Production: Data Distribution Shifts and Monitoring

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$ echo "Data Science Institute"
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Agenda

7.1. Monitoring

- ML System Failures
- Data Distribution Shifts
- Monitoring and Observability

7.2 Continual Learning and Test in Production

- Testing data distribution shifts.

About

- These notes are based on Chapter 6 of *Designing Machine Learning Systems*, by Chip Huyen.

Our Reference Architecture

The Flock Reference Architecture

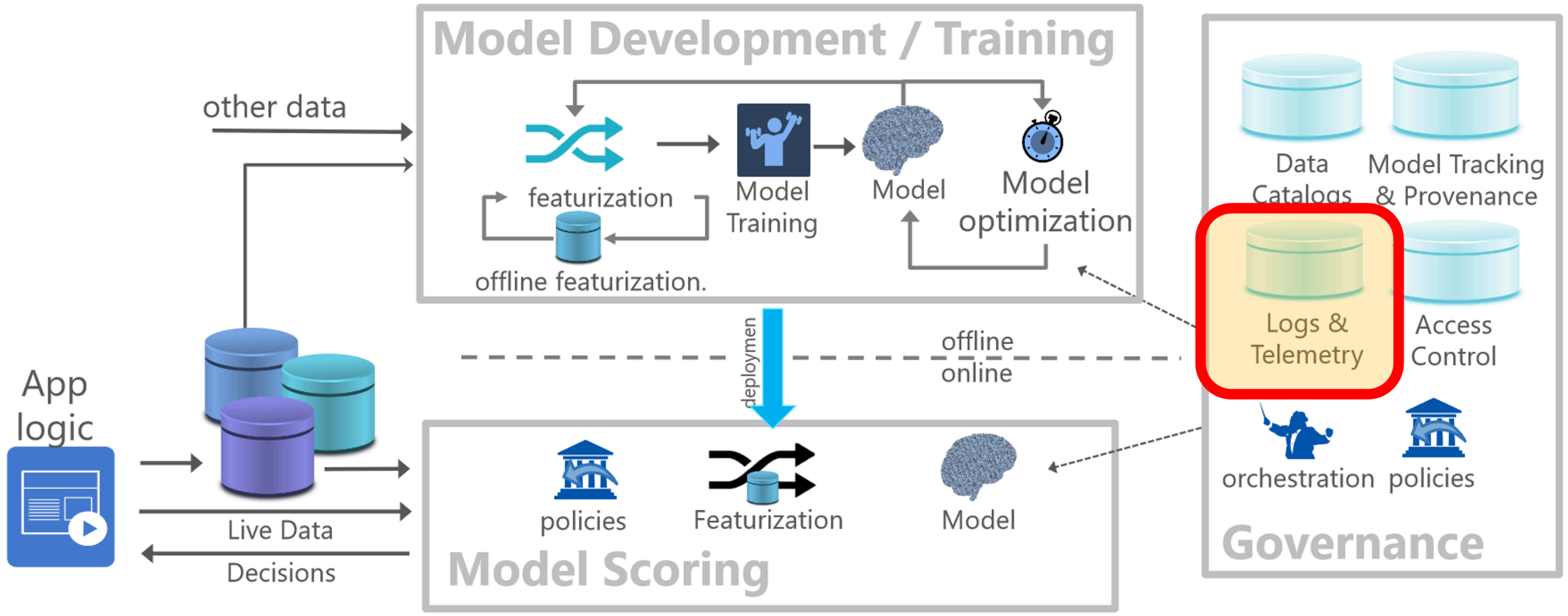


Figure 1: Flock reference architecture for a canonical data science lifecycle.

ML System Failures

What is an ML System Failure? (1/2)

A failure happens when one or more expectations of the system are not met:

- Traditional software expectations: the system executes its logic within the expected metrics, such as latency and throughput.
- ML performance: performance metrics are met, explanations are given, trust in the system (can be achieved by communicating uncertainty), etc.

What is an ML System Failure? (2/2)

- Operational expectations can be easier to detect than ML performance expectations.
- Understanding why ML systems fail can help monitor ML performance.

Software System Failures (1/2)

Dependency failure

- A package or codebase that the system depends on breaks, which leads to system failure.
- Common when the dependency is maintained by a third party.
- Can also happen when our model is a dependency of a downstream consumer.
- Deployment failure
- The root cause is deployment errors: deploying old binaries, permissions are not correctly granted, etc.
- Coding errors and integration errors (interface changes).

Software System Failures (2/2)

Hardware failures

- Hardware used to deploy the model fails.

Downtime or crashing

- Connectivity, security, and other issues may give rise to unreachable servers (AWS, Azure, GCP, etc.)
- Distributed systems are complex systems, and the risk of failure increases with complexity.

ML-Specific Failures (1/3)

Production data is different from training data

- A key assumption is that training and unseen data come from the same distribution.
- When we say that a model *learns* from data, we are saying that the model learns the distribution of the training data to use this information on unseen data.
- When predictions on unseen data are satisfactory, we say the model "generalizes to unseen data".
- The test data used in the model development phase and the cross-validation are *estimates* of the error in unseen (production) data.
- Reasons for difference:
    - Data collection, encoding, and instrumentation.
    - The world changes, and data distributions are not stationary.

ML-Specific Failures (2/3)

Edge cases

- An ML model performs well in most cases but fails in a small minority of cases, generally with catastrophic consequences.
- Data distribution may have shifted if the number of edge cases increases.
- Key concern for safety-critical applications: autonomous vehicles, health systems, risk monitoring, etc.

ML-Specific Failures (3/3)

Degenerate feedback loops

The model's predictions influence the feedback, which in turn influences the next iteration of the model:

- System outputs are used to generate the next set of inputs.
- In user-facing applications, this can drive the options or interactions that a user is offered.
- User interactions with the system are the training data.

Data Distribution Shifts

Types of Data Distribution Shifts (1/3)

Three types of shifts:

- Concept drift
- Covariate shift
- Label shift

Before we begin:

- Assume that we are looking to predict Y given data X.
- To do so, we estimate $P(Y|X)$.
- Our data, shows a distribution P(X, Y) and we know that:

$$P(X,Y) = P(Y|X)P(X) = P(X|Y)P(Y)$$

Types of Distribution Shifts (2/3)

- Covariate shift:
  - $P(X)$ changes.
  - $P(Y|X)$ does not change.
- Label shift:
  - $P(Y)$ changes.
  - $P(X|Y)$ does not change.
- Concept drift:
  - $P(Y|X)$ changes.
  - $P(X)$ does not change.

Types of Distribution Shifts (3/3)

$$P(X,Y) = P(Y|X)P(X) = P(X|Y)P(Y)$$

- $P(X,Y)$ joint distribution.
- $P(Y|X)$ conditional probability of output Y given input X.
- $P(X)$ probability density of input.
- $P(Y)$ probability density of output.

Covariate Shift (1/2)

- Covariate shift:
  - $P(X)$ changes.
  - $P(Y|X)$ does not change.
- Widely studied distribution shifts.
- Covariate is an independent variable that can influence the outcome of a statistical trial but it is not of direct interest.
- Example: while predicting house prices as a function of location, a covariate is square footage.

Covariate Shift (2/2)

Causes:

- Sampling methods: example, oversampling of cancer patients over 40.
- Training data is artificially altered: applied SMOTE and distribution changed.
- Active learning: instead of randomly sampling, use samples most helpful to that model according to some heuristic.
- Major changes in the production environment or application: changes in marketing, for example, induce more clients from a certain demographic not previously represented in training data.

Label Shift

- Label shift:
  - $P(Y)$ changes.
  - $P(Y|X)$ does not change.
- Also known as *prior shift*, *prior probability shift*, or *target shift*.
- The output distribution changes, but for a given output, the input distribution stays the same.
- When a covariate shift happens, it could be followed by a label shift.
- Methods for detecting covariate and label shifts are similar.

Concept Drift

- Concept drift:
  - $P(Y|X)$ changes.
  - $P(X)$ does not change.
- Also known as *posterior drift*.
- Input distribution remains the same, but the conditional distribution of the output given an input changes.
- "Same input, different output."
- Can be cyclic or seasonal.

Detecting Data Distribution Shifts (1/3)

Exploratory Data Analysis

- Compare different quantiles of data distributions and compare: 5th, 25th, 50th, 75th, and 95th.
- Comparing mean, median, and standard deviation only may give partial results:
  - Noticing differences may be indicative of a distribution shift.
  - **Not** noticing differences could hide distribution shifts.

Detecting Data Distribution Shifts (2/3)

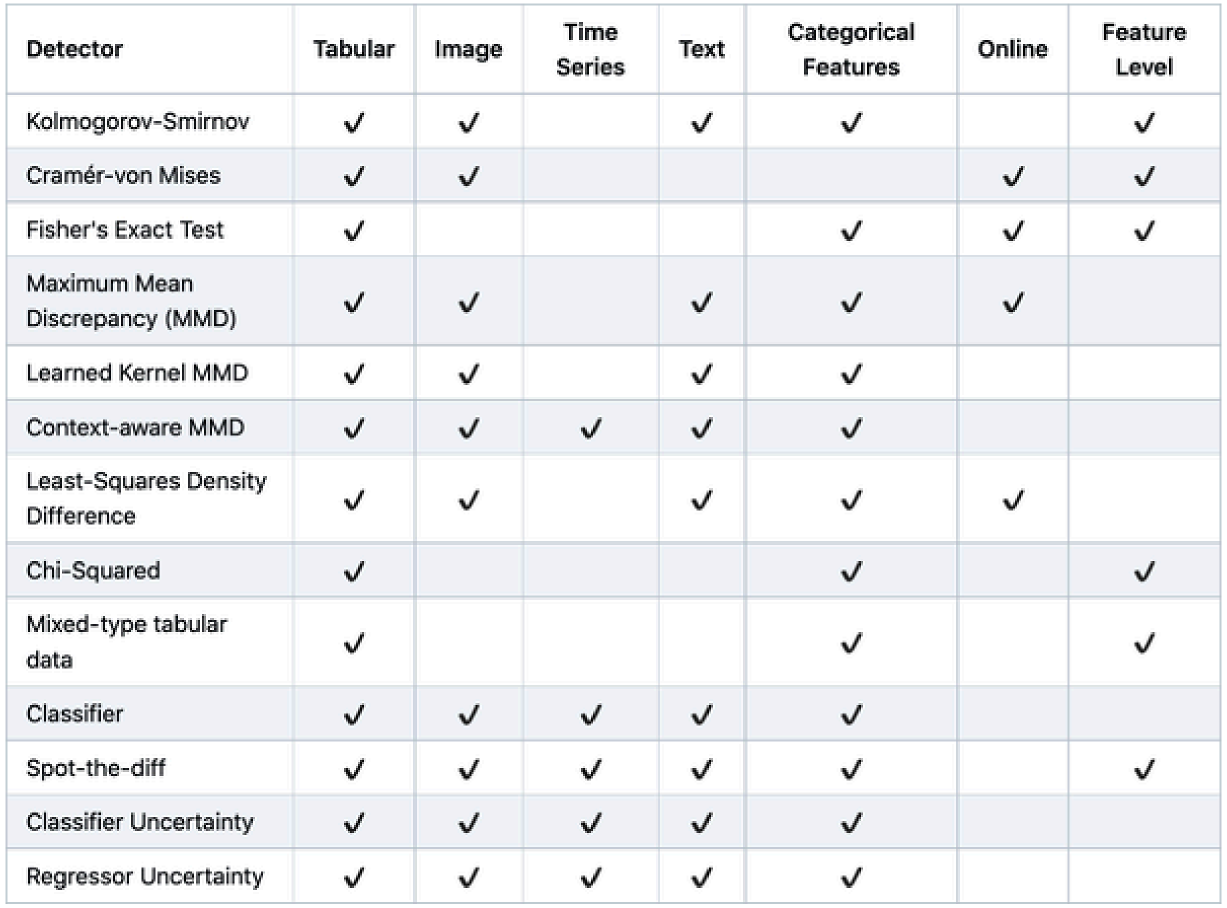
Statistical methods

- A more robust approach is to use two-sample hypothesis tests.
- These tests help us determine if the difference between distributions is statistically significant: if it is, then the probability that the difference is due to random fluctuations is low.
- If a difference is detected, it does not necessarily mean it is important. However, if the difference is noticeable in a small sample, it generally indicates that it is important.

Detecting Data Distribution Shifts (3/3)

- Many methods for univariate data. For example, Kolmogorov-Smirnov test.
- Other methods for multivariate data: Least Squares Density Difference or Maximum Mean Discrepancy.
- In general, these methods are better for low-dimensional data: it may be convenient to reduce the problem's dimensionality.

Drift Detection Methods



Detector	Tabular	Image	Time Series	Text	Categorical Features	Online	Feature Level
Kolmogorov-Smirnov	✓	✓		✓	✓		✓
Cramér-von Mises	✓	✓				✓	✓
Fisher's Exact Test	✓				✓	✓	✓
Maximum Mean Discrepancy (MMD)	✓	✓		✓	✓	✓	
Learned Kernel MMD	✓	✓		✓	✓		
Context-aware MMD	✓	✓	✓	✓	✓		
Least-Squares Density Difference	✓	✓		✓	✓	✓	
Chi-Squared	✓				✓		✓
Mixed-type tabular data	✓				✓		✓
Classifier	✓	✓	✓	✓	✓		
Spot-the-diff	✓	✓	✓	✓	✓		✓
Classifier Uncertainty	✓	✓	✓	✓	✓		
Regressor Uncertainty	✓	✓	✓	✓	✓		

Monitoring and Observability

Monitoring and Observability

Monitoring

- Tracking, measuring, and logging different *metrics* that can help determine when something goes wrong.

Classes of metrics to monitor

- Operational metrics:
    - Convey the health of the system. Operational metrics are related to the network, machine, and application.
    - Ex.: Latency, throughput, prediction requests per unit of time, percentage of successful predictions, CPU/GPU utilization, memory use, etc.
- ML-specific metrics: Model performance, predictions, features, and raw inputs.

Monitoring and Observability

Observability

- Setting up a system in a way that affords us visibility into its inner workings to help us investigate it to solve bugs and produce enhancements.
- Logs and reporting.
- Instrumentation and telemetry.

Monitoring ML Systems

Monitoring model performance

- Prediction correctness is only part of the story.
- Collect performance in terms of usability and trust (preferences).
- Collect inferred metrics (clicks, accepted recommendations, etc.)

Monitoring predictions

- Monitor distribution shifts.
- Slice analysis, backtesting, etc.

Monitoring Data (1/2)

Monitoring features

- Monitor input features and transformed features.
- Easier to validate than raw data because a defined schema exists for features.
- Common validation tests:
    - Min, max, median, and other quantile values.
    - Values satisfy a certain regular expression.
    - Values belong to a predefined set.
    - Values of a feature are always positive, less than one, greater than another feature's value, etc.

Monitoring Data (2/2)

Monitoring raw data

- Generally, a responsibility of the data engineering team or data governance.
- Automated pipelines and data quality verification.

References

References

- Agrawal, A. et al. "Cloudy with a high chance of DBMS: A 10-year prediction for Enterprise-Grade ML." arXiv preprint arXiv:1909.00084 (2019).
- Huyen, Chip. "Designing machine learning systems." O'Reilly Media, Inc.(2021).