DADS7305: MLOPs

Northeastern University

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These materials have been prepared and sourced for the course **MLOPs** at Northeastern University. Every effort has been made to provide proper citations and credit for all referenced works.

If you believe any material has been inadequately cited or requires correction, please contact me at:

`r.mohammadi@northeastern.edu`

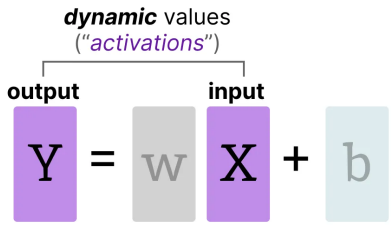
Thank you for your understanding and collaboration.

ML Experiments Management and Workflow Automation

Experiment Tracking

Why experiment tracking?

- ML projects have far more branching and experimentation
- Debugging in ML is difficult and time consuming
- Small changes can lead to drastic changes in a model's performance and resource requirements
- Running experiments can be time consuming and expensive

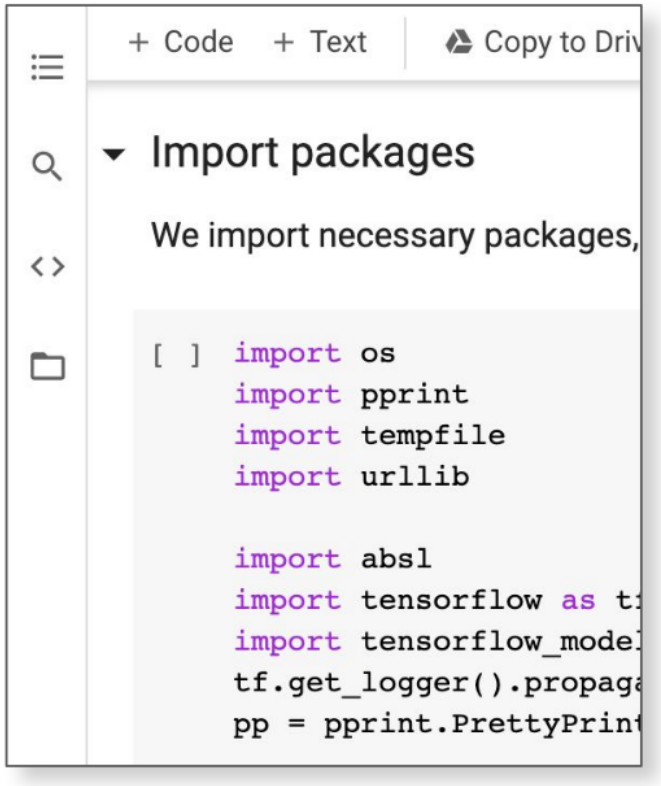


What does it mean to track experiments?

- Enable you to duplicate a result
- Enable you to meaningfully compare experiments
- Manage code/data versions, hyperparameters, environment, and metrics
- Organize experiments in a meaningful way
- Make them accessible for collaboration within your organization

Simple Experiments with Notebooks

- Notebooks are great tools
- Notebook code is usually not promoted to production
- Tools for managing notebook code:
  - `nbconvert` (.ipynb → .py conversion)
  - `nbdime` (diffing)
  - `jupytext` (conversion + versioning)
  - `neptune-notebooks` (versioning + diffing + sharing)



Smoke testing for Notebooks

```
jupyter nbconvert --to script train_model.ipynb python train_model.py;

python train_model.py
```

Not Just One Big File

- Modular code, not monolithic
- Collections of interdependent and versioned files
- Directory hierarchies or monorepos
- Code repositories and commits

Tracking Runtime Parameters

Config files

```
data:
    train_path: '/path/to/my/train.csv'
    valid_path: '/path/to/my/valid.csv'

model:
    objective: 'binary'
    metric: 'auc'
    learning_rate: 0.1
    num_boost_round: 200
    num_leaves: 60
    feature_fraction: 0.2
```

Command line

```
python train_evaluate.py \
    --train_path '/path/to/my/train.csv' \
    --valid_path '/path/to/my/valid.csv' \
    -- objective 'binary' \
    -- metric 'auc' \
    -- learning_rate 0.1 \
    -- num_boost_round 200 \
    -- num_leaves 60 \
    -- feature_fraction 0.2
```

Log Runtime Parameters

```
parser = argparse.ArgumentParser()
parser.add_argument('--number_trees')
parser.add_argument('--learning_rate')
args = parser.parse_args()

neptune.create_experiment(params=vars(args))
...
# experiment logic
...
```

ML Experiments Management and Workflow Automation

Tools for Experiment Tracking

Data Versioning

- Data reflects the world, and the world changes
- Experimental changes include changes in data
- Tracking, understanding, comparing, and duplicating experiments includes data

Tools for Data Versioning

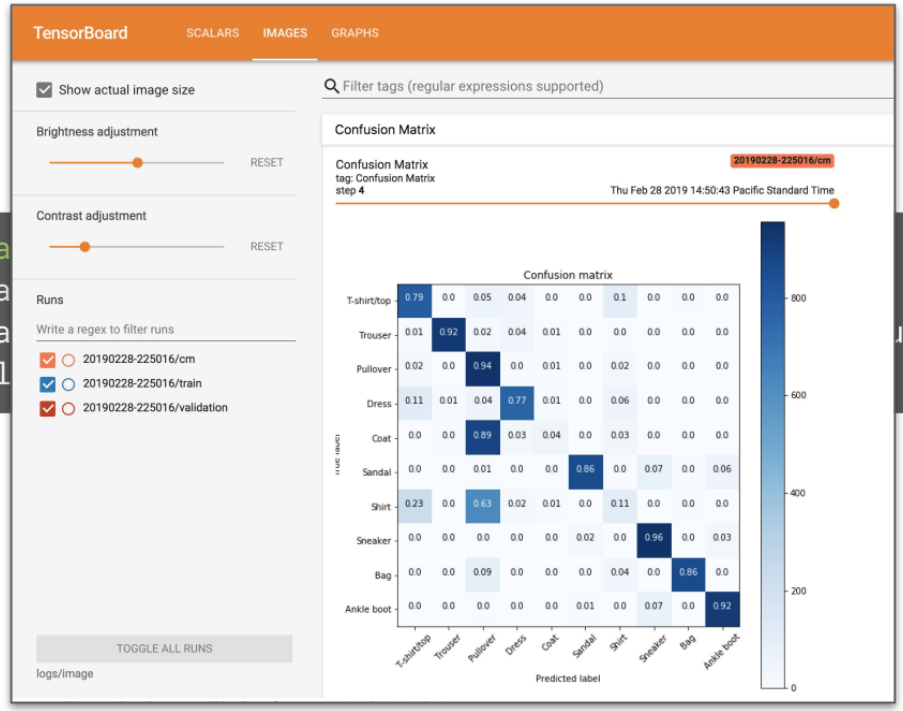
- Neptune
- Dolt
- Pachyderm
- lakeFS
- Delta Lake
- DVC
- Git LFS
- ML-Metadata

Experiment tracking to compare results

Name (50 visualized)	Tags	acc	Sweep	optimizer	epoch	batch_size	n_train	n_valid	n_conv_lay	loss	GPU
batch 64 4 GPU	4GPU b_64_c	0.4305	-	rmsprop	49	64	5000	800	1	1.632	-
batch 64 (V2, 5K train	2GPU b_64_c	0.4343	-	rmsprop	49	64	5000	800	1	1.63	-
50K examples (b 64)		0.4042	-	rmsprop	49	64	50000	8000	1	1.76	-
batch 32 4 GPU	4GPU b_32_c	0.4032	-	rmsprop	49	32	5000	800	1	1.714	-
batch 64 1 GPU	1GPU GCP	0.4465	-	rmsprop	49	64	5000	800	5	1.615	1
batch 128 (5K train)	2GPU b_128	0.4181	-	rmsprop	49	128	5000	800	1	1.658	-
batch 256 4 GPU	4GPU keras	0.3882	-	rmsprop	49	256	5000	800	1	1.751	-

Example: Logging metrics using TensorBoard

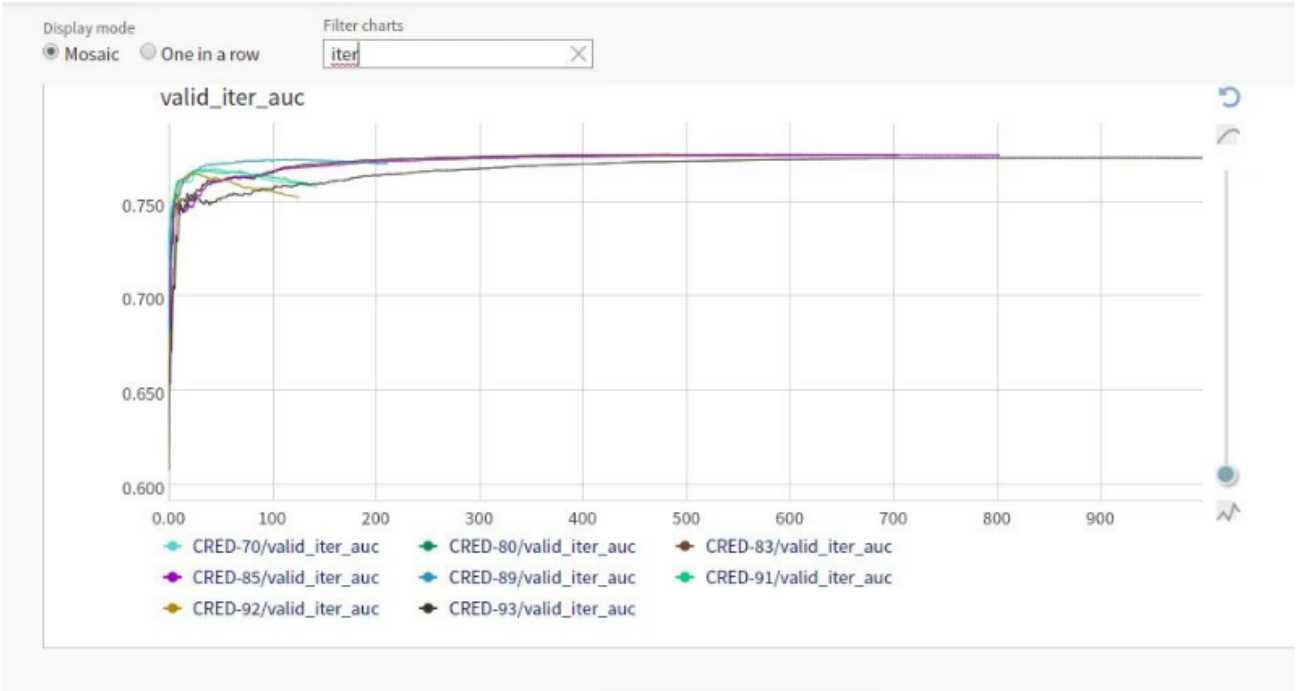
```
logdir = "logs/ima                                    histogram_freq=1)
tensorboard_callba                                    usion_matrix)
cm_callback = kera
model.fit(... call
```



Organizing model development

- Search through and visualize all experiments
- Organize into something digestible
- Make data shareable and accessible
- Tag and add notes that will be meaningful to your team

Tooling for Teams

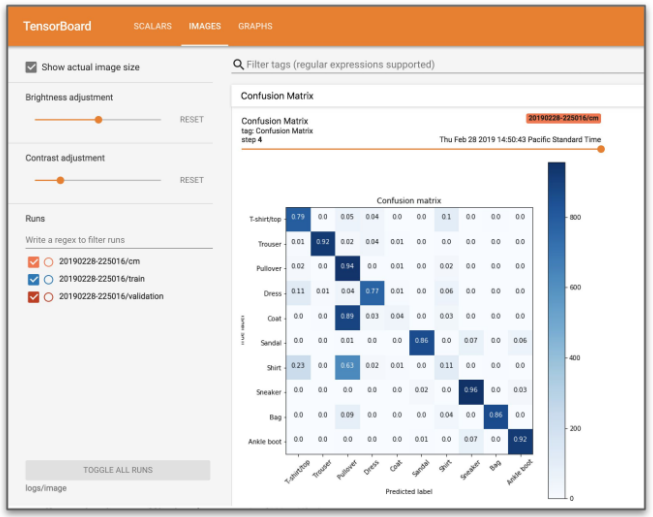


Short ID	Owner	Tags	valid_auc	train_auc	features_...	train_spli...	valid_spli...
CRED-93	kamil	lgbm, features_v1	0.773536	0.807047	e1f5a473fe...	41bf231b7...	4b61d05c0...
CRED-92	kamil	lgbm, features_v1	0.765647	0.790213	e1f5a473fe...	41bf231b7...	4b61d05c0...
CRED-91	kamil	lgbm, features_v1	0.767254	0.78022	e1f5a473fe...	41bf231b7...	4b61d05c0...
CRED-89	kamil	lgbm, features_v1	0.772704	0.788251	e1f5a473fe...	41bf231b7...	4b61d05c0...
CRED-85	jakub-czakon	lgbm, features_v1	0.775187	0.797085	e1f5a473fe...	41bf231b7...	4b61d05c0...

Tooling for Teams

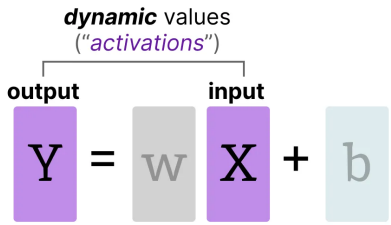
Vertex TensorBoard

- Managed service with enterprise-grade security, privacy, and compliance
- Persistent, shareable link to your experiment dashboard
- Searchable list of all experiments in a project



Experiments are iterative in nature

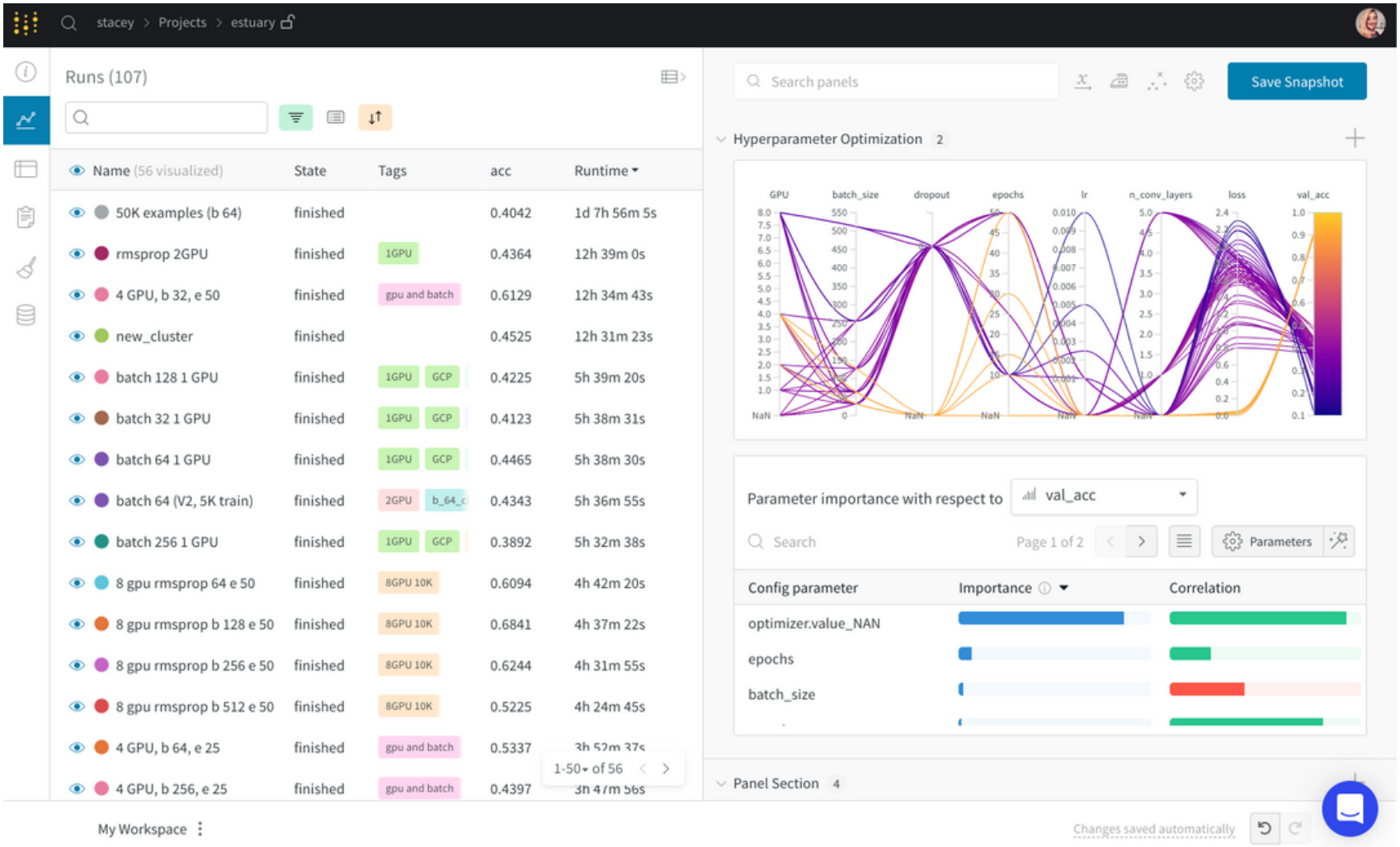
- Creative iterations for ML experimentation
- Define a baseline approach
- Develop, implement, and evaluate to get metrics
- Assess the results, and decide on next steps
- Consider latency, cost, fairness, etc.



Weights & Biases

- **Purpose:** Centralized platform for tracking ML experiments, datasets, and models
- **Experiment logging:** Track hyperparameters, metrics, system stats, and outputs in real-time
- **Visualization:** Interactive dashboards to compare runs, view loss curves, and analyze results
- **Collaboration:** Share experiment results, notes, and visualizations with your team
- **Integrations:** Works with PyTorch, TensorFlow, Scikit-learn, Hugging Face, and more
- **Additional features:** Dataset versioning, model registry, and hyperparameter sweeps

WandB Dashboard



ML Experiments Management and Workflow Automation

Introduction to MLOps

Data Scientists vs. Software Engineers

Data Scientists

- Often work on fixed datasets
- Focused on model metrics
- Prototyping on Jupyter notebooks
- Expert in modeling techniques and feature engineering
- Model size, cost, latency, and fairness are often ignored

Data Scientists vs. Software Engineers

Software Engineers

- Build a product
- Concerned about cost, performance, stability, schedule
- Identify quality through customer satisfaction
- Must scale solution, handle large amounts of data
- Detect and handle error conditions, preferably automatically
- Consider requirements for security, safety, fairness
- Maintain, evolve, and extend the product over long periods

Growing Need for ML in Products and Services

- Large datasets
- Inexpensive on-demand compute resources
- Increasingly powerful accelerators for ML
- Rapid advances in many ML research fields (such as computer vision, natural language understanding, and recommendation systems)
- Businesses are investing in their data science teams and ML capabilities to develop predictive models that can deliver business value to their customers

Key problems affecting ML efforts today

We've been here before

- In the 90s, Software Engineering was siloed
- Weak version control, CI/CD didn't exist
- Software was slow to ship; now it ships in minutes
- Is that ML today?

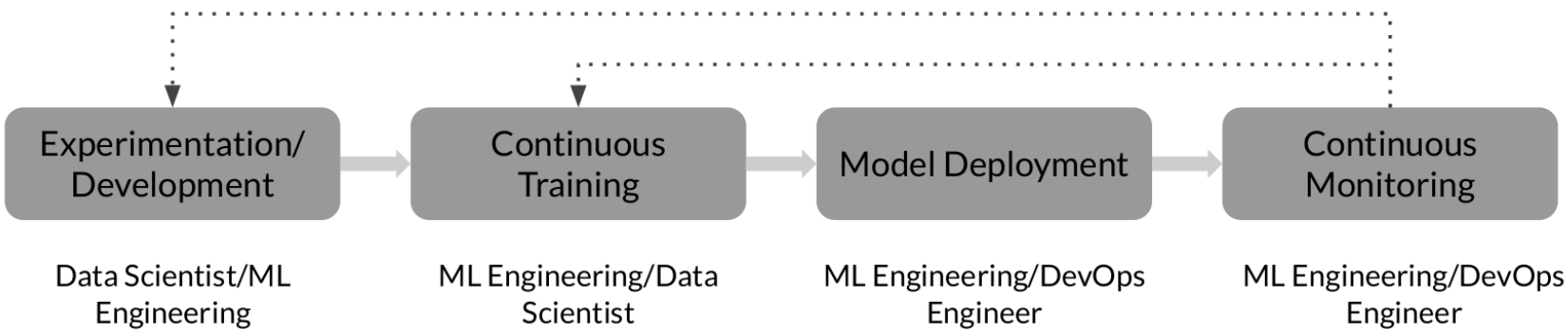
Today's perspective

- Models blocked before deployment
- Slow to market
- Manual tracking
- No reproducibility or provenance
- Inefficient collaboration
- Unmonitored models

Bridging ML and IT with MLOps

- **Continuous Integration (CI):** Testing and validating code, components, data, data schemas, and models
- **Continuous Delivery (CD):** Not only about deploying a single software package or service, but a system which automatically deploys another service (model prediction service)
- **Continuous Training (CT):** A new process, unique to ML systems, that automatically retrains candidate models for testing and serving
- **Continuous Monitoring (CM):** Catching errors in production systems, and monitoring production inference data and model performance metrics tied to business outcomes

ML Solution Lifecycle



Standardizing ML processes with MLOps

- ML Lifecycle Management
- Model Versioning & Iteration
- Model Monitoring and Management
- Model Governance
- Model Security
- Model Discovery

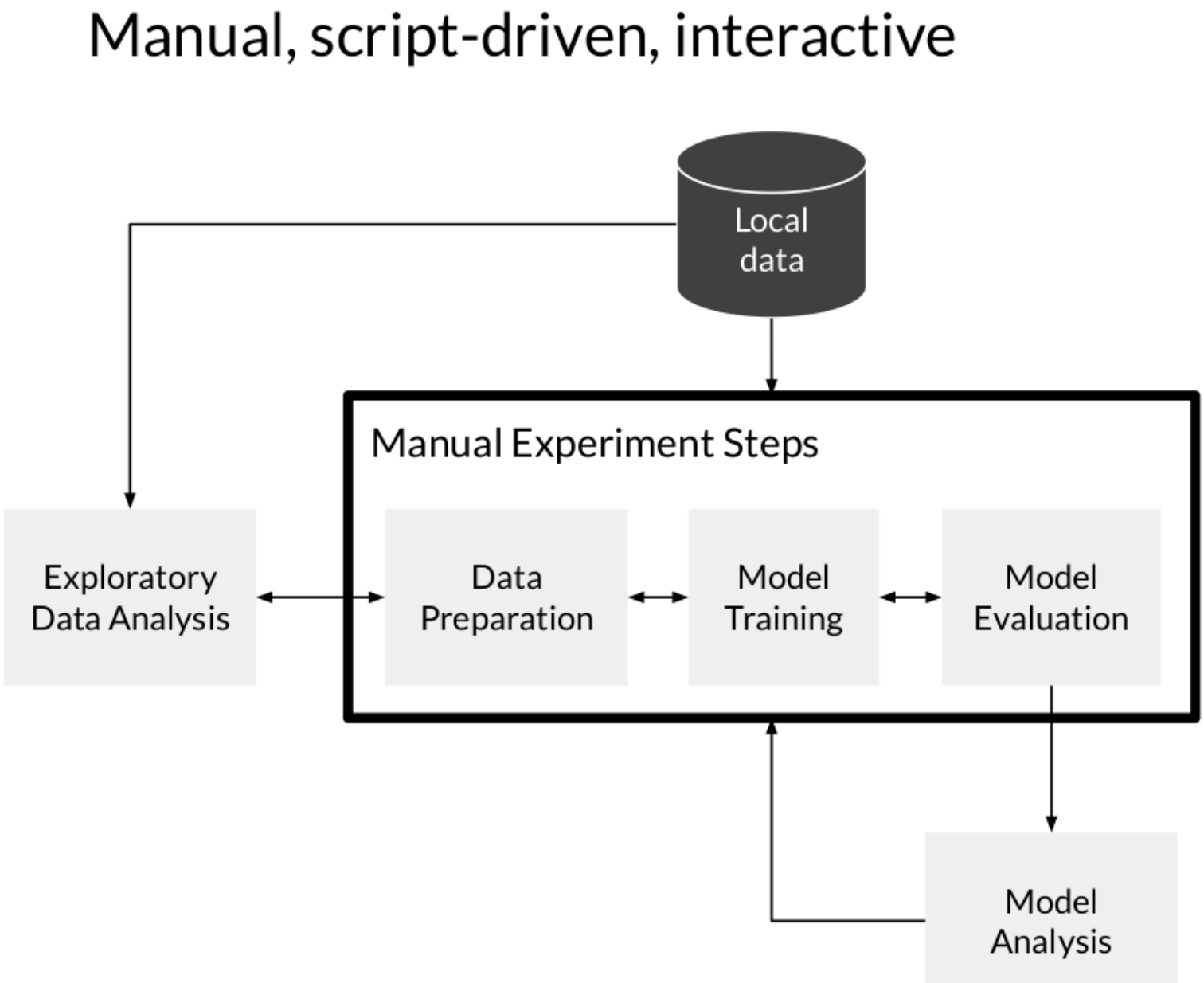
MLOps Methodology

MLOps Level 0

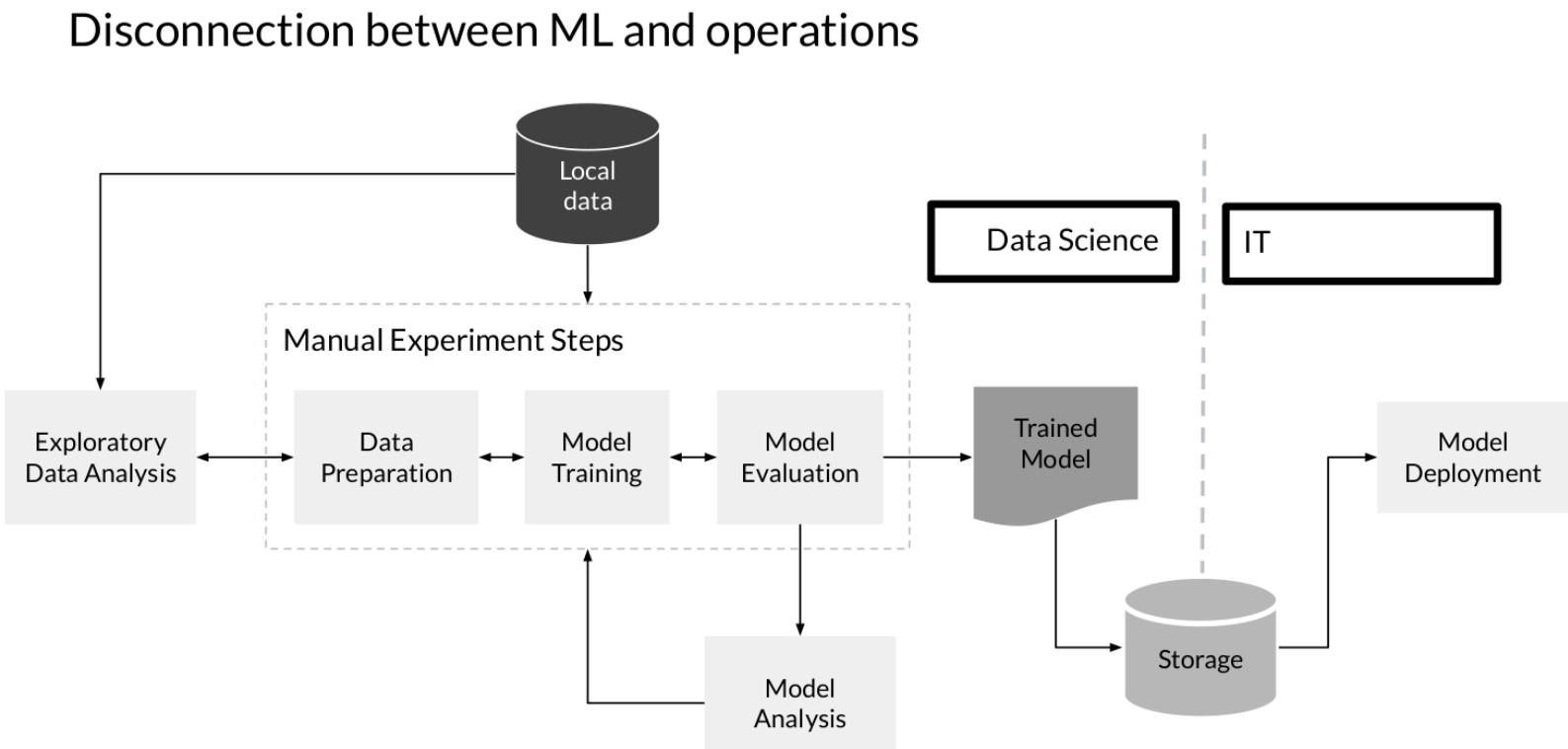
What defines an MLOps process' maturity?

- The level of automation of ML pipelines determines the maturity of the MLOps process
- As maturity increases, the available velocity for the training and deployment of new models also increases
- Goal is to automate training and deployment of ML models into the core software system, and provide monitoring

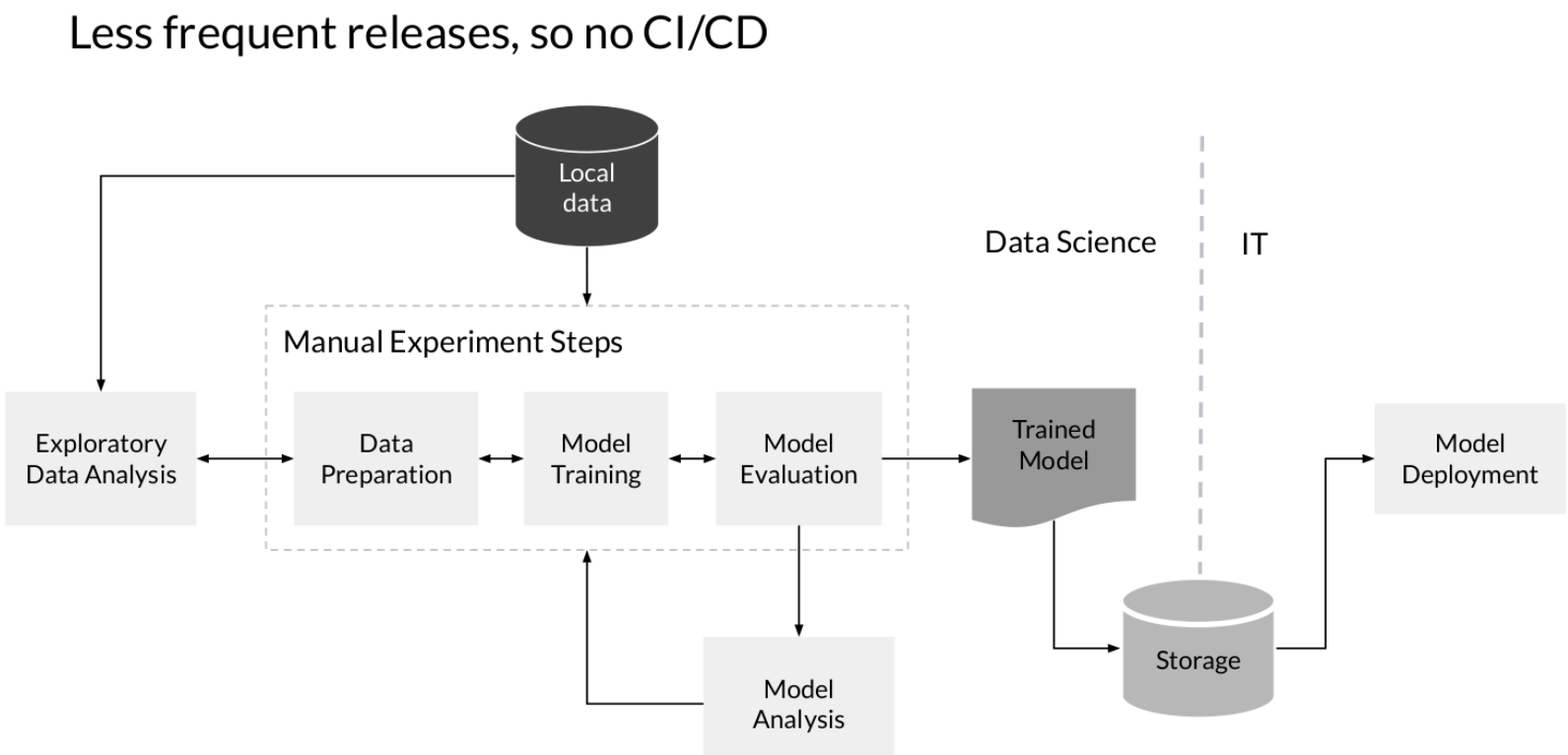
MLOps level 0: Manual process



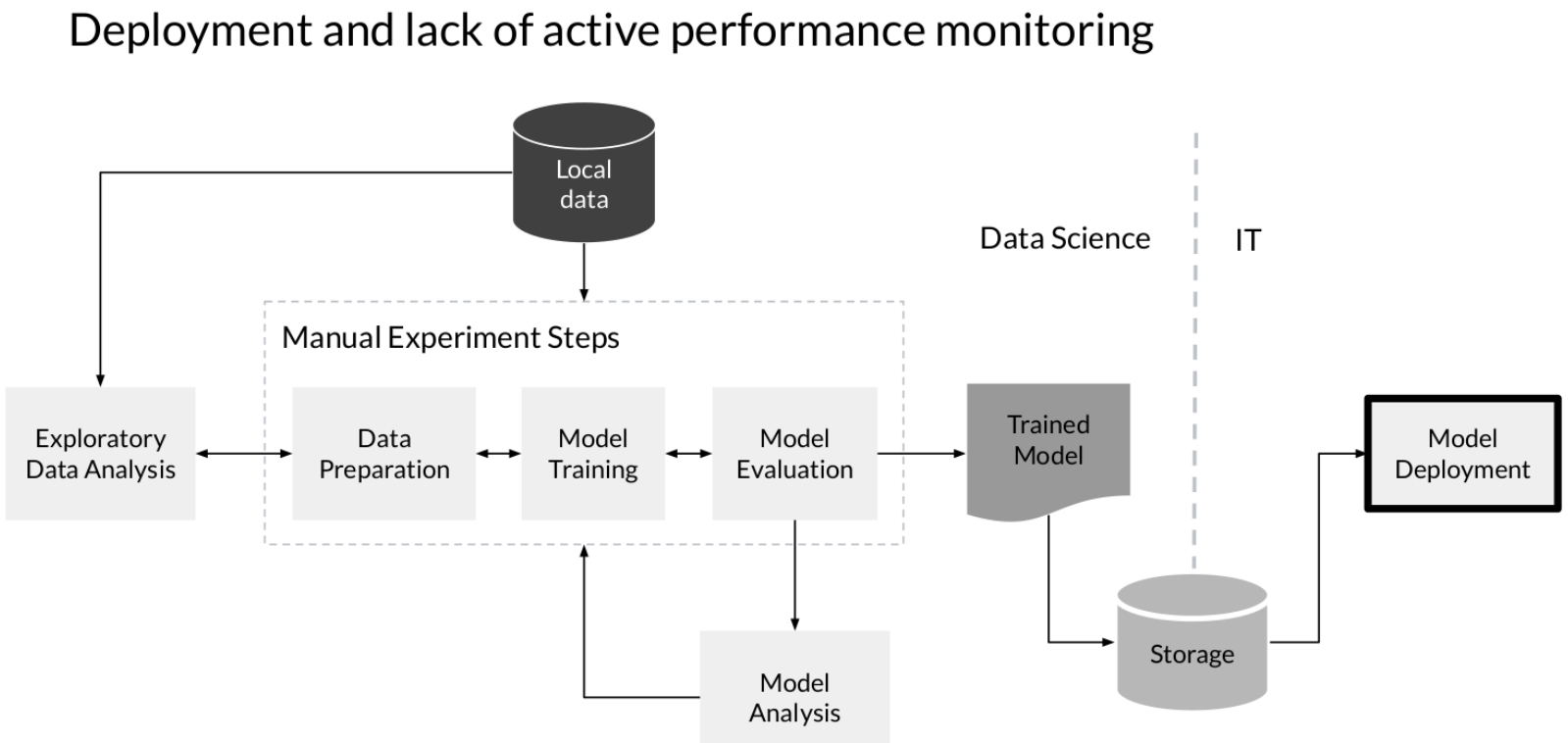
MLOps level 0: Manual process



MLOps level 0: Manual process



How do you scale?



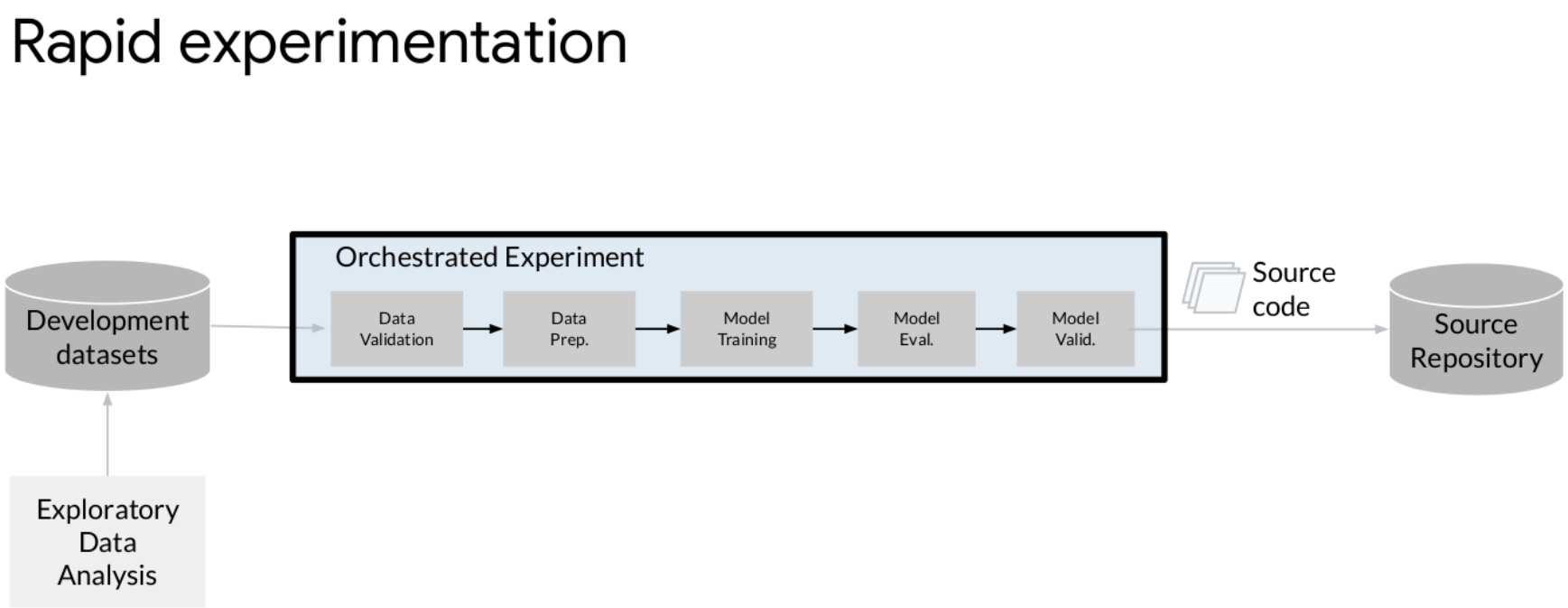
Challenges for MLOps Level 0

- Need for actively monitoring the quality of your model in production
- Retraining your production models with new data
- Continuously experimenting with new implementations to improve the data and model

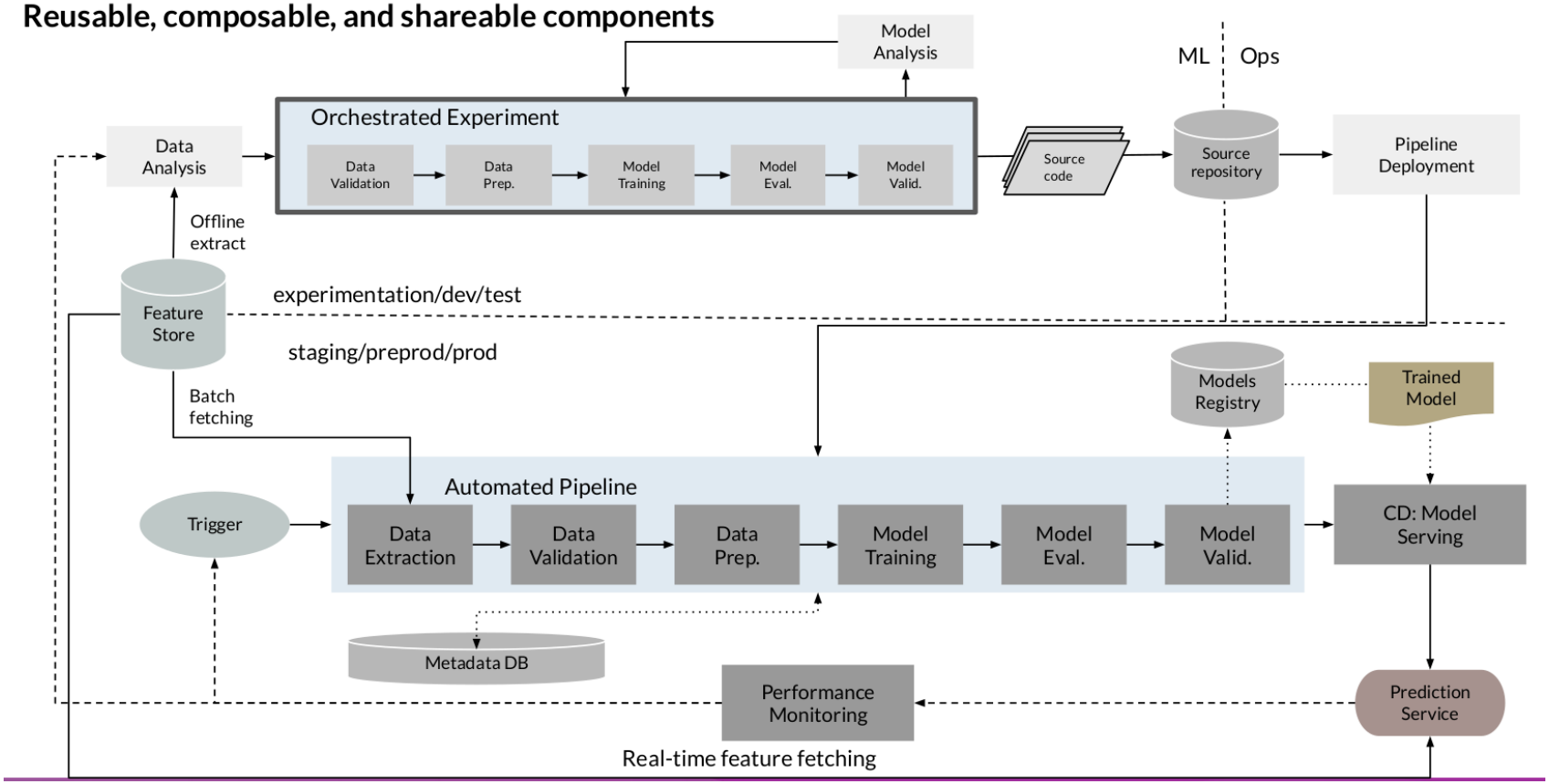
MLOps Methodology

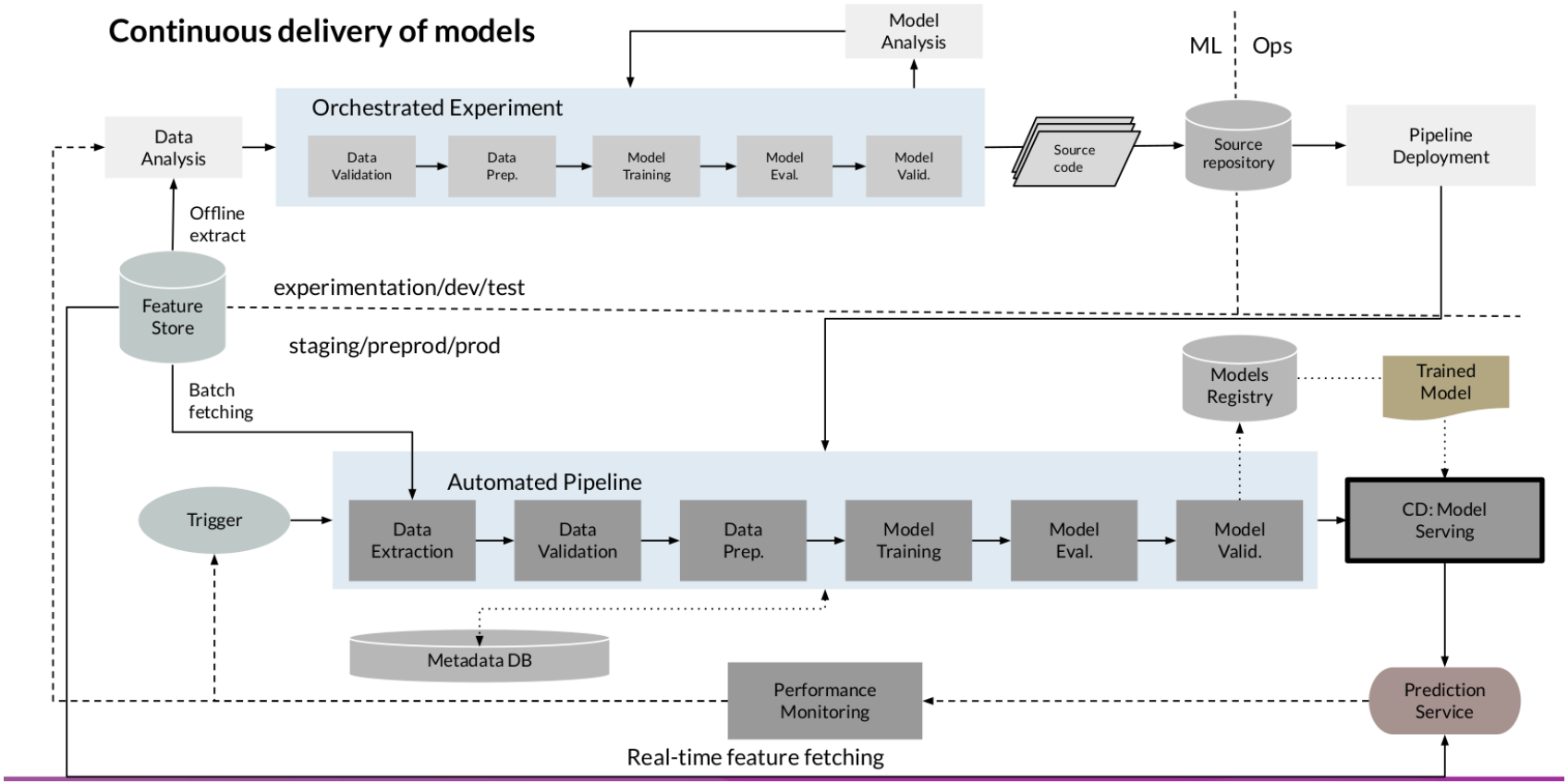
MLOps levels 1 and 2

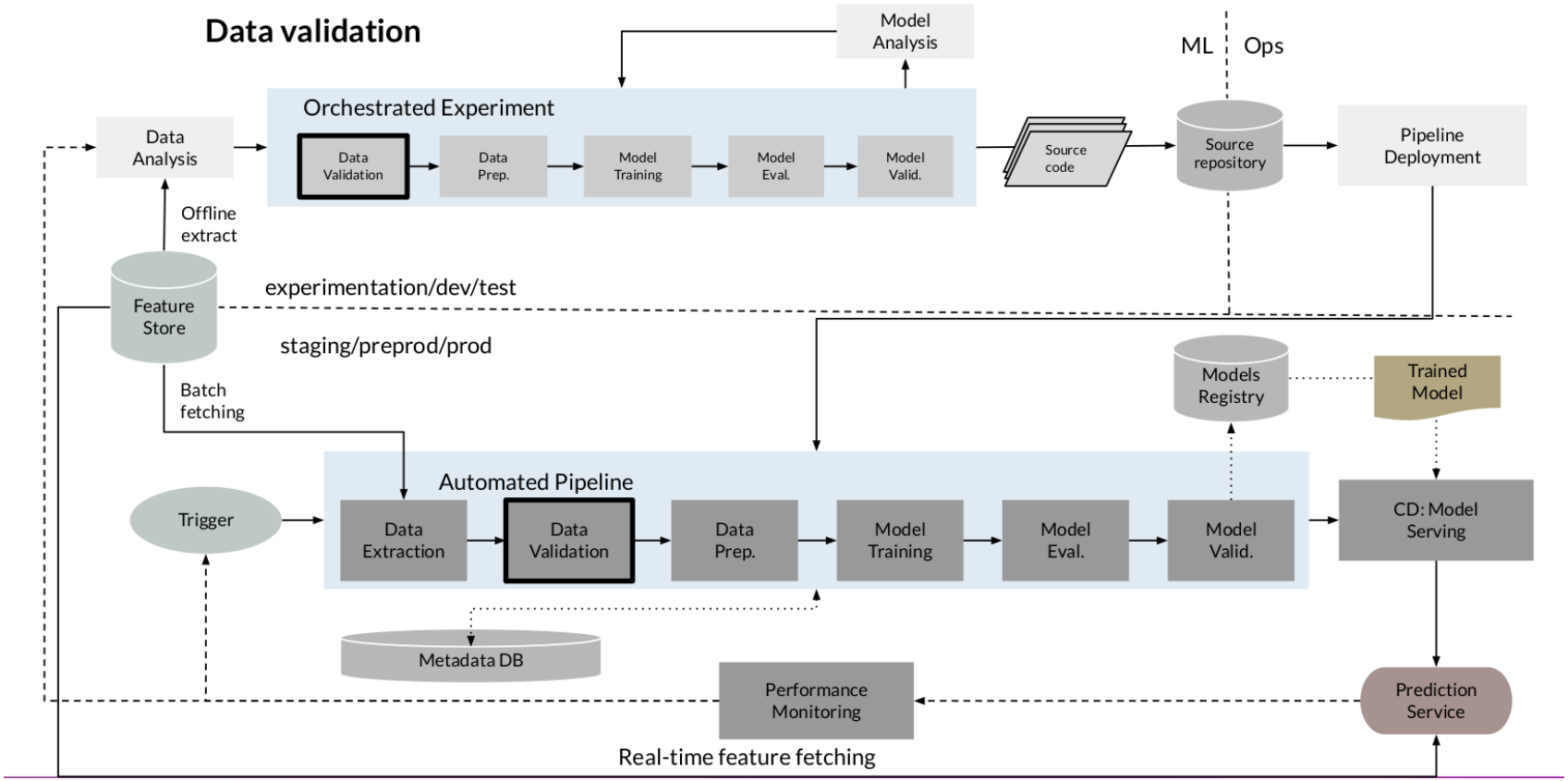
MLOps level 1: ML pipeline automation



Reusable, composable, and shareable components




Continuous delivery of models
Model Analysis
ML
Ops
Orchestrated Experiment
Data Analysis
Data Validation
Data Prep.
Model Training
Model Eval.
Model Valid.
Source code
Source repository
Pipeline Deployment
Offline extract
Feature Store
experimentation/dev/test
staging/preprod/prod
Batch fetching
Models Registry
Trained Model
Automated Pipeline
Trigger
Data Extraction
Data Validation
Data Prep.
Model Training
Model Eval.
Model Valid.
CD: Model Serving
Metadata DB
Performance Monitoring
Prediction Service
Real-time feature fetching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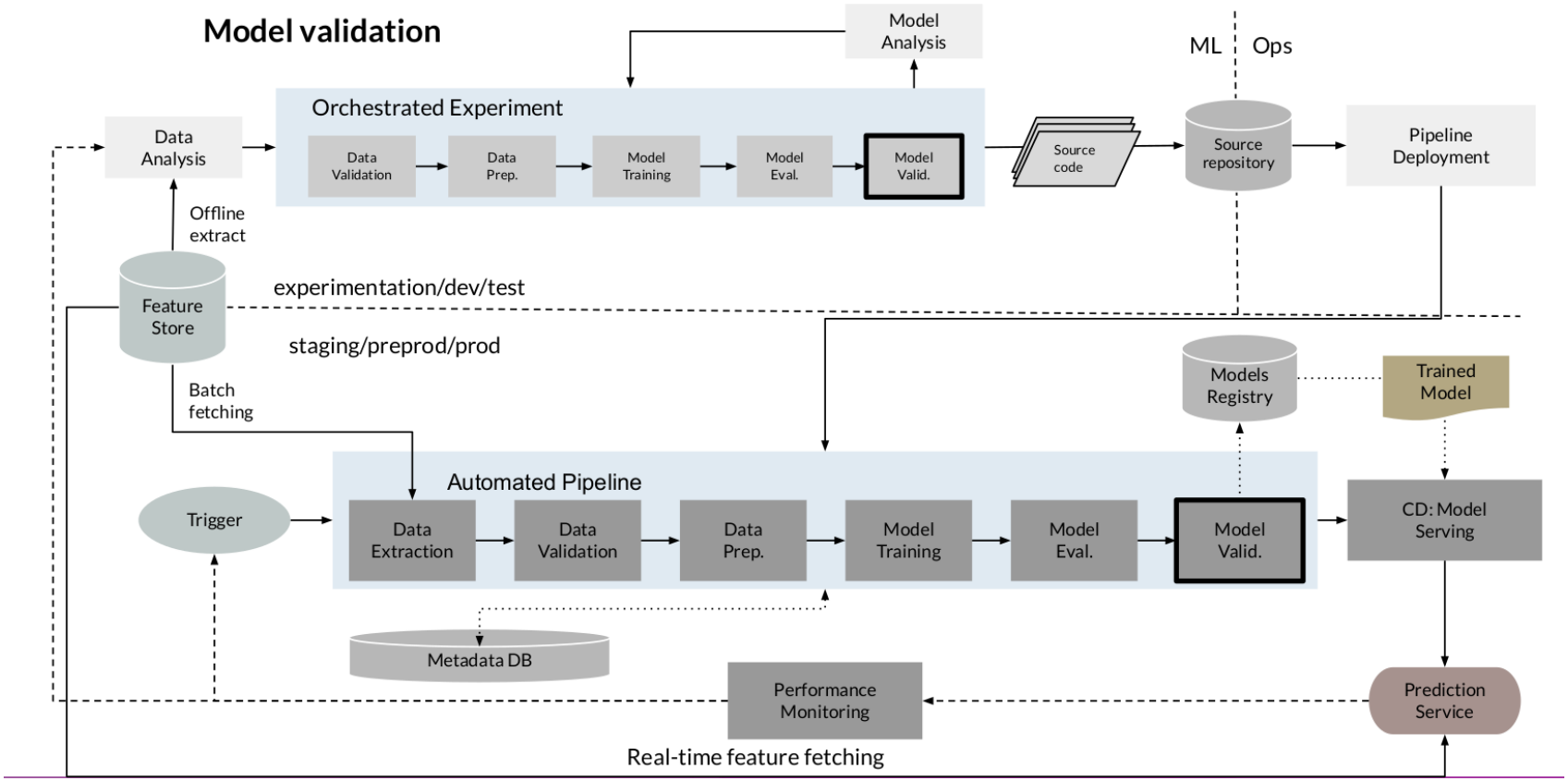
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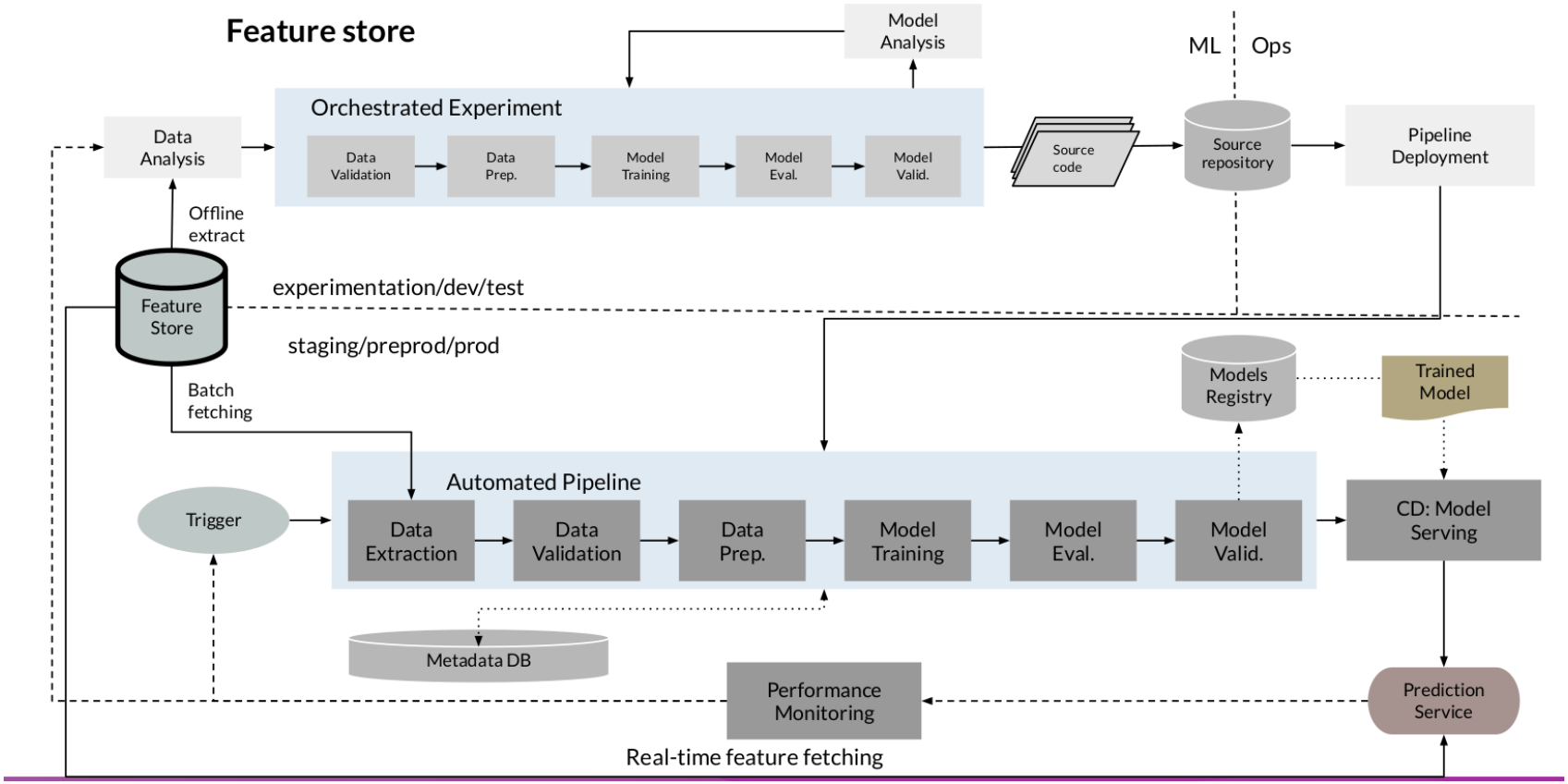
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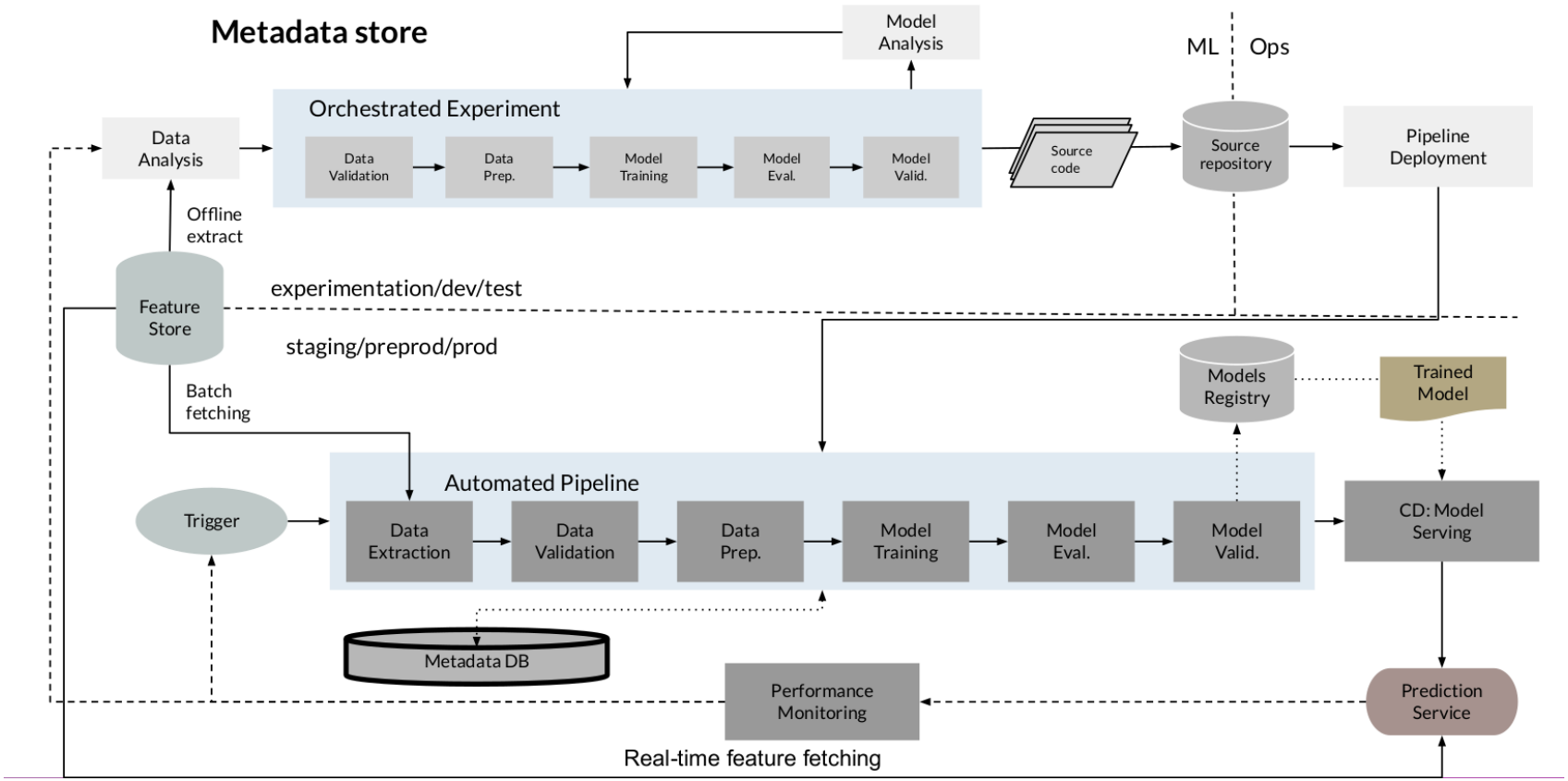
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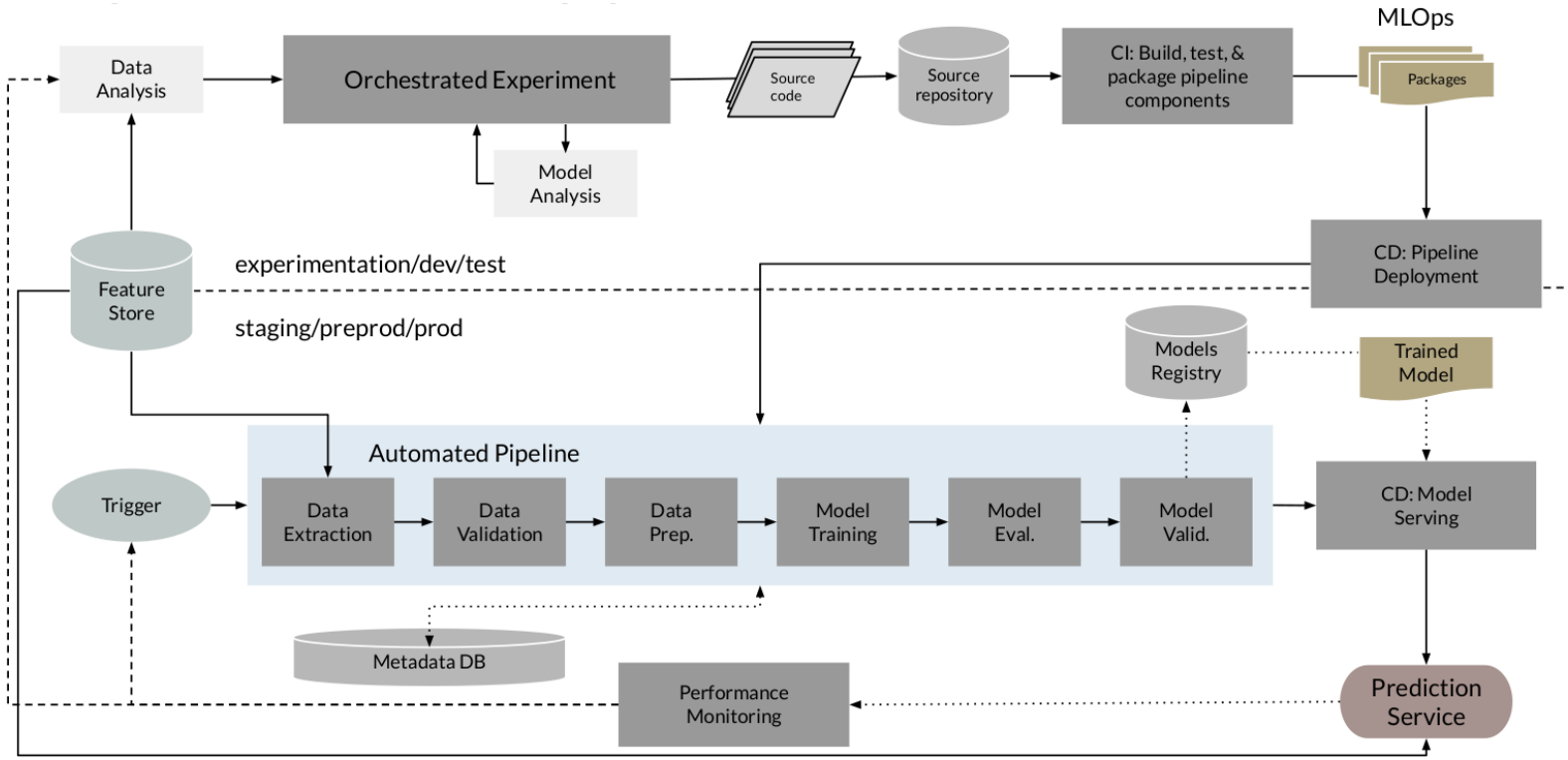
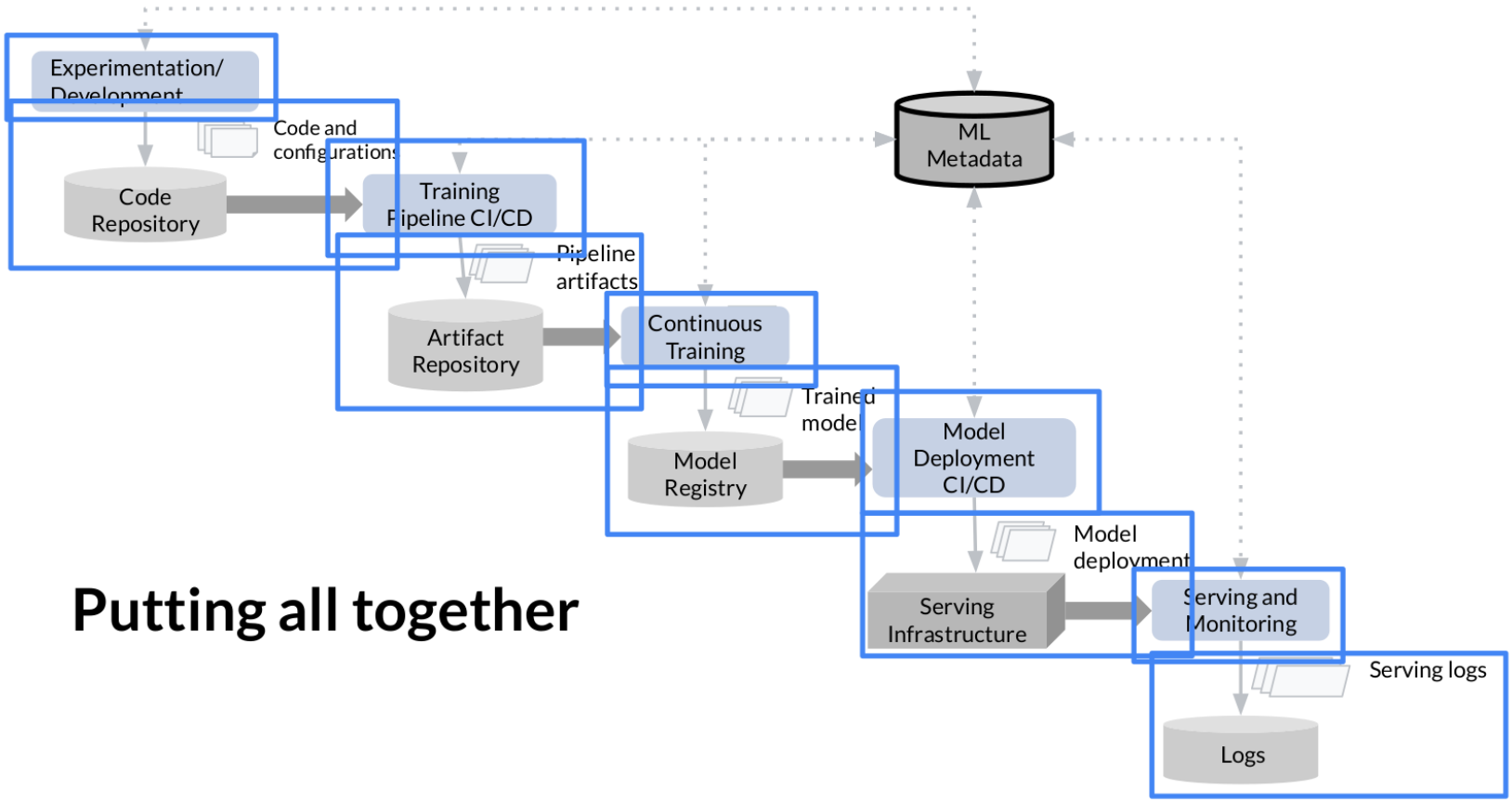
MLOps level 2: CI/CD pipeline automation



Putting all together



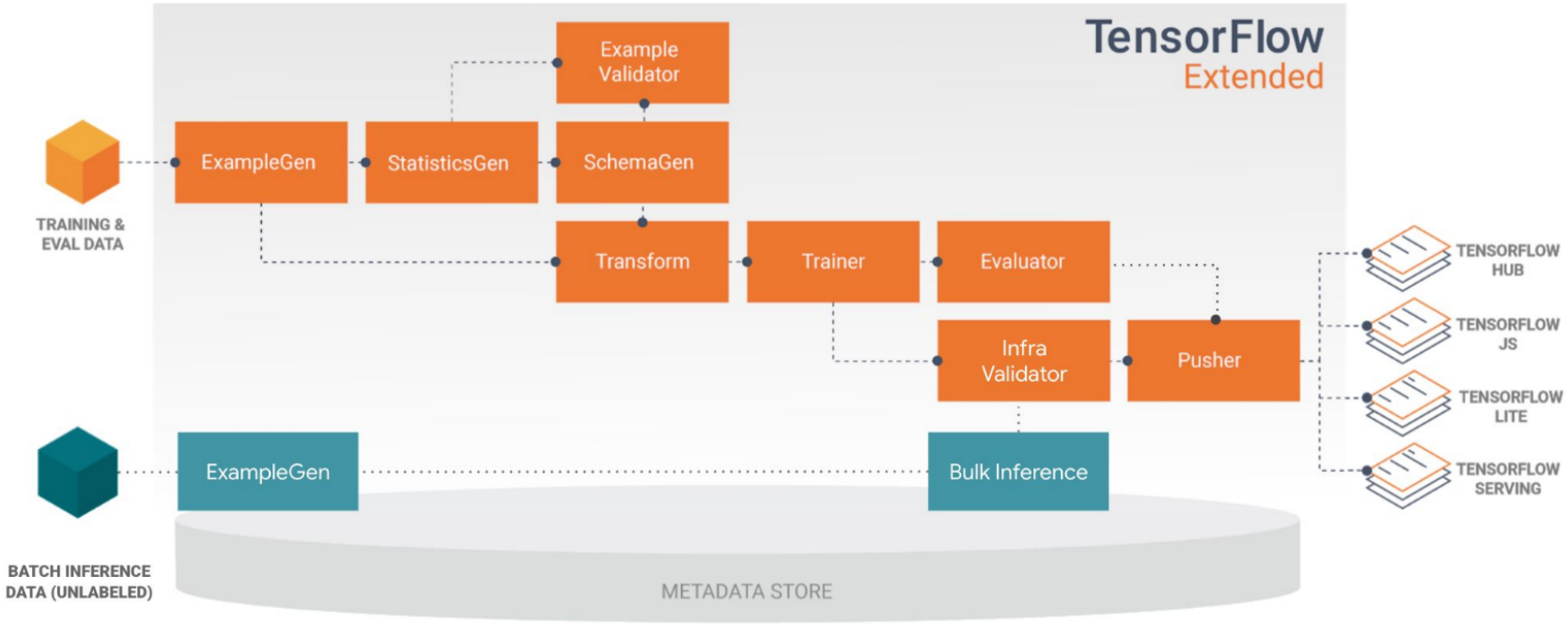
MLOps Methodology

Developing components for an orchestrated workflow

Orchestrate your ML workflows with TFX

- Pre-built and standard components, and 3 styles of custom components
- Components can also be containerized
- Examples of things you can do with TFX components:
  - Data augmentation, upsampling, or downsampling
  - Anomaly detection based on confidence intervals or autoencoder reproduction error
  - Interfacing with external systems like help desks for alerting and monitoring
  - . . . and more!

Hello TFX


TensorFlow
Extended
Example Validator
ExampleGen
StatisticsGen
SchemaGen
TRAINING & EVAL DATA
Transform
Trainer
Evaluator
Infra Validator
Pusher
TENSORFLOW HUB
TENSORFLOW JS
TENSORFLOW LITE
TENSORFLOW SERVING
ExampleGen
Bulk Inference
BATCH INFERENCE DATA (UNLABELED)
METADATA STORE

Anatomy of a TFX Component

Component Specification

- The component's input and output contract

Executor Class

- Implementation of the component's processing

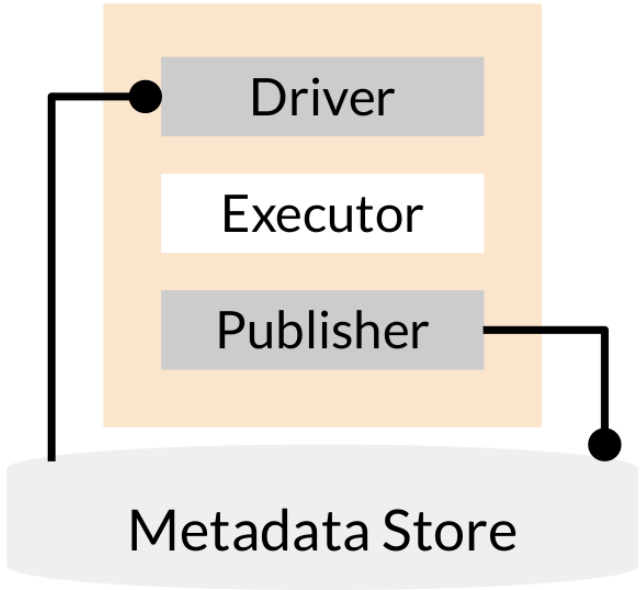
Component Class

- Combines the specification with the executor to create a TFX component

TFX components at runtime

Types of custom components

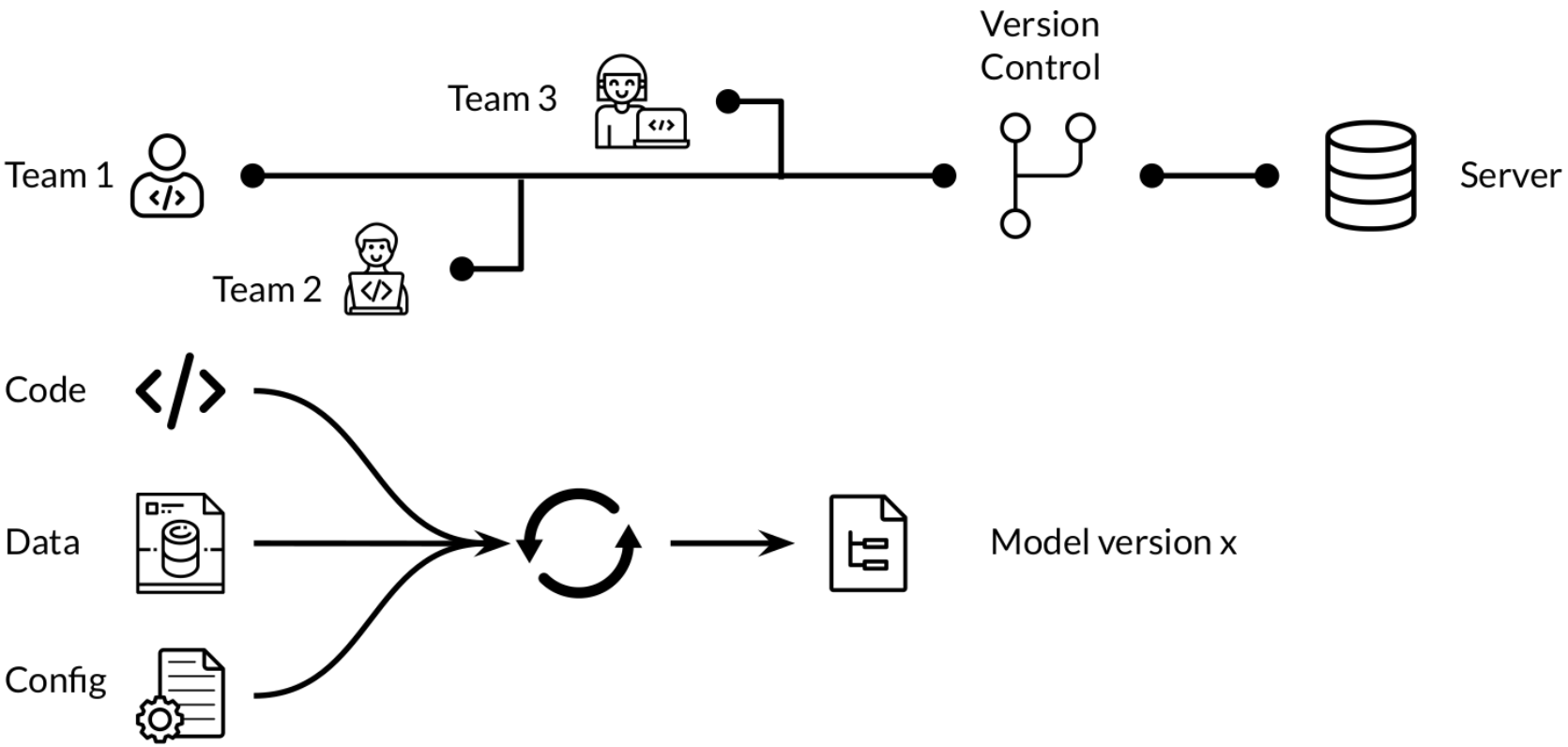
- Fully custom components combine the specification with the executor
- Python function-based components use a decorator and argument annotations
- Container-based components wrap the component inside a Docker container



Model Management and Deployment Infrastructure

Managing Model Versions

Why versioning ML Models?



How ML Models are versioned?

How software is versioned?

- Version format: `MAJOR.MINOR.PATCH`
- **MAJOR:** Contains incompatible API changes
- **MINOR:** Adds functionality in a backwards compatible manner
- **PATCH:** Makes backwards compatible bug fixes

ML Models versioning

- No uniform standard accepted yet
- Different organizations have different meanings and conventions

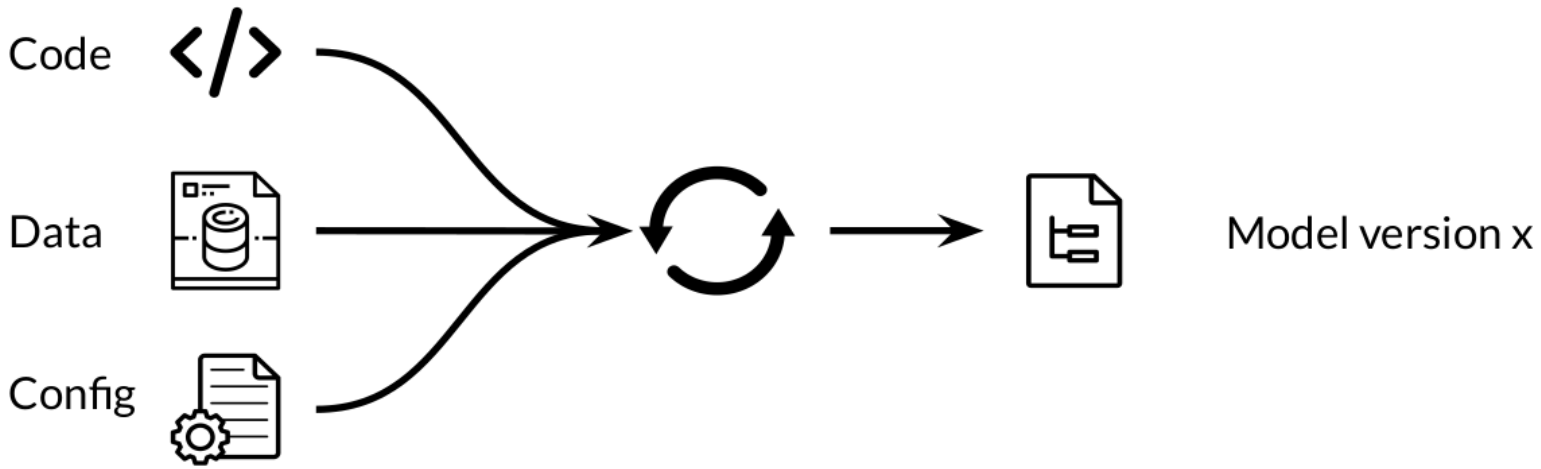
A Model Versioning Proposal

- Version format: `MAJOR.MINOR.PIPELINE`
- **MAJOR:** Incompatibility in data or target variable
- **MINOR:** Model performance is improved
- **PIPELINE:** Pipeline of model training is changed

Retrieving older models

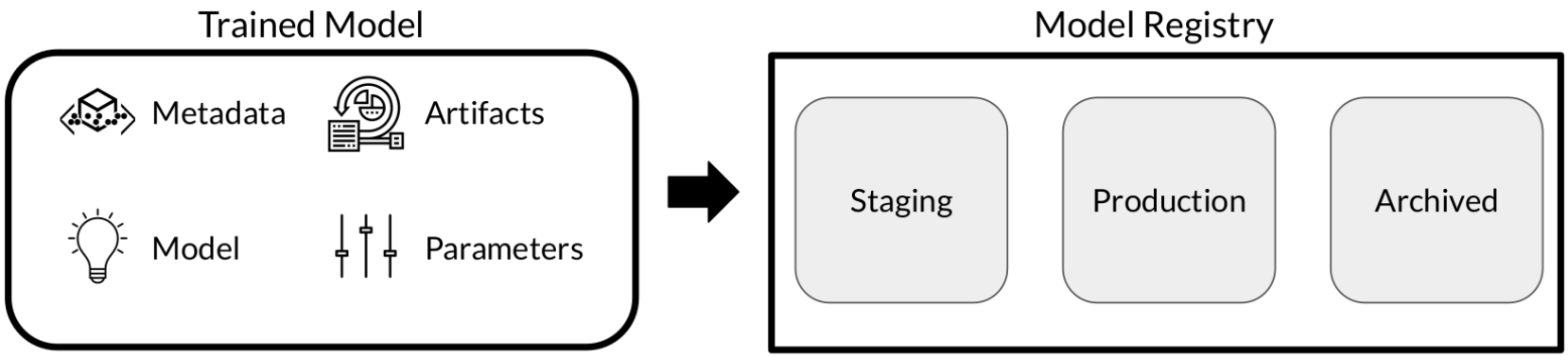
- Can ML framework be leveraged to retrieve previously trained models?
- ML framework may internally be versioning models

What is model lineage?



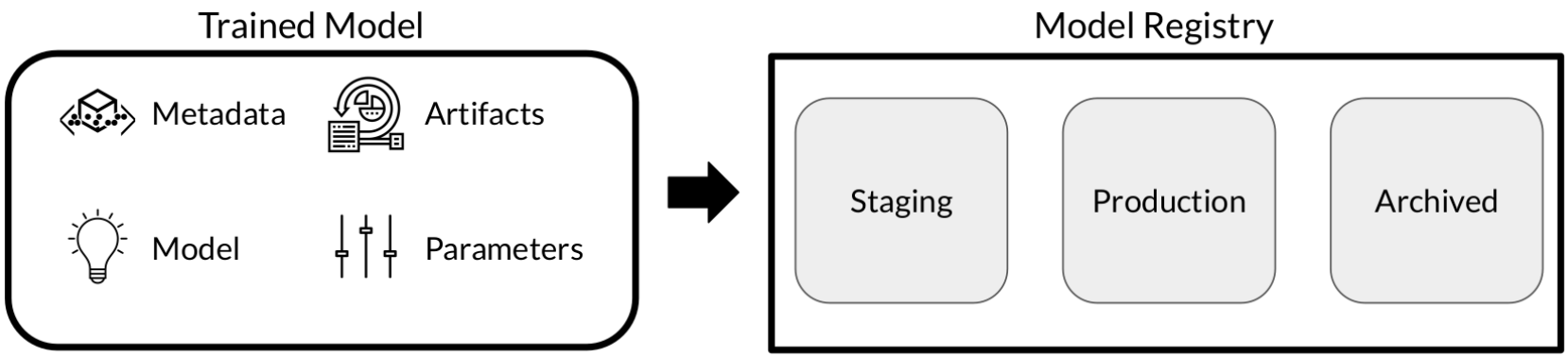
- **Artifacts:** Information needed to preprocess data and generate result (code, data, config, model)
- ML orchestration frameworks may store operations and data artifacts to recreate model
- Post-training artifacts and operations are usually not part of lineage

What is a model registry?



- Central repository for storing trained ML models
- Provides various operations of ML model development lifecycle
- Promotes model discovery, model understanding, and model reuse
- Integrated into OSS and commercial ML platforms

What is a model registry?



- Model versions
- Model serialized artifacts
- Free text annotations and structured properties
- Links to other ML artifact and metadata stores

Capabilities Enabled by Model Registries

- Model search/discovery and understanding
- Approval/Governance
- Collaboration/Discussion
- Streamlined deployments
- Continuous evaluation and monitoring
- Staging and promotions

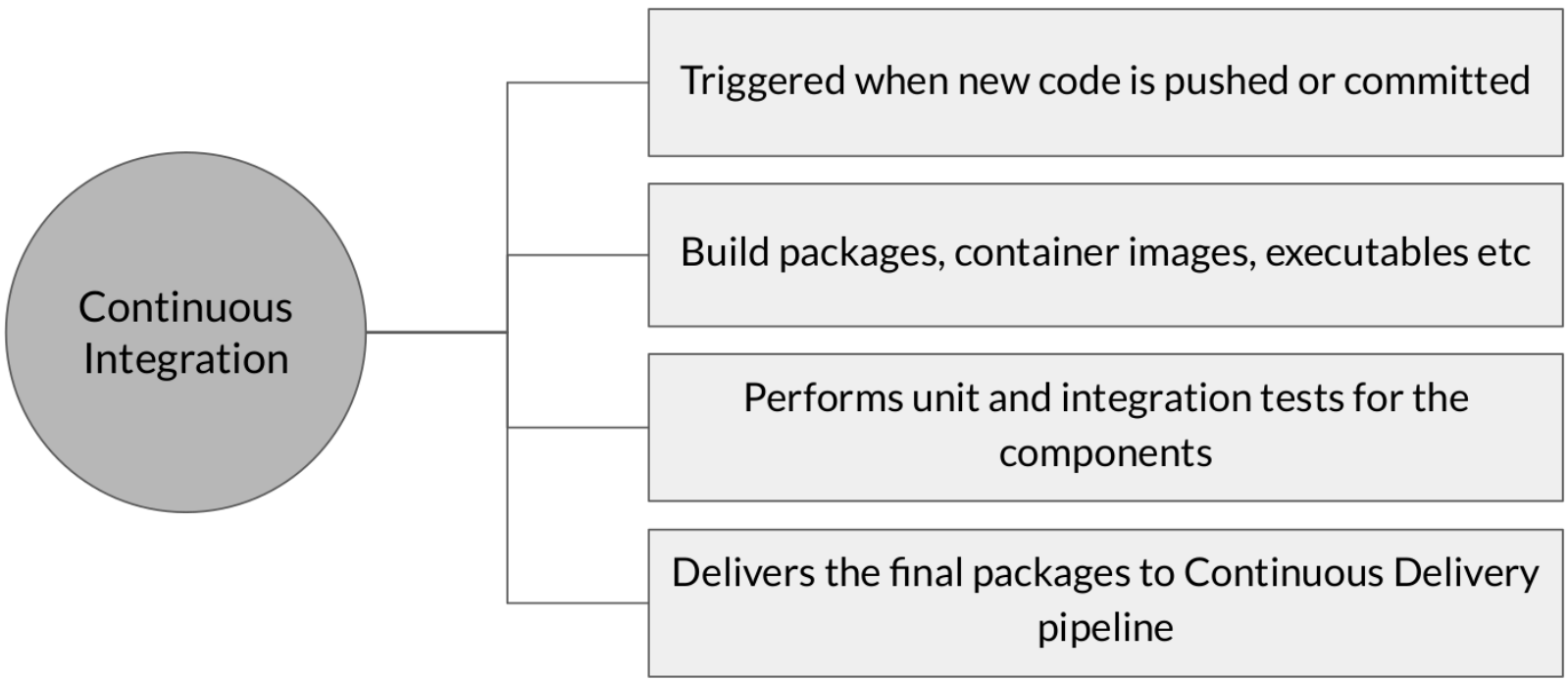
Examples of Model Registries

- Azure ML Model Registry
- SAS Model Manager
- MLflow Model Registry
- Google AI Platform
- Algorithmia

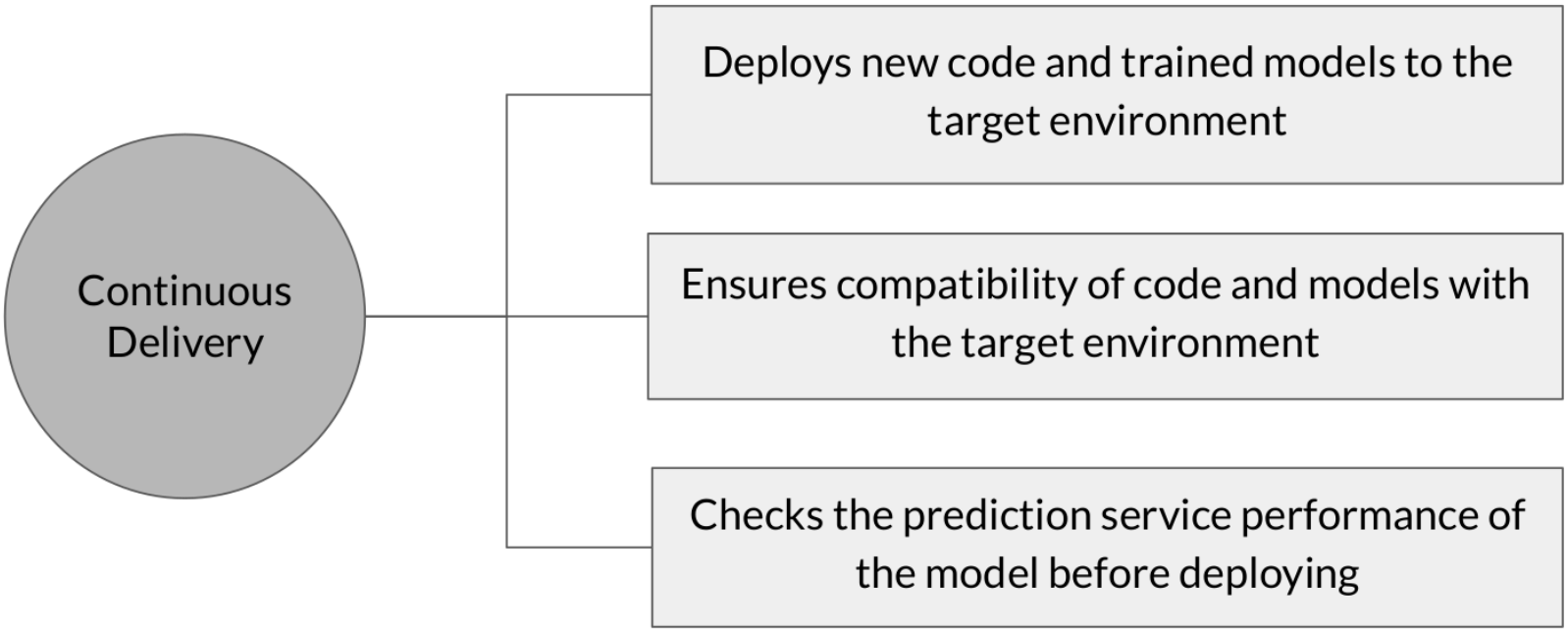
Model Management and Deployment Infrastructure

Continuous Delivery

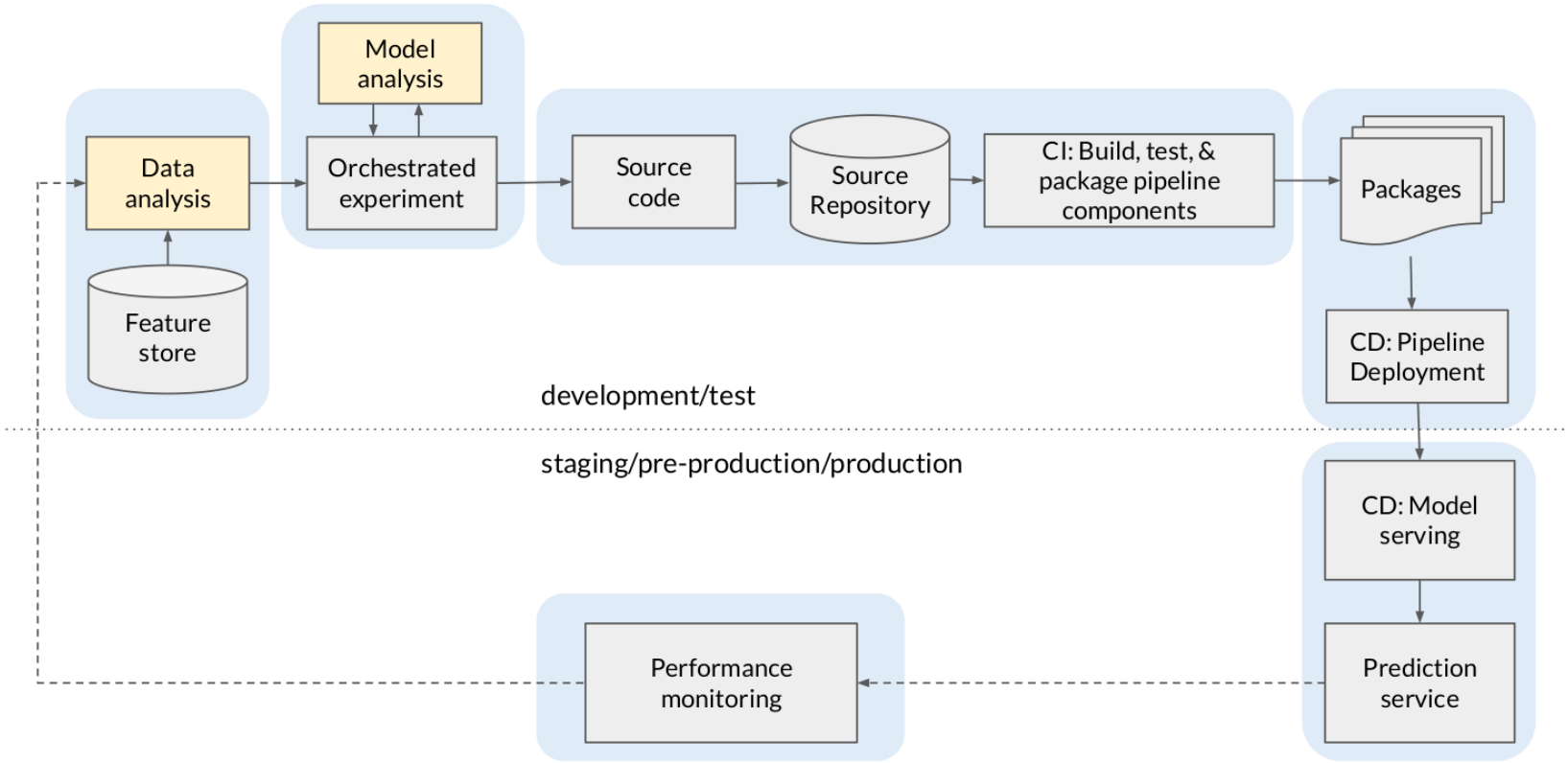
What is Continuous Integration (CI)



What is Continuous Integration (CI)

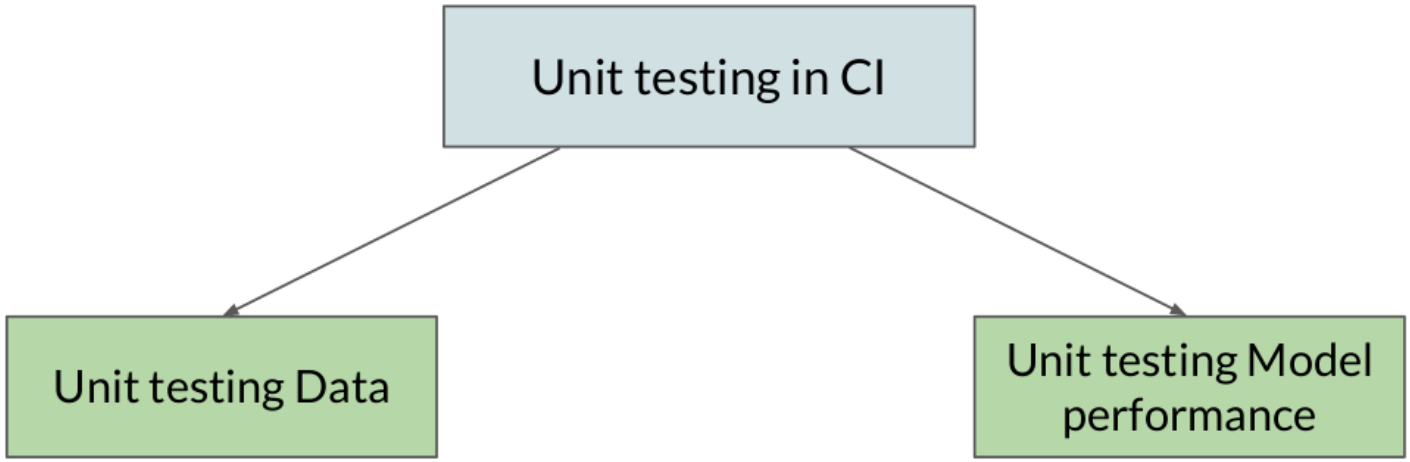


CI/CD Infrastructure

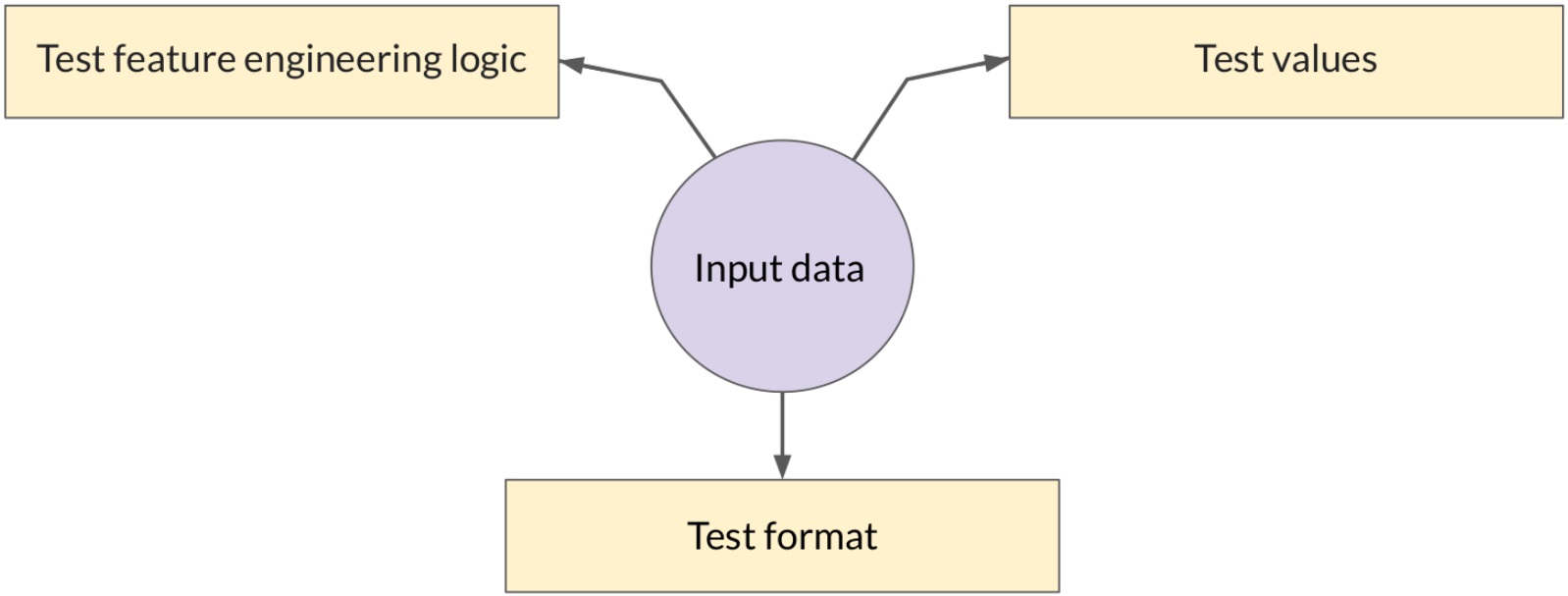


Unit Testing in CI

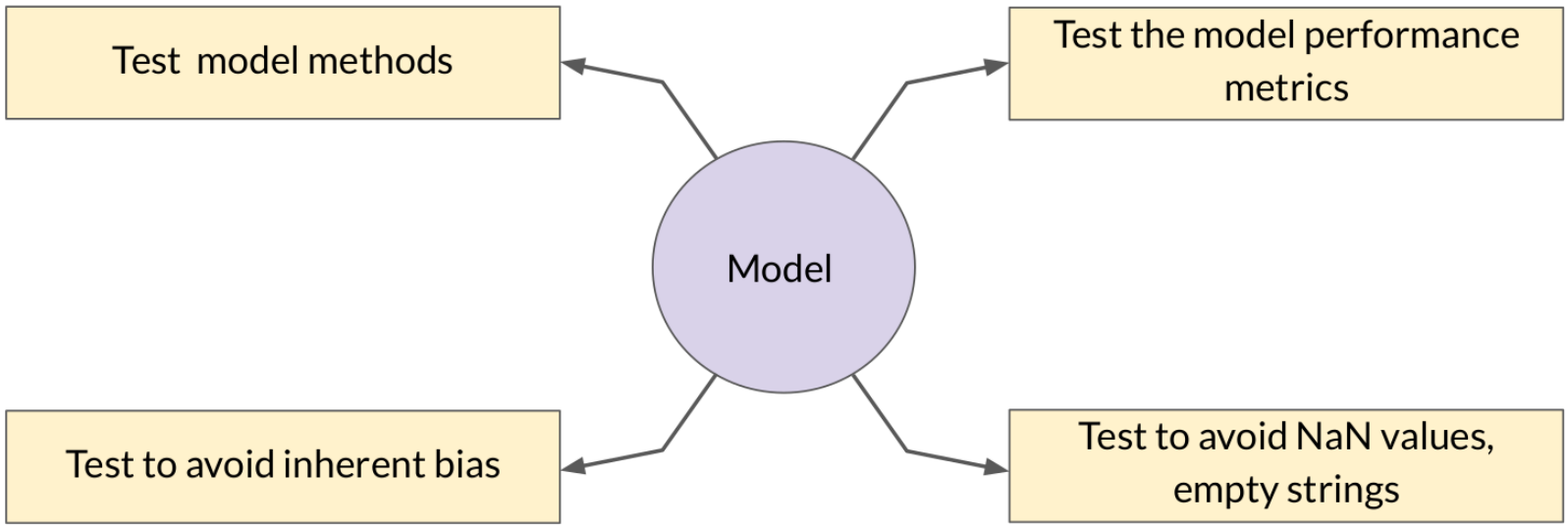
Testing that each component in the pipeline produces the expected artifacts.



Unit Testing Input Data



Unit Testing Model Performance



ML Unit Testing Considerations

Mocking

Mocks of datasets are especially important for ML. They should cover edge and corner cases.

Data Coverage

Your mocks should sparsely cover the same space as your data, but with a much smaller dataset.

Code Coverage

Use code coverage libraries to make sure that you are not missing unit tests for any part of our code.

Infrastructure validation

When to apply infrastructure validation

- Before starting CI/CD as part of model training
- Can also occur as part of CI/CD as a last check to verify that the model is deployable to the serving infrastructure

TFX InfraValidator

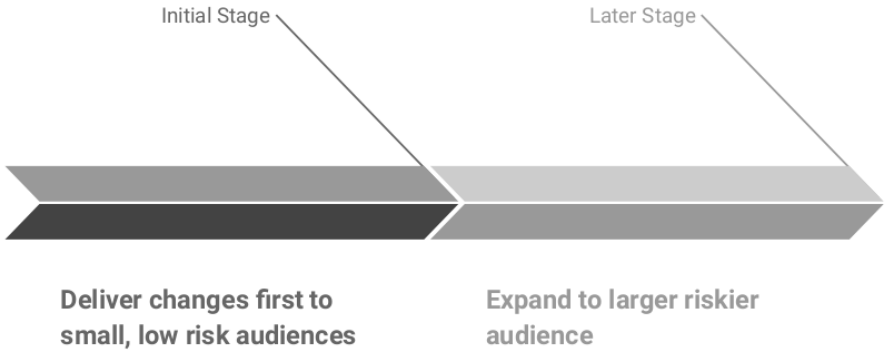
- Takes the model, launches a sand-boxed model server with the model, and checks if it can be successfully loaded and optionally queried
- Uses the same model server binary, same resources, and same server configuration as production

Model Management and Deployment Infrastructure

Progressive Delivery

Progressive Delivery

Progressive Delivery is essentially an improvement over Continuous Delivery

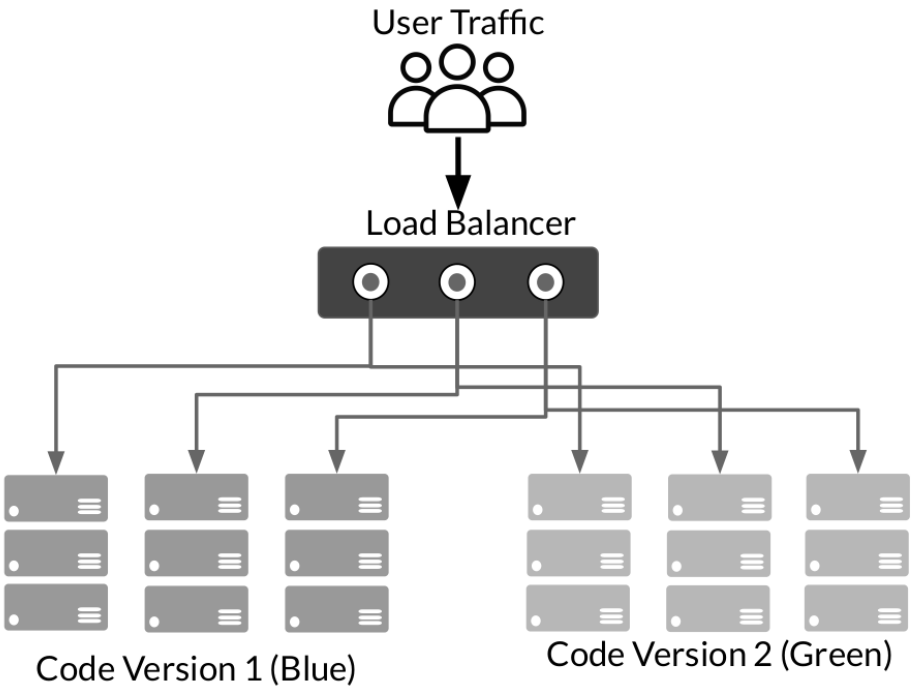


- Decrease deployment risk
- Faster deployment
- Gradual rollout and ownership

Complex Model Deployment Scenarios

- You can deploy multiple models performing the same task
- Deploying competing models, as in A/B testing
- Deploying as shadow models, as in Canary testing

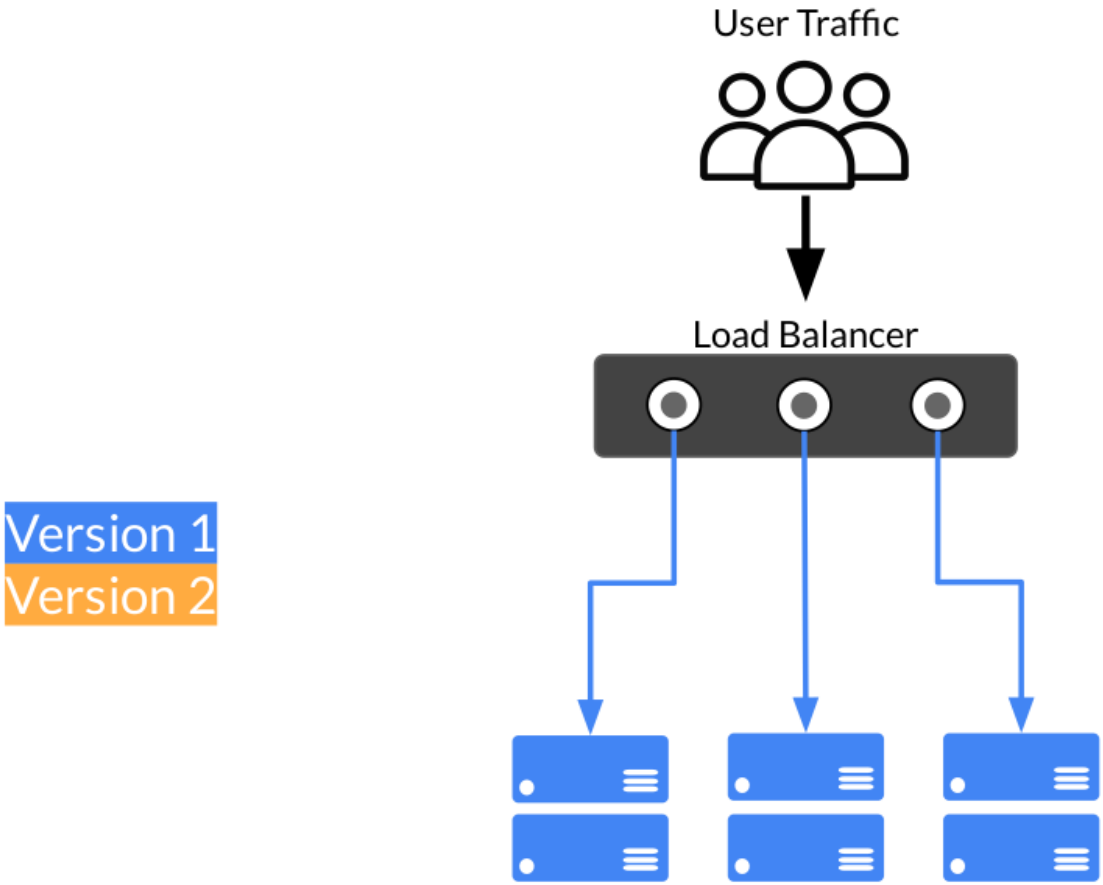
Blue/Green deployment



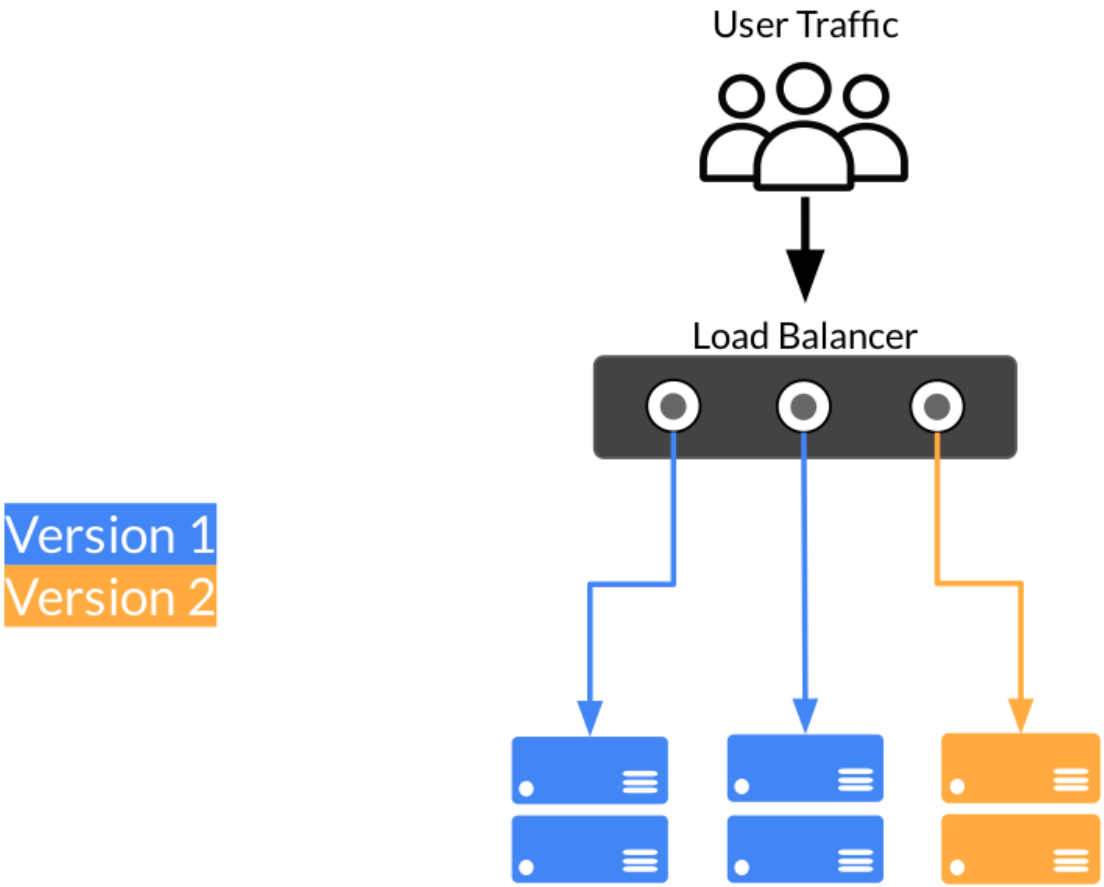
- No downtime
- Quick rollback & reliable
- Smoke testing in production environment

The diagrams are illustrations based on:
https://dev.to/mostlyjason/intro-to-deployment-strategies-blue-green-canary-and-more-3a3#

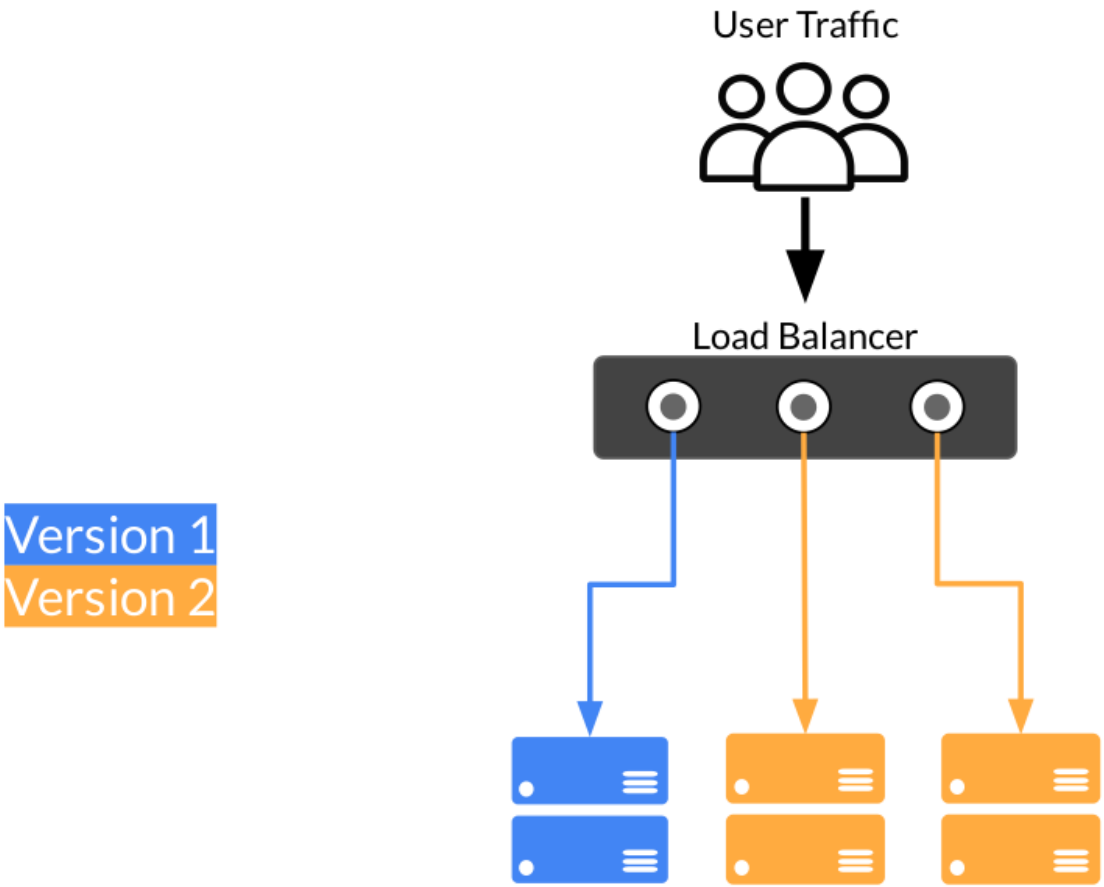
Canary deployment



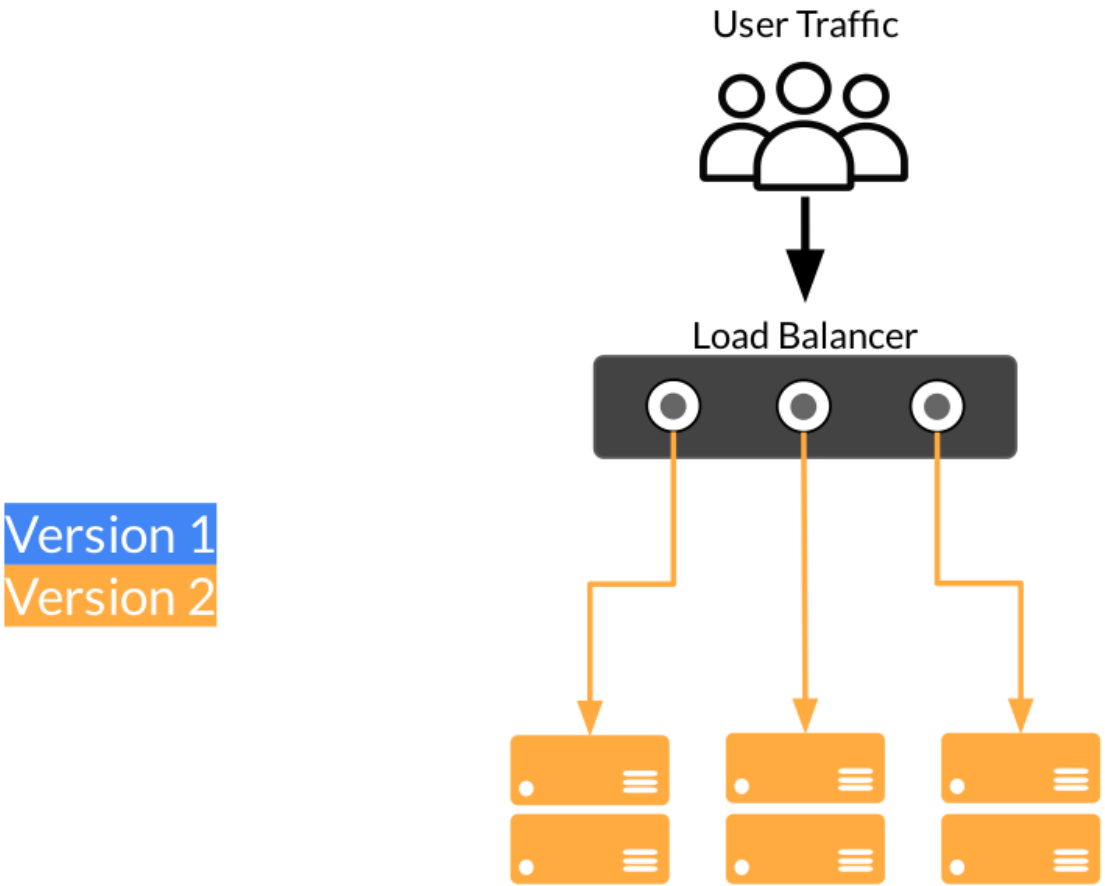
Canary deployment



Canary deployment

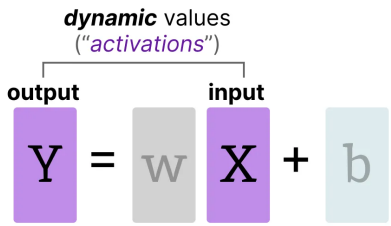


Canary deployment



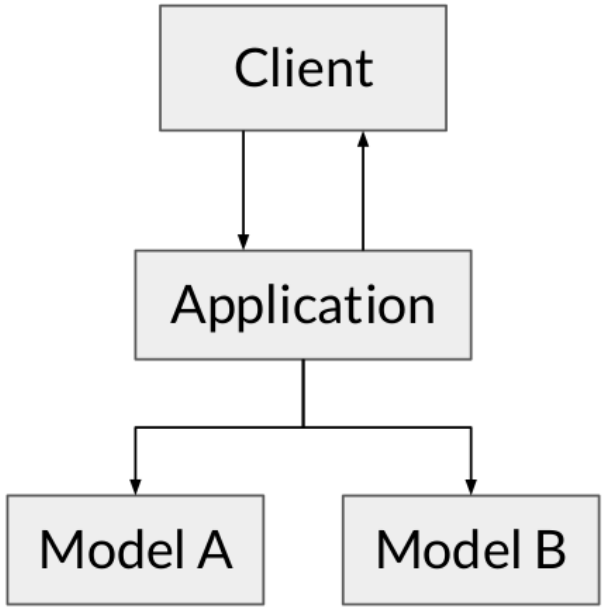
Live Experimentation

- Model metrics are usually not exact matches for business objectives
- **Example:** Recommender systems
  - Model trained on clicks
  - Business wants to maximize profit
  - Example: Different products have different profit margins

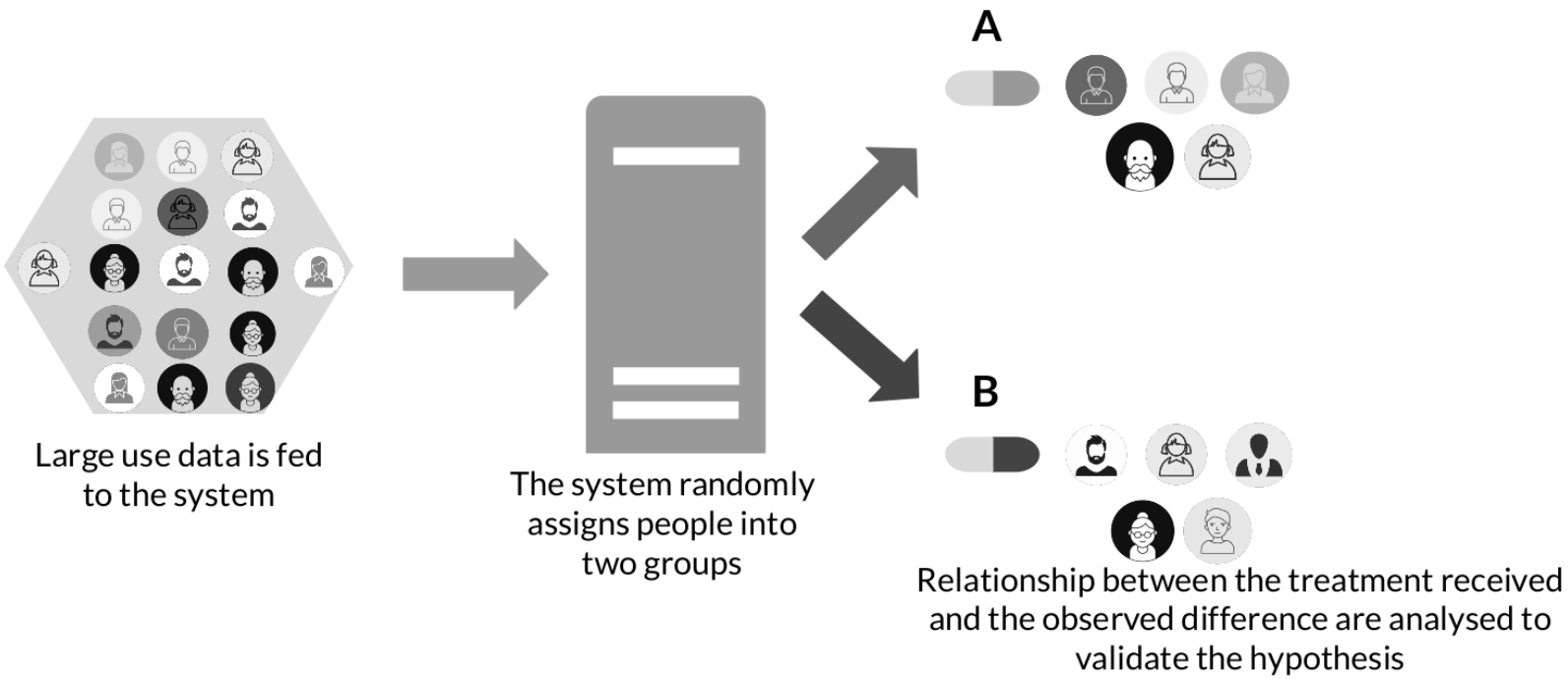


Live Experimentation: A/B Testing

- Users are divided into two groups
- Users are randomly routed to different models in the environment
- Business results from each model are gathered to see which one performs better



Live Experimentation: A/B Testing

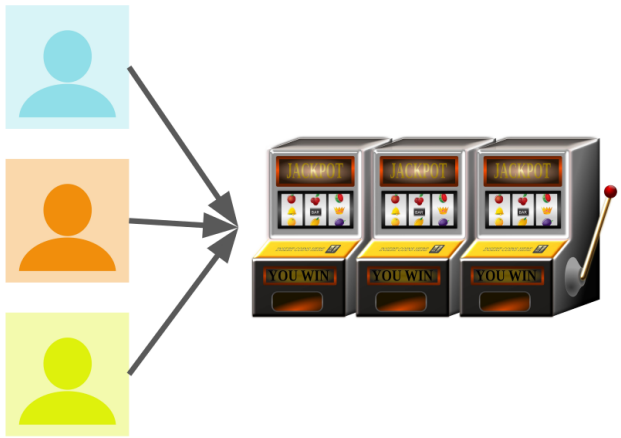


Live Experimentation: Multi-Armed Bandit (MAB)

- Uses ML to learn from test results during the test
- Dynamically routes requests to winning models
- Eventually all requests are routed to one model
- Minimizes use of low-performing models

Live Experimentation: Contextual Bandit

- Similar to multi-armed bandit, but also considers context of request
- Example: Users in different climates



Labs for This Week

Objective

Briefly describe the learning goal for this week's lab(s).

Lab Activities:

- Lab 7: [WandB] — [WandB Tutorial]
- Lab 7: [MLFlow] — [MLFlow Tutorial]
- Lab 7: [HyperOpt] — [HyperOpt Tutorial]

Submission Deadline: [Before the next class]

- Assignment 7: [WandB] — [Create a experiment of your choice]
- Assignment 7: [MLFlow] — [Create a experiment of your choice]
- Assignment 7: [HyperOpt] — [Create a experiment of your choice]

Reading Materials

This Week's Theme

Topic focus: [People + AI Guidebook - Data Collection + Evaluation.pdf]
You should use the worksheet related to this pdf to your project and submit it when its requested.

Required Readings:

- [On the Reliable Detection of Concept Drift from Streaming Unlabeled Data]

Be prepared to discuss highlights and open questions in class.

Sources


DeepLearning.AI


The People + AI Guidebook