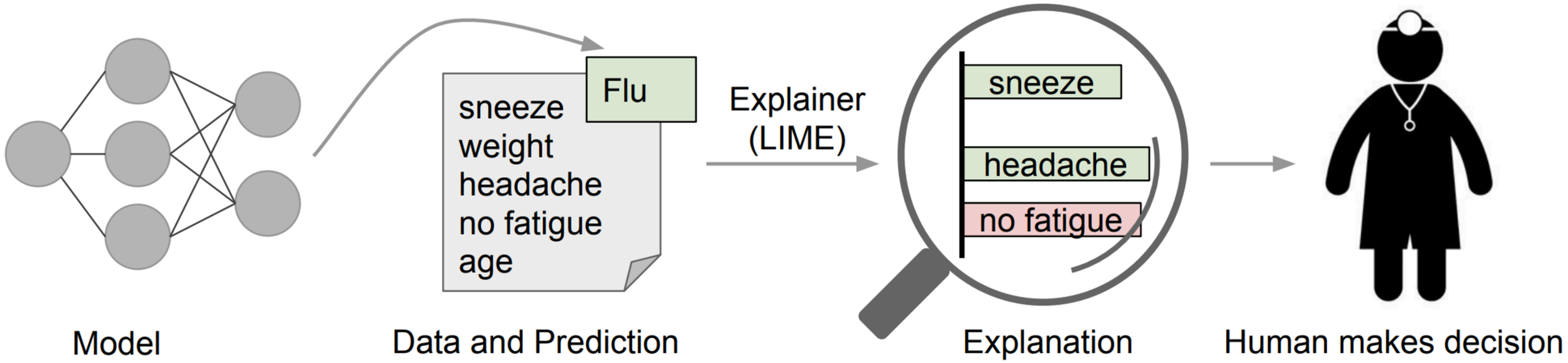
“Why Should I Trust You?”

Explaining the Predictions of Any Classifier



Explaining individual predictions

A model predicts that a patient has the flu, and LIME highlights the symptoms in the patient's history that led to the prediction



ML Model Monitoring

How models perform in production and rollback mechanisms

- **Model outputs and decisions**:
  - What predictions our models are making given the production input data, and also which decisions are being made with those predictions.
  - Sometimes the application might choose to ignore the model and make a decision based on pre-defined rules (or to avoid future bias).

ML Model Monitoring

How models perform in production and rollback mechanisms

- **User action and rewards**:
  - Based on further user action, we can capture reward metrics to understand if the model is having the desired effect.
  - For example, if we display product recommendations, we can track when the user decides to purchase the recommended product as a reward.

A pipeline for model monitoring
ELK

- **Elasticsearch**: an open source *search* engine.
- **Logstash**: an open source data collector for unified *logging* layer.
- **Kibana**: an open source web UI that makes it easy to explore and *visualize* the data indexed by Elasticsearch.

A pipeline for model monitoring

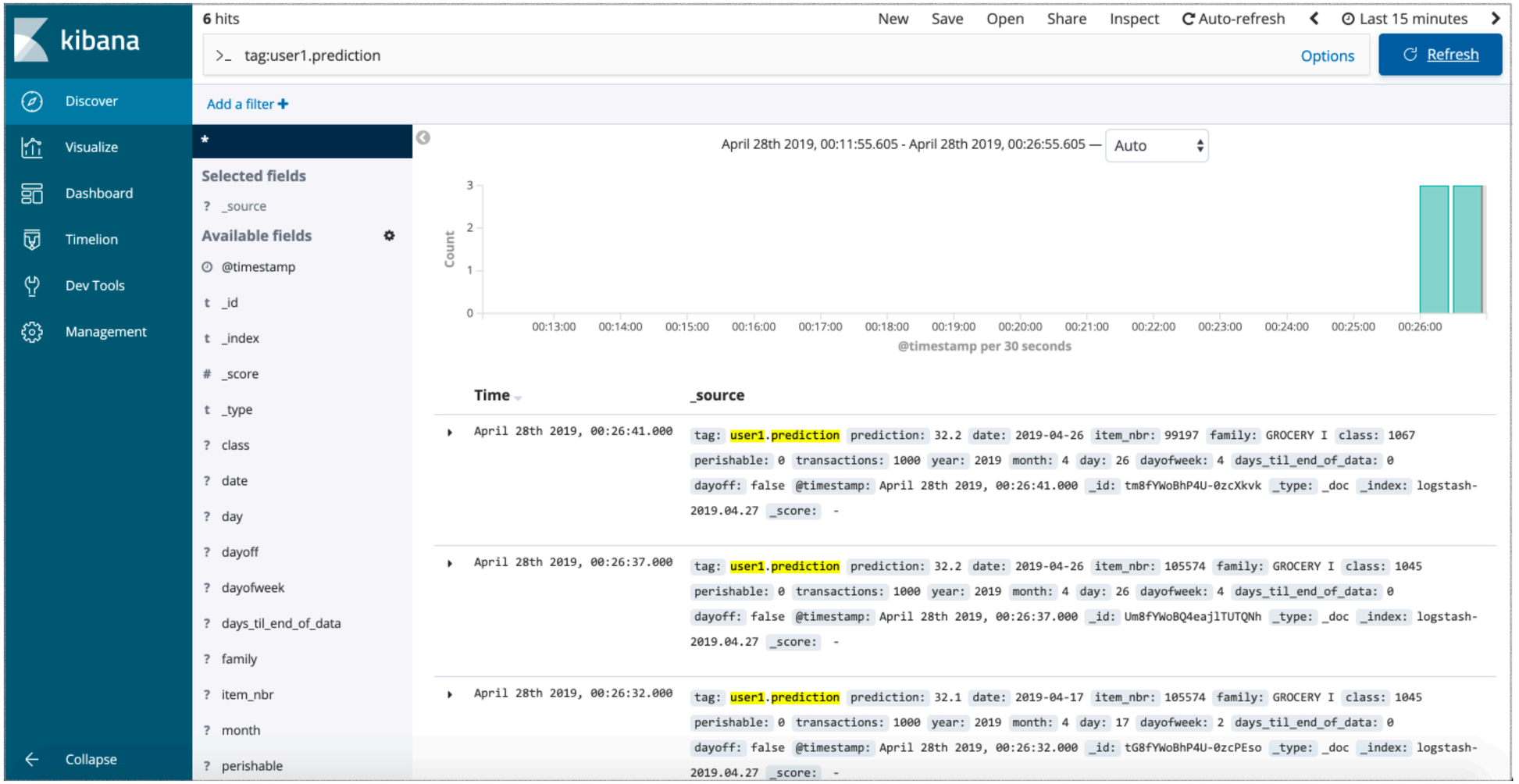
ELK

Logging

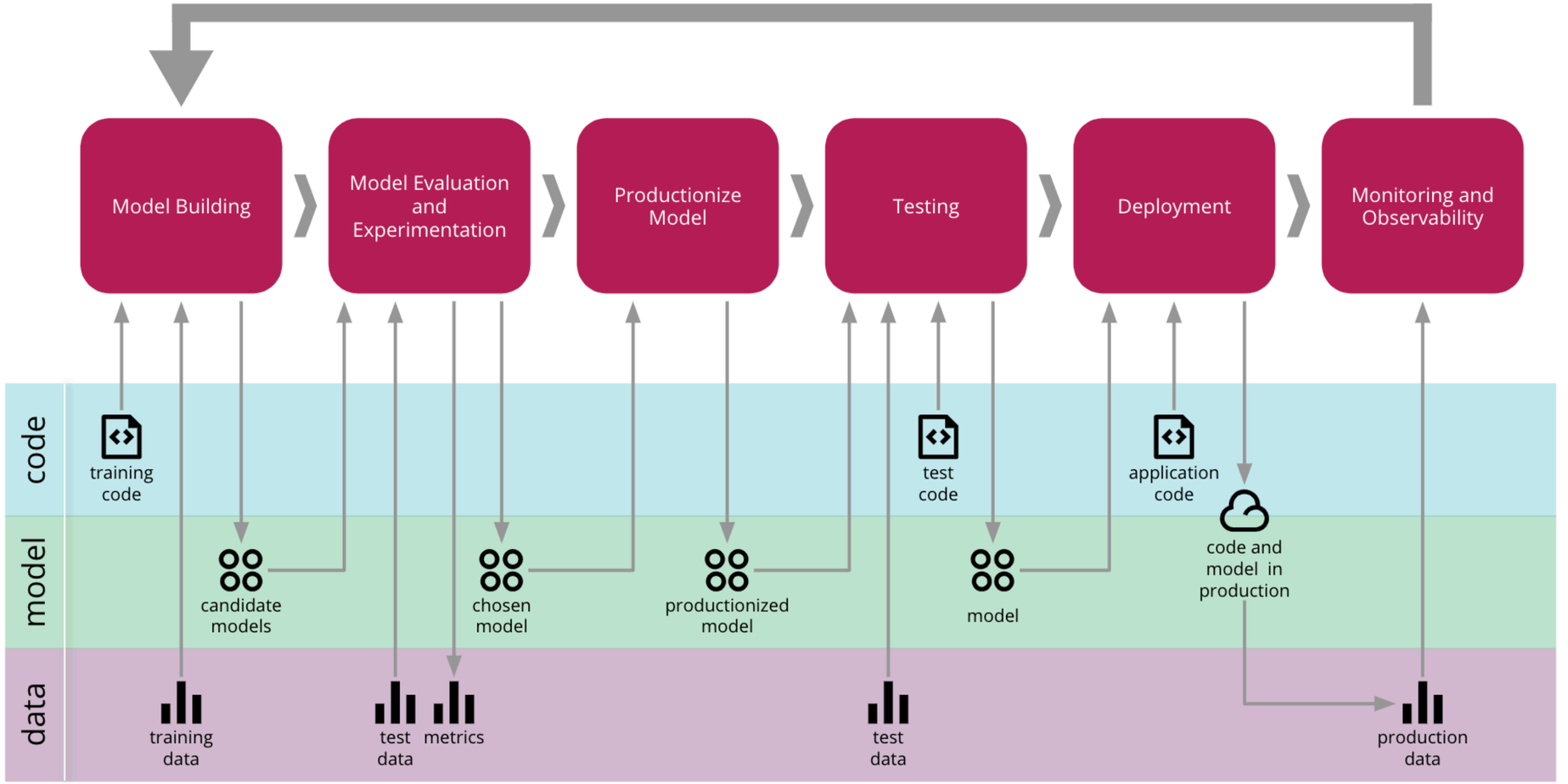
predict_with_logging.py...

```
df = pd.DataFrame(data=data, index=['row1'])
df = decision_tree.encode_categorical_columns(df)
pred = model.predict(df)
logger = sender.FluentSender(TENANT, host=FLUENTD_HOST, port=int(FLUENTD_PORT))
log_payload = {'prediction': pred[0], **data}
logger.emit('prediction', log_payload)
```

A pipeline for model monitoring



An End-to-End ML Building Process



Continuous Delivery for Machine Learning

PyTorch: An Imperative Style, High-Performance Deep Learning Library

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TensorFlow: A System for Large-Scale Machine Learning

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https://www.usenix.org/conference/osdi16/technical-sessions/presentation/abadi

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