Scalable Machine Learning with Apache Spark™

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Introductions

- Instructor Introduction
- Student Introductions
  - Name
  - Spark and Databricks Experience
  - Professional Responsibilities
  - Fun Personal Interest/Fact
  - Expectations for the Course

Course Objectives

1. Create data processing pipelines with Spark
2. Build and tune machine learning models with Spark ML
3. Track, version, and deploy machine learning models with MLflow
4. Perform distributed hyperparameter tuning with Hyperopt
5. Scale the inference of single-node models with Spark

Agenda

Day 1

1. *Spark Review**
2. *Delta Lake Review**
3. *ML Overview**
4. Break
5. **Data Cleansing**
6. **Data Exploration Lab**
7. Break
8. **Linear Regression, pt. 1**

Day 2

1. **Linear Regression, pt. 1 Lab**
2. **Linear Regression, pt. 2**
3. Break
4. **Linear Regression, pt. 2 Lab**
5. **MLflow Tracking**
6. Break
7. **MLflow Model Registry**
8. **MLflow Lab**

Day 3

1. **Decision Trees**
2. Break
3. **Random Forest and Hyperparameter Tuning**
4. Break
5. **Hyperparameter Tuning Lab**
6. **Hyperopt**

Day 4

1. **Hyperopt Lab**
2. *MLlib Deployment Options**
3. *XGBoost**
4. Break
5. **Inference with Pandas UDFs**
6. **Training with Pandas UDFs**
7. **Pandas UDFs Lab**
8. **Koalas**
9. Break
10. *Capstone Project**

*Optional

Survey

Apache Spark

Machine Learning

Programming Language

LET'S GET STARTED

Apache Spark™ Overview

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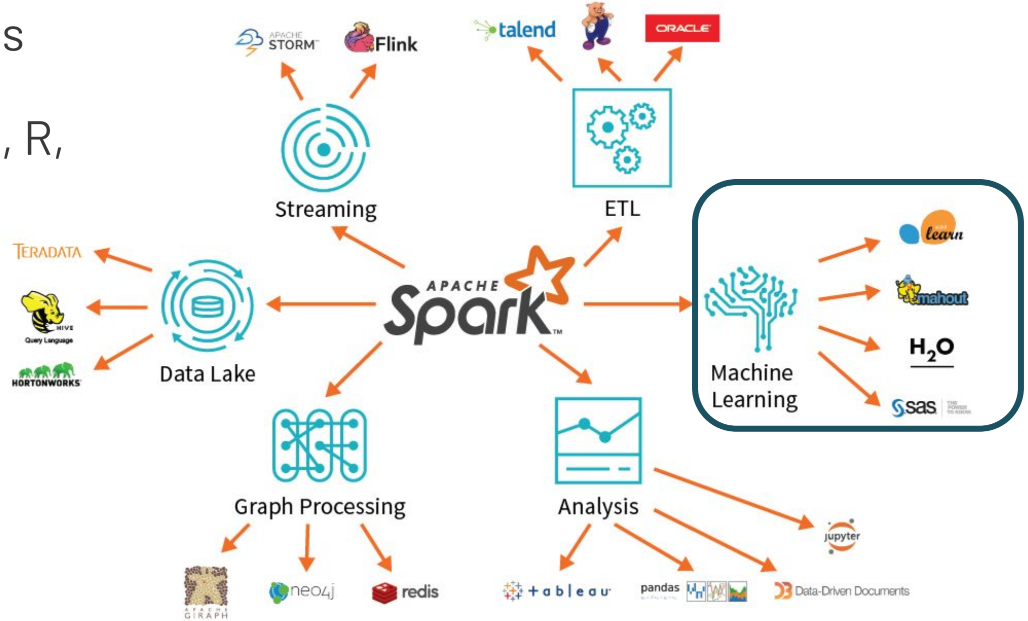
Apache Spark Background

- Founded as a research project at UC Berkeley in 2009
- Open-source unified data analytics engine for big data
- Built-in APIs in SQL, Python, Scala, R, and Java



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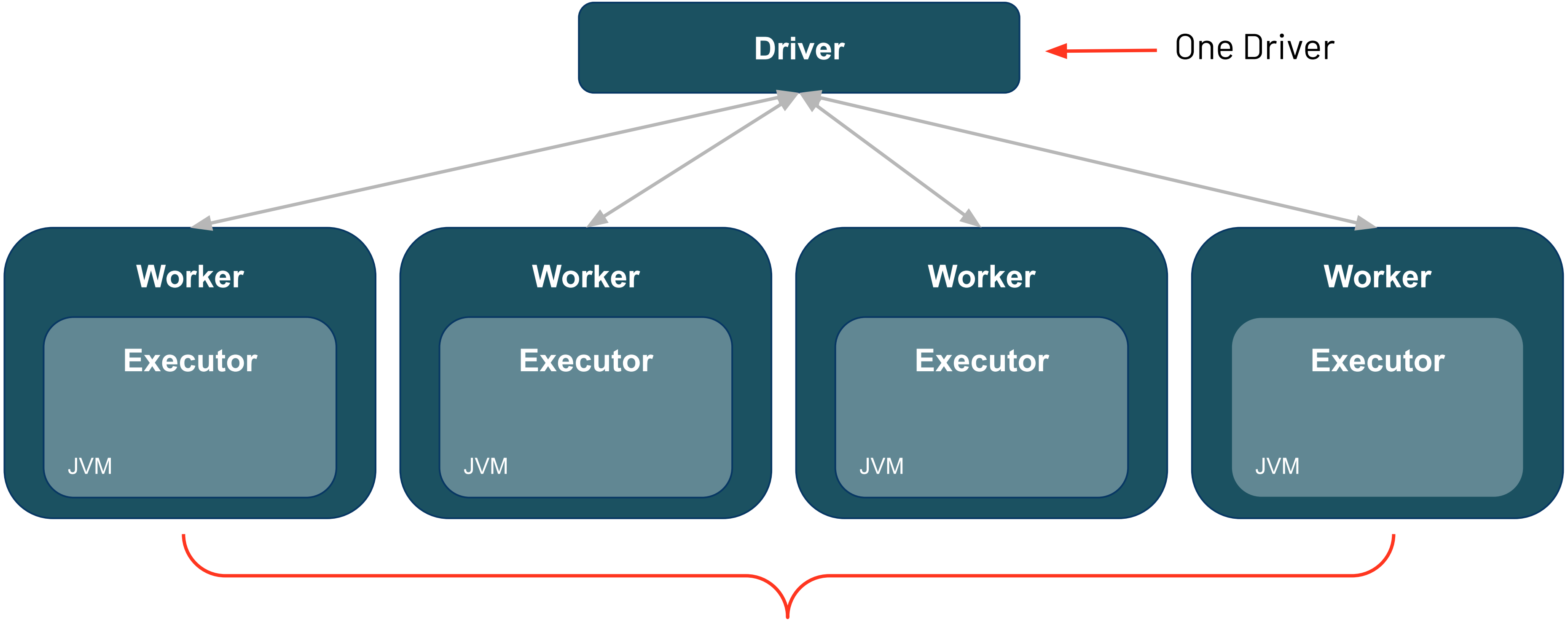
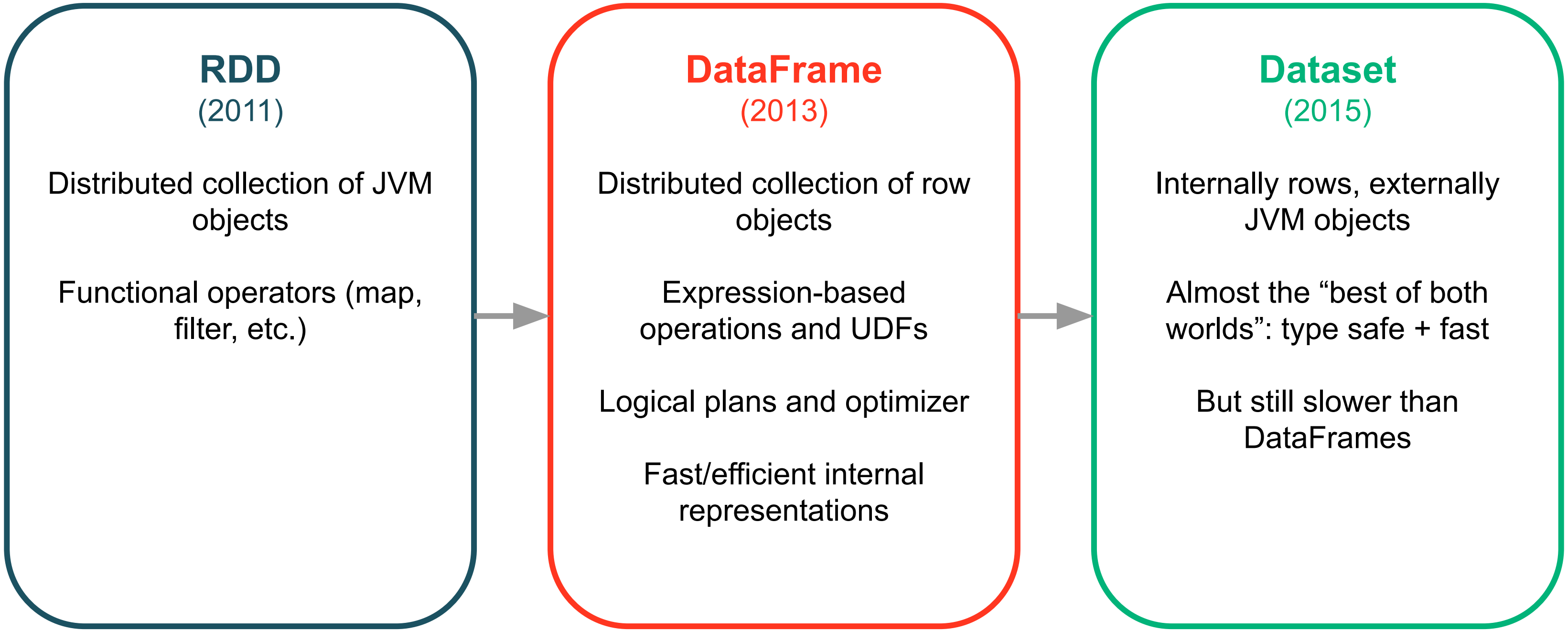
Have you ever counted the number of M&Ms in a jar?

Spark Cluster



Spark’s Structured Data APIs



RDD
(2011)

Distributed collection of JVM objects

Functional operators (map, filter, etc.)

DataFrame
(2013)

Distributed collection of row objects

Expression-based operations and UDFs

Logical plans and optimizer

Fast/efficient internal representations

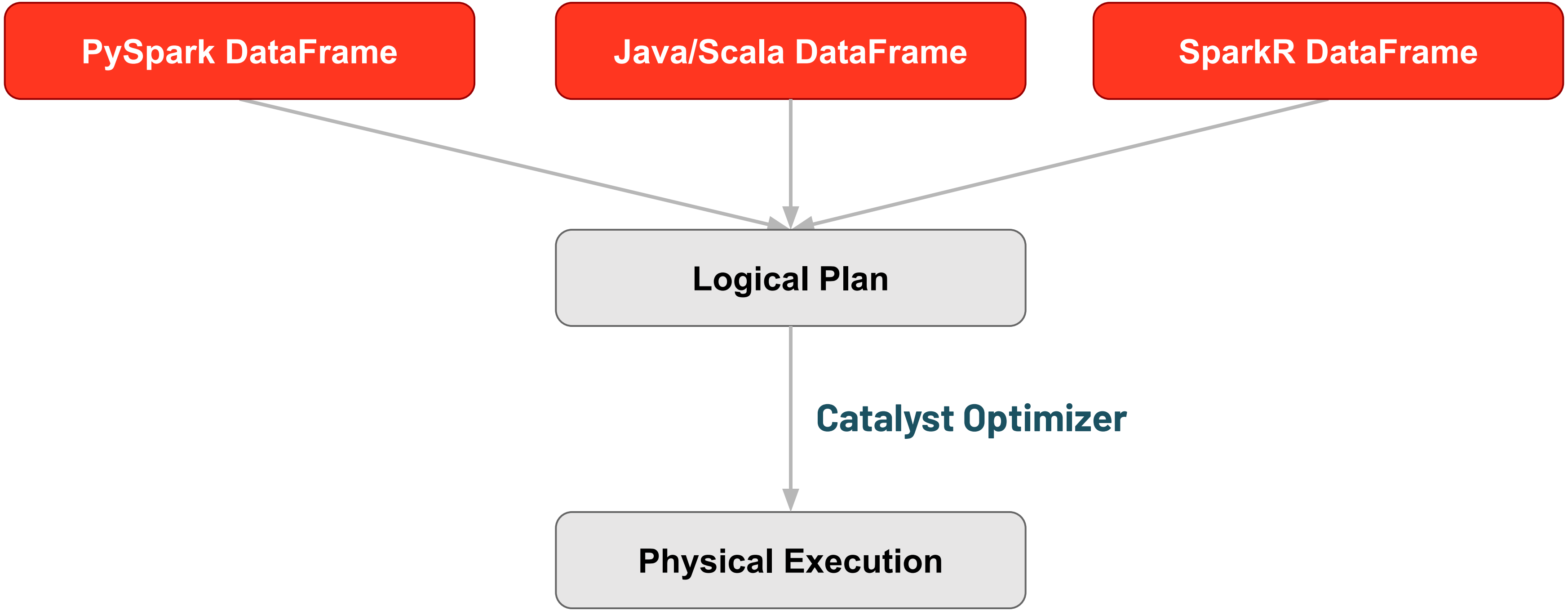
Dataset
(2015)

Internally rows, externally JVM objects

Almost the “best of both worlds”: type safe + fast

But still slower than DataFrames

Spark DataFrame Execution



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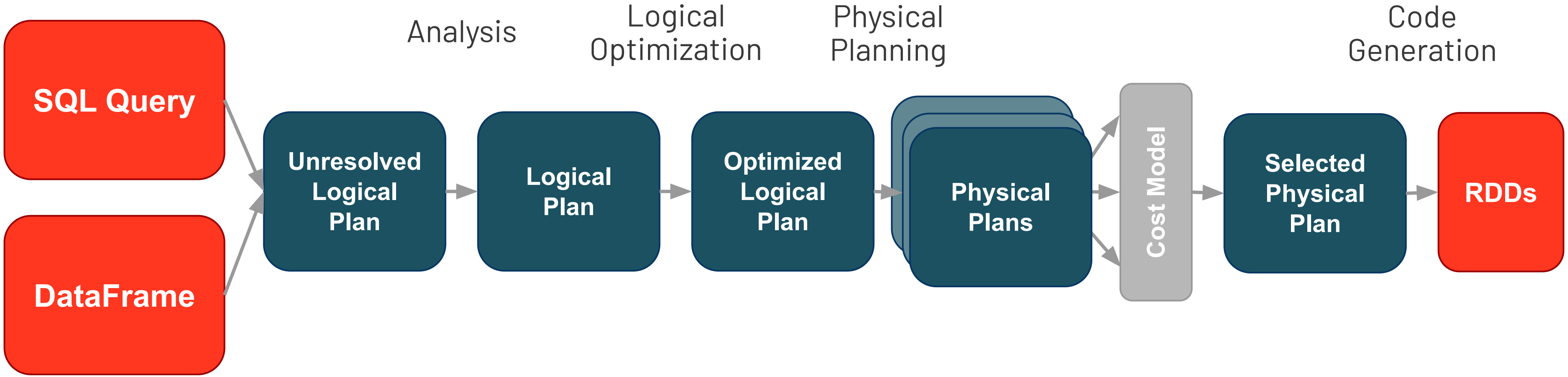
Under the Catalyst Optimizer’s Hood



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When to Use Spark

Scaling Out

Data or model is too large to process on a single machine, commonly resulting in out-of-memory errors

Speeding Up

Data or model is processing slowly and could benefit from shorter processing times and faster results

Delta Lake Overview

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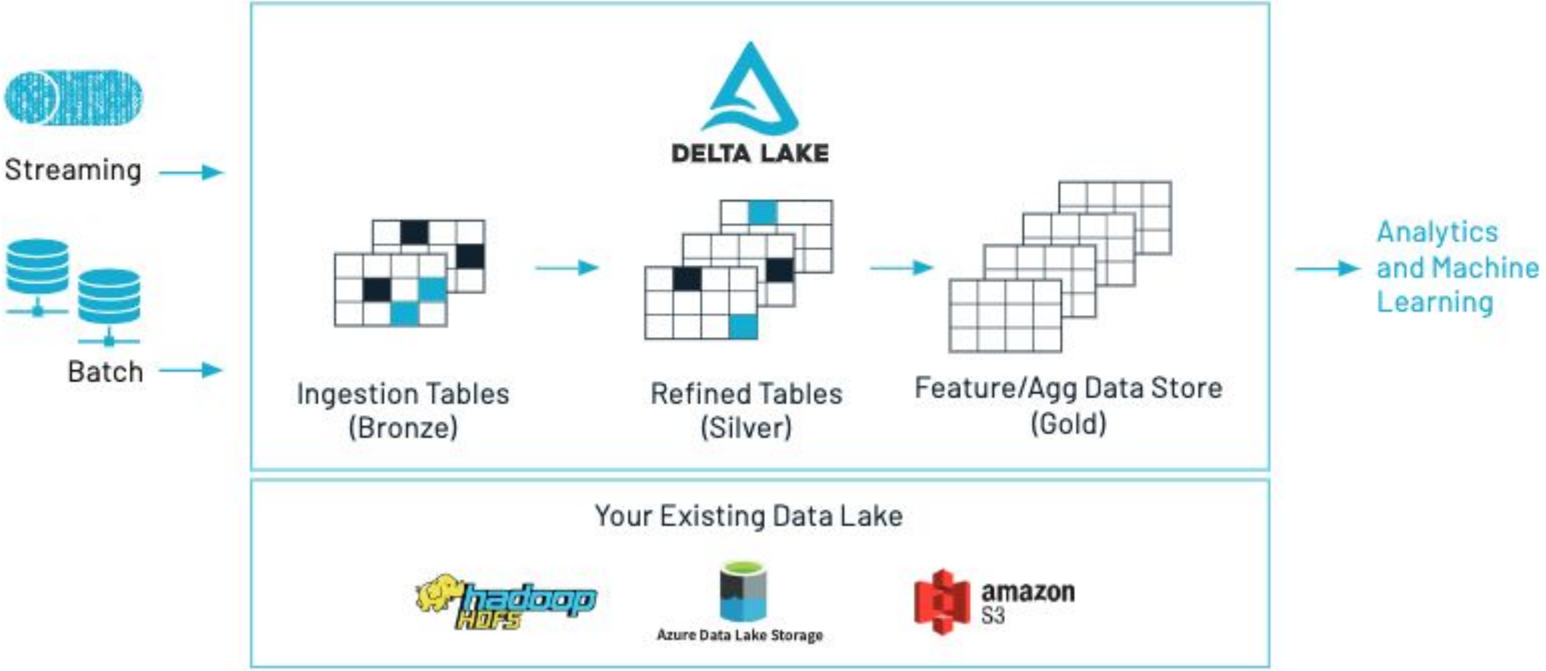
Open-source Storage Layer



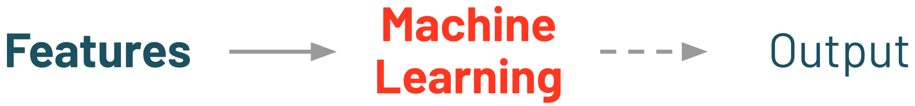
Delta Lake’s Key Features

- ACID transactions
- Time travel (data versioning)
- Schema enforcement and evolution
- Audit history
- Parquet format
- Compatible with Apache Spark API

Machine Learning Overview

What is Machine Learning

- Learn **patterns** and **relationships** in your data without explicitly programming them
- Derive an approximation function to map **features** to an **output** or relate them to each other

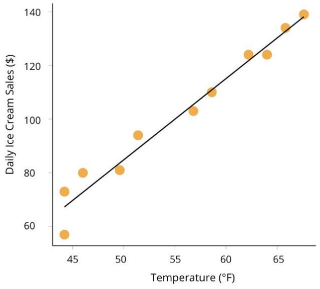


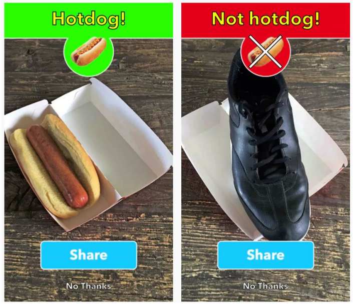
Features → **Machine Learning** - - -> Output

Types of Machine Learning

Supervised Learning

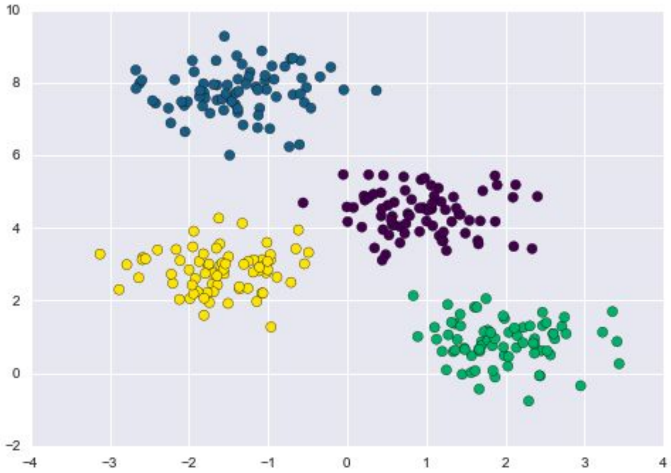
- Labeled data (known function output)
- Regression (a continuous/ordinal-discrete output)
- Classification (a categorical output)





Unsupervised Learning

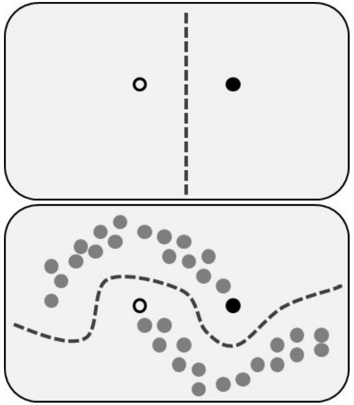
- Unlabeled data (no known function output)
- Clustering (categorize records based on features)
- Dimensionality reduction (reduce feature space)



Types of Machine Learning

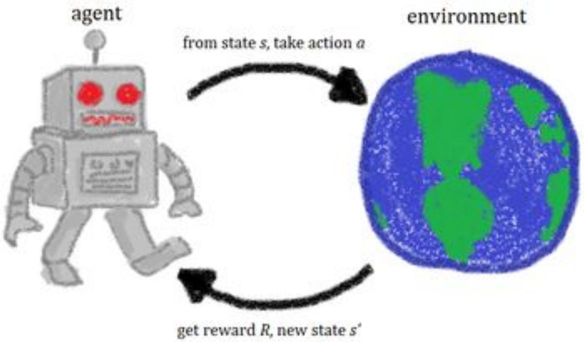
Semi-supervised Learning

- Labeled and unlabeled data, mostly unlabeled
- Combines supervised learning and unsupervised learning
- Commonly trying to label the unlabeled data to be used in another round of training



Reinforcement Learning

- States, actions, and rewards
- Useful for exploring spaces and exploiting information to maximize expected cumulative rewards
- Frequently utilizes neural networks and deep learning


agent
environment
from state s, take action a
get reward R, new state s'

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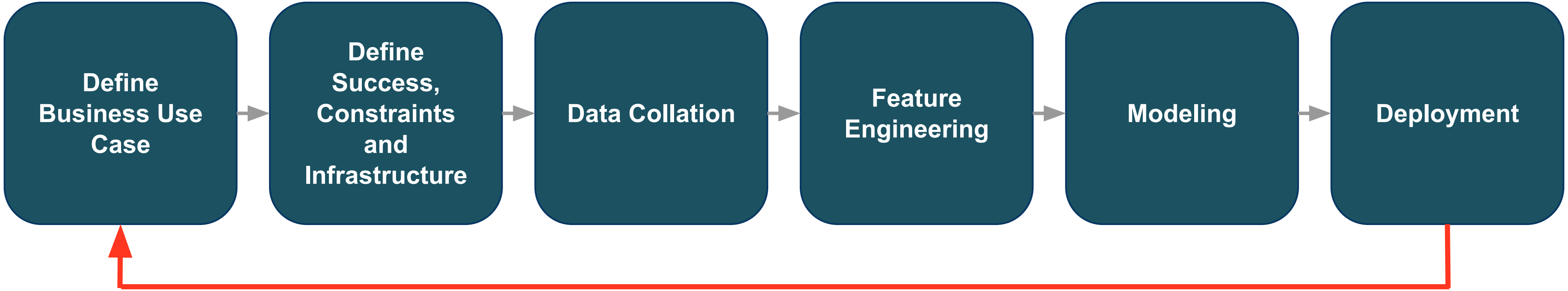
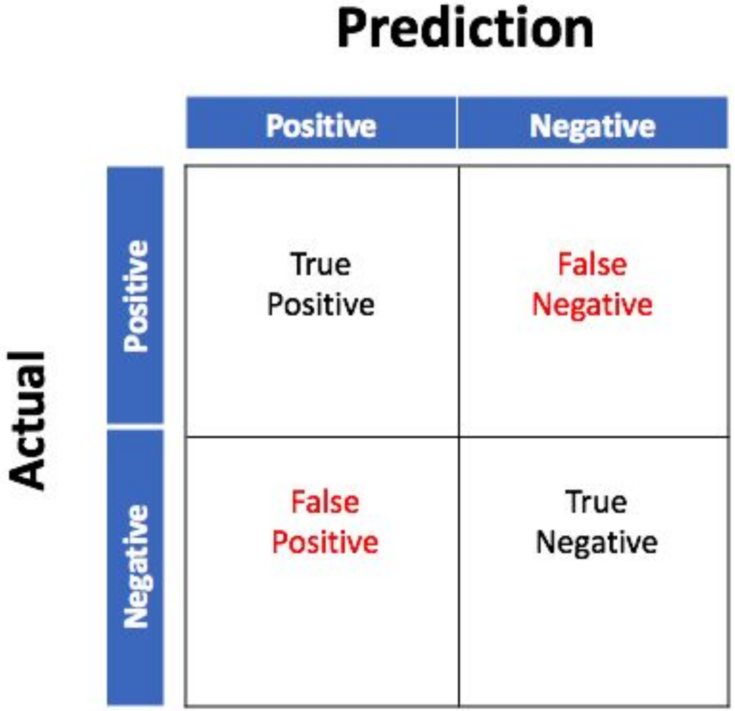
Machine Learning Workflow



Business Use Cases

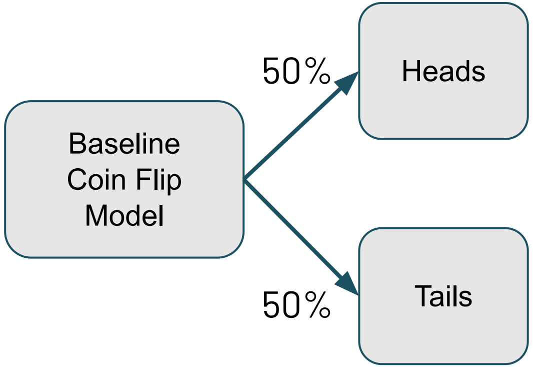
What business use cases do you have?

Defining and Measuring Success



		Prediction	
		Positive	Negative
Actual	Positive	True Positive	False Negative
	Negative	False Positive	True Negative

Baseline Models



- Simple, dummy model
- Examples include:
  - Most common case (not hot dog)
  - Target variable mean
- Point-of-reference

Algorithm Selection

How do we decide which machine learning algorithms to use?

- Data distribution
- Feature interactions
- Missing values
- Target variable type
- Deployment considerations
- Speed of training
- Need for accuracy
- Need for interpretability

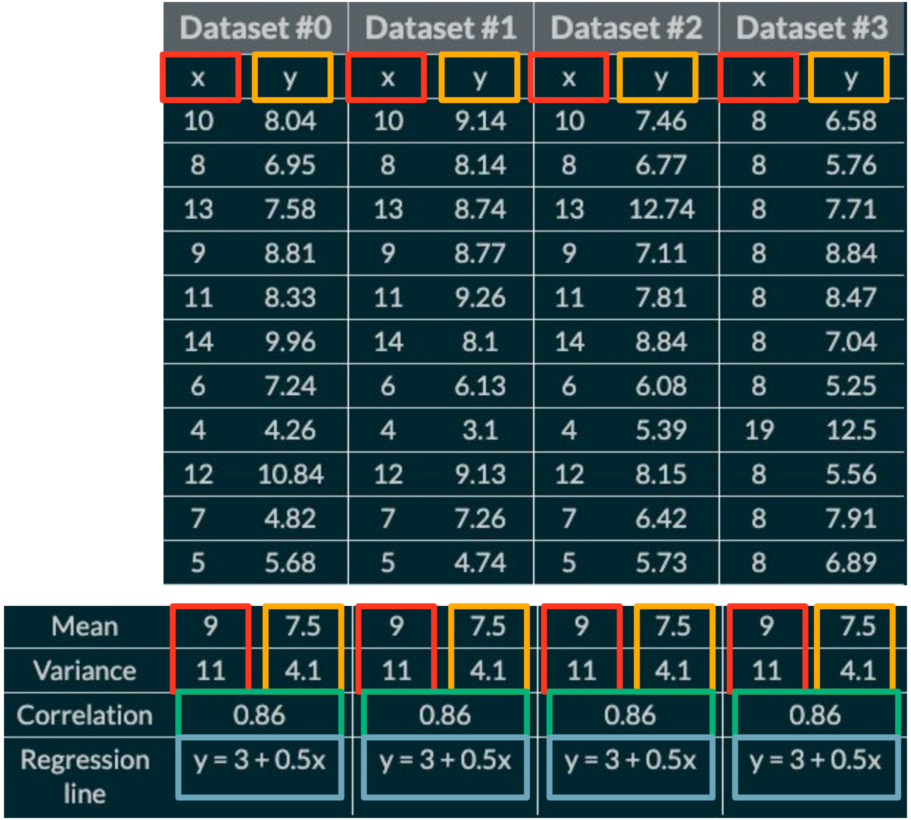
Note: Be aware of any interpretability requirements due to data regulations like the General Data Protection Regulation.

How do we get this information?

- Exploratory data analysis
  - Data visualization
  - Data cleaning
  - Data summaries
  - Data relationships

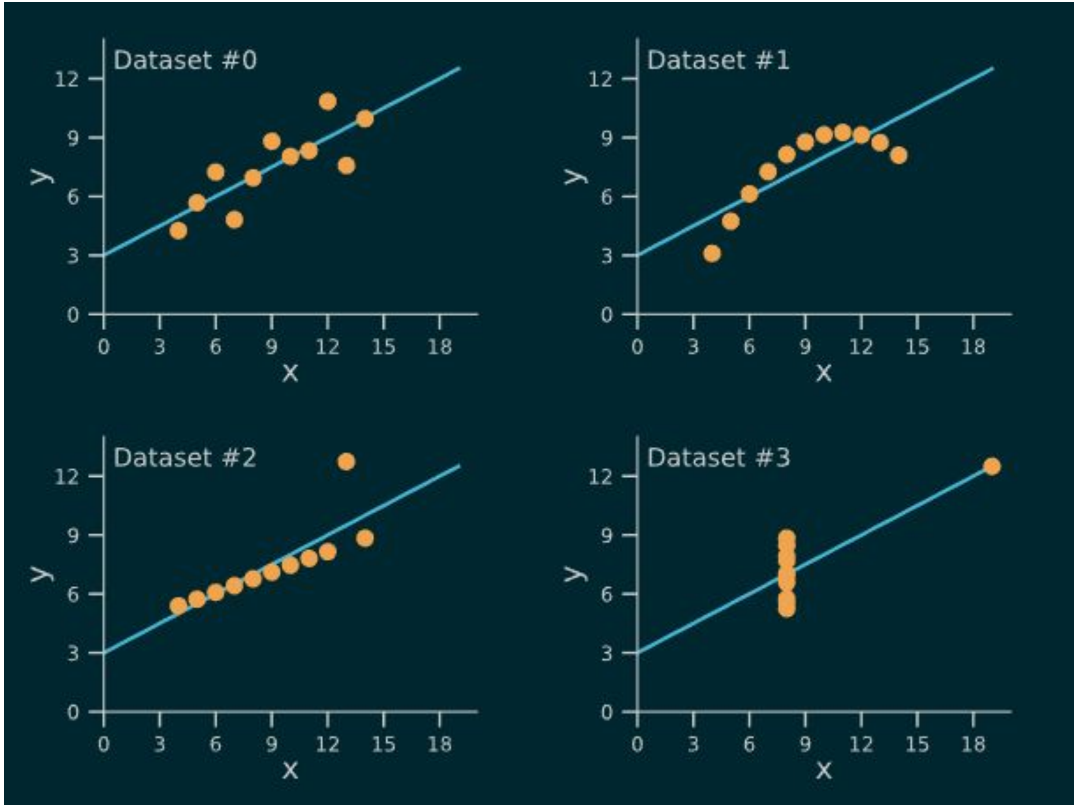
DATA CLEANSING DEMO

Importance of Data Visualization

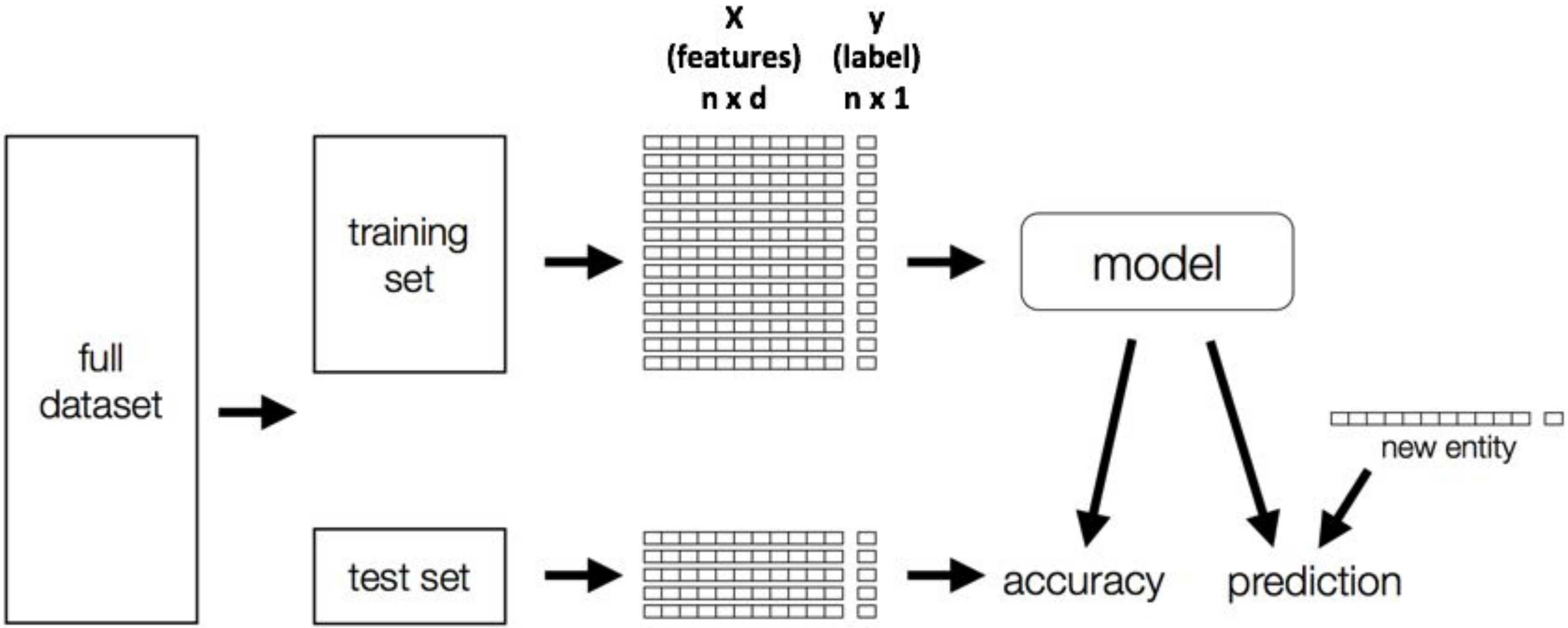


	Dataset #0		Dataset #1		Dataset #2		Dataset #3	
	x	y	x	y	x	y	x	y
	10	8.04	10	9.14	10	7.46	8	6.58
	8	6.95	8	8.14	8	6.77	8	5.76
	13	7.58	13	8.74	13	12.74	8	7.71
	9	8.81	9	8.77	9	7.11	8	8.84
	11	8.33	11	9.26	11	7.81	8	8.47
	14	9.96	14	8.1	14	8.84	8	7.04
	6	7.24	6	6.13	6	6.08	8	5.25
	4	4.26	4	3.1	4	5.39	19	12.5
	12	10.84	12	9.13	12	8.15	8	5.56
	7	4.82	7	7.26	7	6.42	8	7.91
	5	5.68	5	4.74	5	5.73	8	6.89
Mean	9	7.5	9	7.5	9	7.5	9	7.5
Variance	11	4.1	11	4.1	11	4.1	11	4.1
Correlation	0.86		0.86		0.86		0.86	
Regression line	y = 3 + 0.5x		y = 3 + 0.5x		y = 3 + 0.5x		y = 3 + 0.5x	

Importance of Data Visualization



How do we build and evaluate models?



DATA EXPLORATION LAB

Linear Regression

Linear Regression

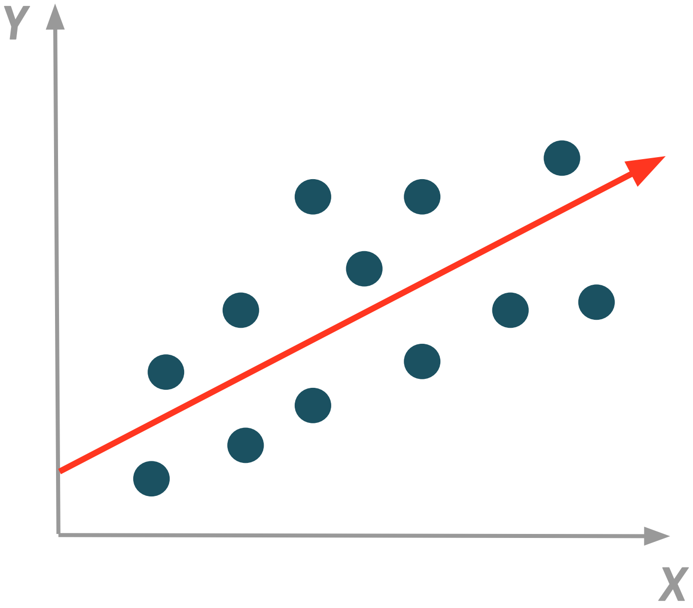
Goal: Find the *line of best fit*.

$$\hat{y} = w_0 + w_1 x$$

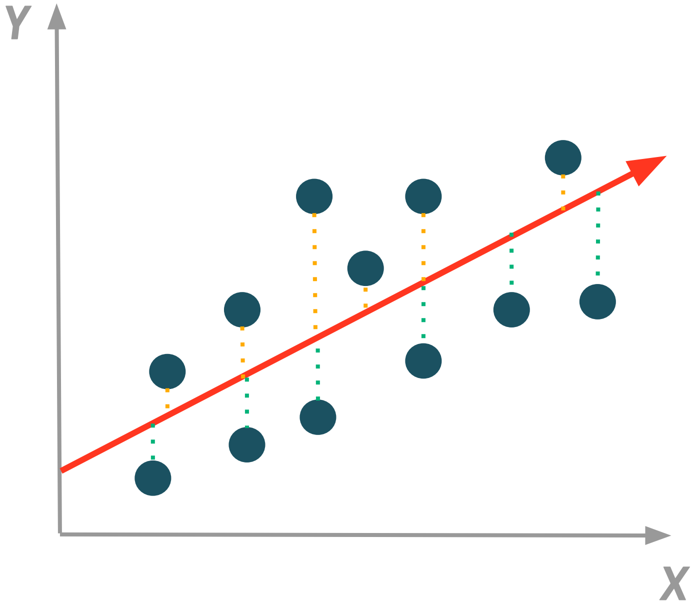
$$y \approx \hat{y} + \epsilon$$

where...

x: feature
y: label
w_0: y-intercept
w_1: slope of the line of best fit



Minimizing the Residuals



- **Blue point**: True value
- **Green-dotted line**: Positive residual
- **Orange-dotted line**: Negative residual
- **Red line**: Line of best fit

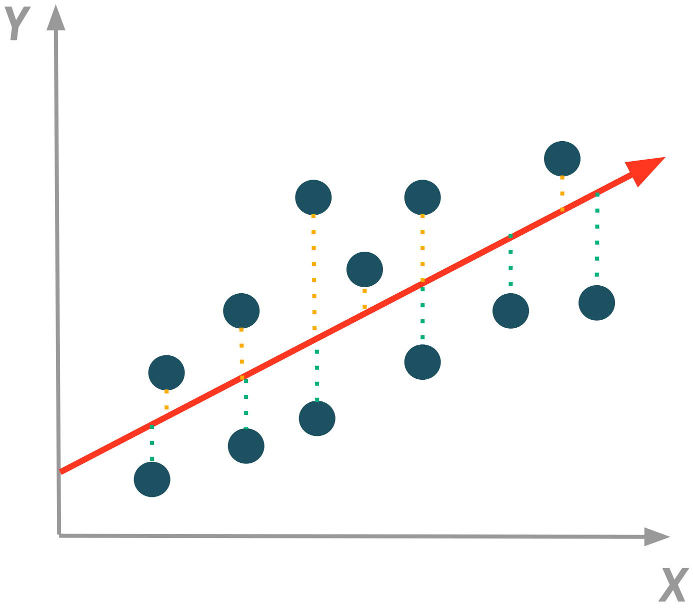
The goal is to draw a line that minimizes the sum of the squared residuals.

Regression Evaluators

Measure the "closeness" between the **actual value** and the **predicted value**.

Evaluation Metrics

- **Loss:** $(y - \hat{y})$
- **Absolute loss:** $|y - \hat{y}|$
- **Squared loss:** $(y - \hat{y})^2$



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Evaluation Metric: Root mean-squared-error (RMSE)

$$Error = (y_i - \hat{y}_i)$$

$$SE = (y_i - \hat{y}_i)^2$$

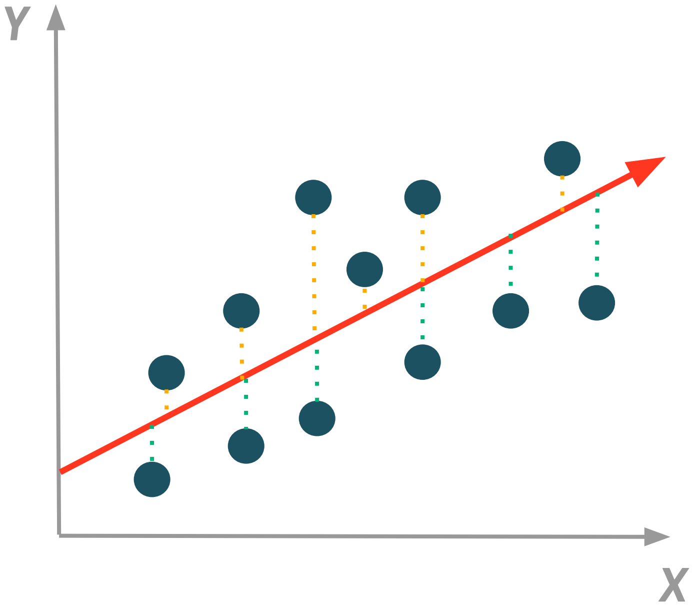
$$SSE = \sum_{i=1}^{n} (y_i - \hat{y}_i)^2$$

$$MSE = \frac{1}{n} \sum_{i=1}^{n} (y_i - \hat{y}_i)^2$$

$$\boxed{RMSE = \sqrt{\frac{1}{n} \sum_{i=1}^{n} (y_i - \hat{y}_i)^2}}$$

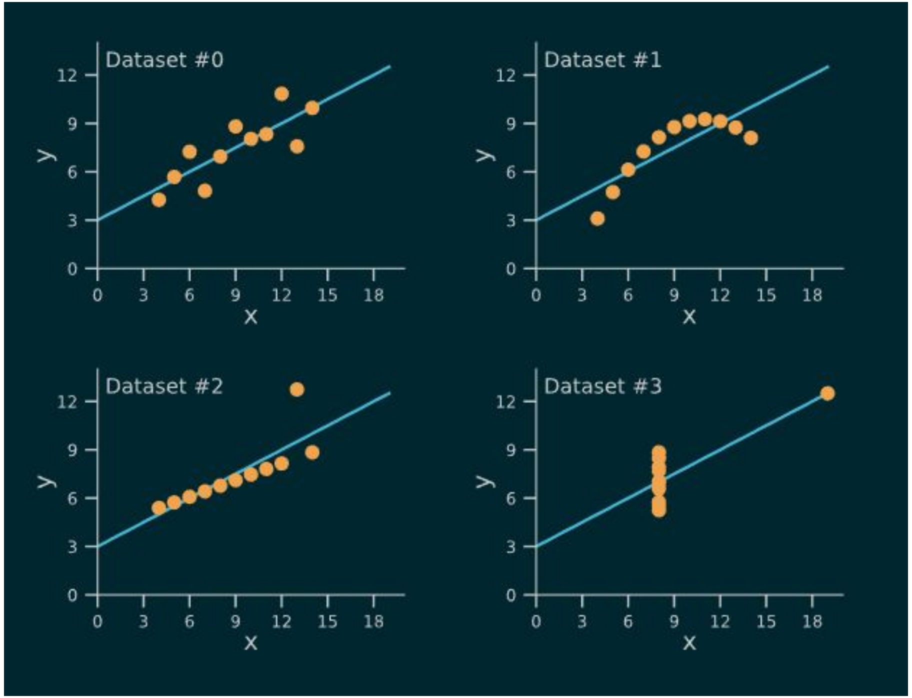
Linear Regression Assumptions

- Linear relationship between each feature and y
- Observations are independent from one another
- Features are independent from one another
- The value of residuals is not dependent on the feature values

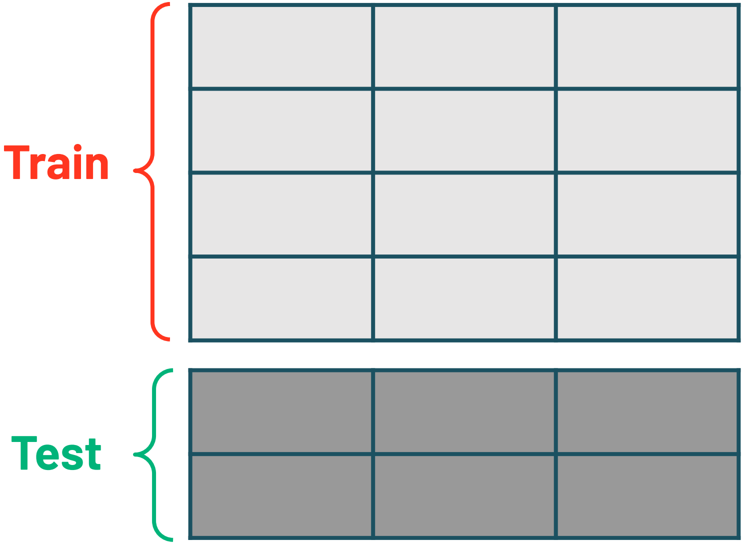


Linear Regression Assumptions

So, which datasets are suited for linear regression?



Train vs. Test RMSE



Which is more important? Why?

$$RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}$$

Evaluation Metric: R^2

$$SS_{tot} = \sum_{i=1}^{n} (y_i - \bar{y})^2$$

$$SS_{res} = \sum_{i=1}^{n} (y_i - \hat{y}_i)^2$$

$$R^2 = 1 - \frac{SS_{res}}{SS_{tot}}$$

What is the range of R^2?

Do we want it to be higher or lower?

Machine Learning Libraries

scikit learn

Scikit-learn is a popular single-node machine learning library.

But what if our data or model get too big?

APACHE Spark™

Machine Learning in Spark

Scale Out and **Speed Up**

Machine learning in Spark allows us to work with **bigger data** and train models **faster** by **distributing the data and computations** across **multiple workers.**

Spark Machine Learning Libraries

MLlib

Original ML API for Spark

Based on RDDs

Maintenance Mode

Spark ML

Newer ML API for Spark

Based on DataFrames

Supported API

LINEAR REGRESSION DEMO I

LINEAR REGRESSION LAB I

Non-numeric Features

Two primary types of non-numeric features

Categorical Features

A series of categories of a single feature

No intrinsic ordering

e.g. Dog, Cat, Fish

Ordinal Features

A series of categories of a single feature

Relative ordering, but not necessarily consistent spacing

e.g. Infant, Toddler, Adolescent, Teen, Young Adult, etc.

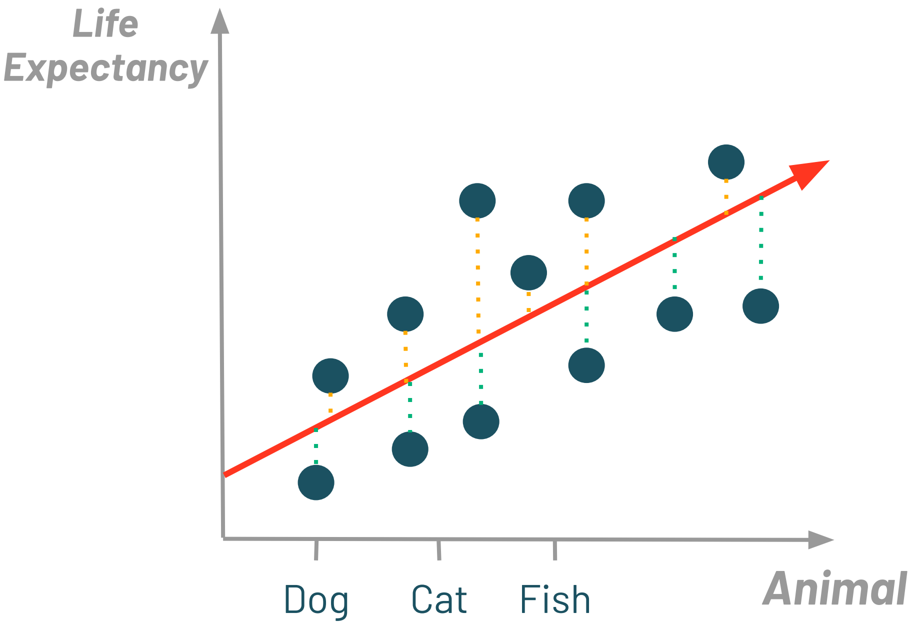
Non-numeric Features in Linear Regression

How do we handle non-numeric features for linear regression?

- X-axis is numeric, so features need to be numeric
- Convert our non-numeric features to numeric features?

Could we assign numeric values to each of the categories

- "Dog" = 1, "Cat" = 2, "Fish" = 3, etc.
- Does this make sense?



This implies 1 Cat is equal to 2 Dogs!

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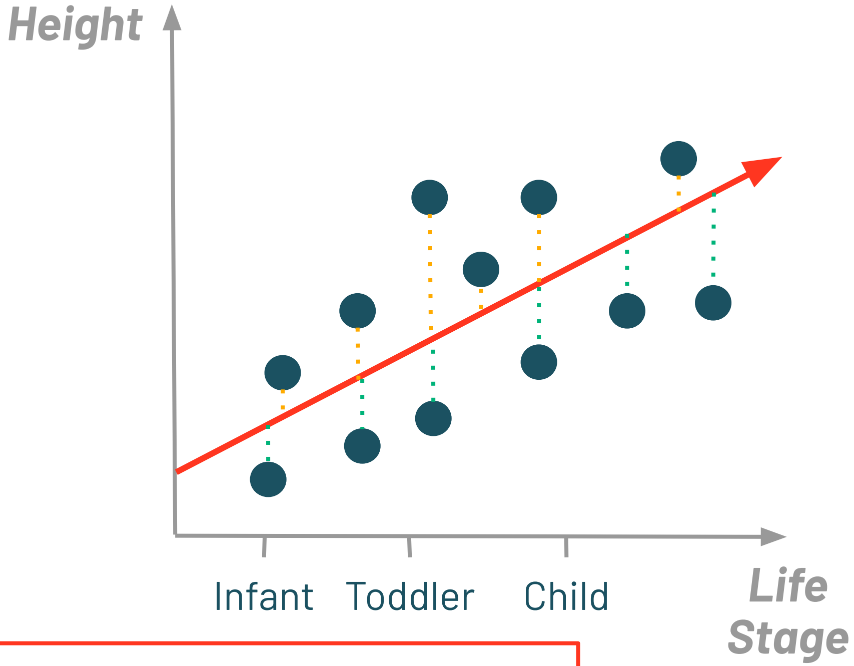
Non-numeric Features in Linear Regression

What about with ordinal variables?

- Since ordinal variables have an order just like numbers, could this work?
- “Infant” = 1, “Toddler” = 2, “Child” = 3, etc.
- Does this make sense?



Remember that the ordinal categories aren’t necessarily evenly spaced, so it’s still not perfect and not particularly scalable.

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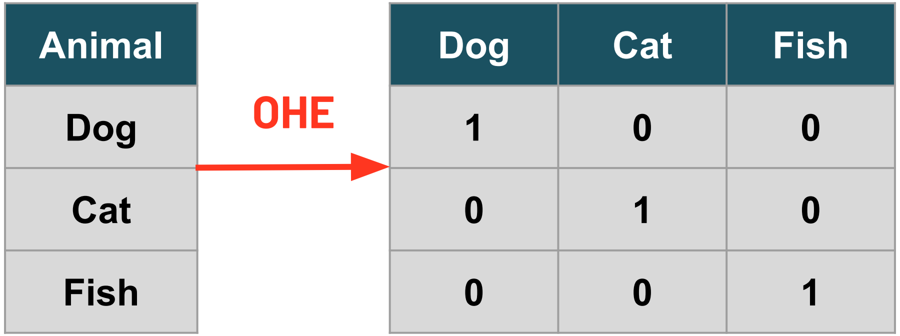
Non-numeric Features in Linear Regression

Instead, we commonly use a practice known as one-hot encoding (OHE).

- Creates a binary "dummy" feature for each category



Animal
Dog
Cat
Fish

OHE

Dog	Cat	Fish
1	0	0
0	1	0
0	0	1

- Doesn't force a uniformly-spaced, ordered numeric representation

One-hot Encoding at Scale

You might be thinking...

- Okay, I see what's happening here ... this works for a handful of animals.
- But what if we have an entire zoo of animals? That would result in really wide data!

Spark uses sparse vectors for this...

```
DenseVector(0, 0, 0, 7, 0, 2, 0, 0, 0, 0)
SparseVector(10, [3, 5], [7, 2])
```

- Sparse vectors take the form:

(Number of elements, [indices of non-zero elements], [values of non-zero elements])

LINEAR REGRESSION DEMO II

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LINEAR REGRESSION LAB II

MLflow Tracking

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MLflow

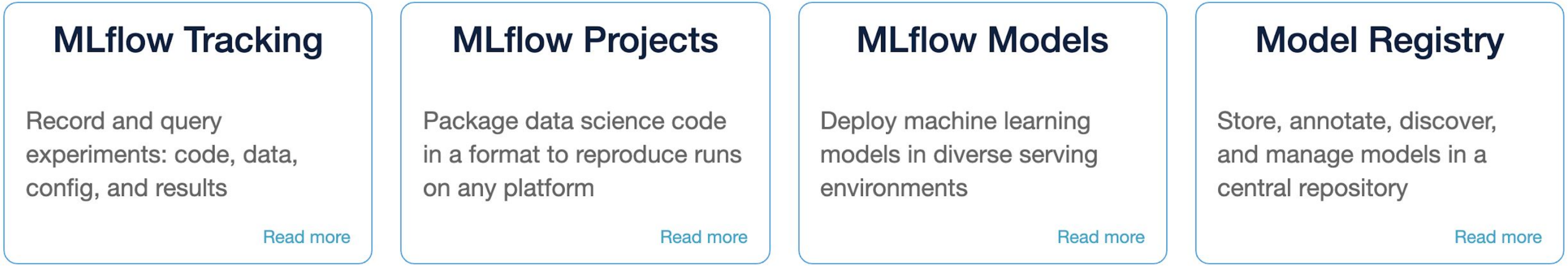
- Open-source platform for machine learning lifecycle
- Operationalizing machine learning
- Developed by Databricks
- Pre-installed on the Databricks Runtime for ML

Core Machine Learning Issues

- Keeping track of experiments or model development
- Reproducing code
- Comparing models
- Standardization of packaging and deploying models

MLflow addresses these issues.

MLflow Components



MLflow Tracking

Record and query experiments: code, data, config, and results

Read more

MLflow Projects

Package data science code in a format to reproduce runs on any platform

Read more

MLflow Models

Deploy machine learning models in diverse serving environments

Read more

Model Registry

Store, annotate, discover, and manage models in a central repository

Read more

- APIs: CLI, Python, R, Java, REST

MLflow Tracking

- Logging API
- Specific to machine learning
- Library and environment agnostic

Runs

Executions of data science code

E.g. a model build, an optimization run

Experiments

Aggregations of runs

Typically correspond to a data science project

What Gets Tracked

- Parameters
  - Key-value pairs of parameters (e.g. hyperparameters)
- Metrics
  - Evaluation metrics (e.g. RMSE)
- Artifacts
  - Arbitrary output files (e.g. images, pickled models, data files)
- Source
  - The source code from the run

Examining Past Runs

- Querying Past Runs via the API
  - MLflowClient Object
  - List experiments
  - Search runs
  - Return run metrics
- MLflow UI
  - Built in to Databricks platform

MLFLOW TRACKING DEMO

MLflow Model Registry

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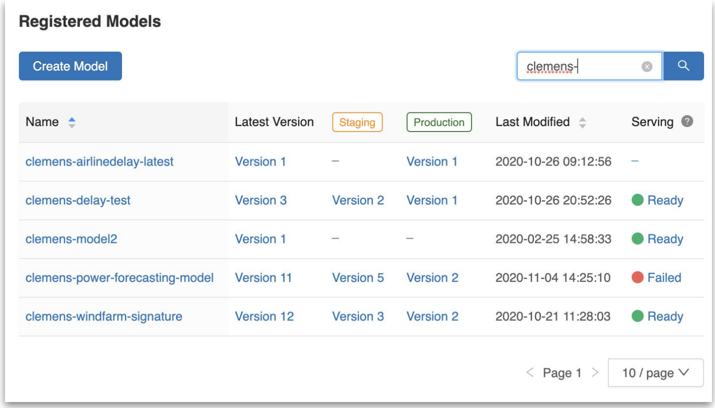
MLflow Model Registry

- Collaborative, centralized model hub
- Facilitate experimentation, testing, and production
- Integrate with approval and governance workflows
- Monitor ML deployments and their performance

Databricks MLflow Blog Post

One Collaborative Hub for Model Management

Centralized Model Management and Discovery

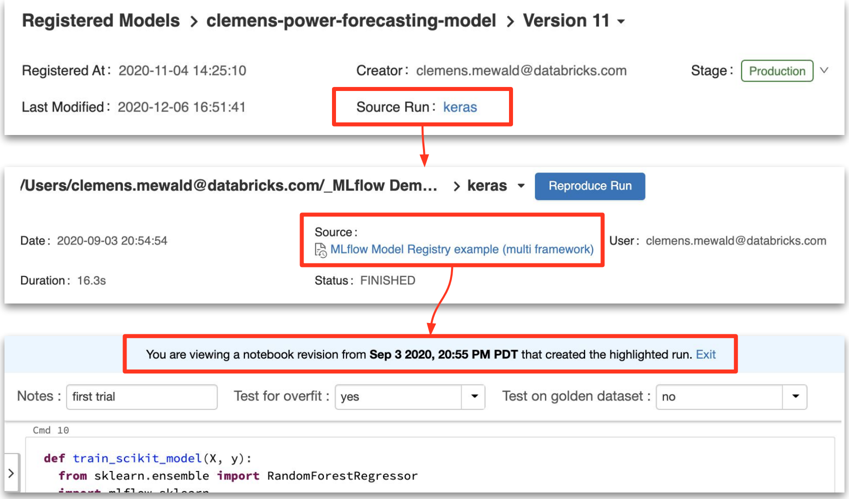


Registered Models

Name	Latest Version	Staging	Production	Last Modified	Serving
clemens-airlinedelay-latest	Version 1	–	Version 1	2020-10-26 09:12:56	–
clemens-delay-test	Version 3	Version 2	Version 1	2020-10-26 20:52:26	● Ready
clemens-model2	Version 1	–	–	2020-02-25 14:58:33	● Ready
clemens-power-forecasting-model	Version 11	Version 5	Version 2	2020-11-04 14:25:10	● Failed
clemens-windfarm-signature	Version 12	Version 3	Version 2	2020-10-21 11:28:03	● Ready

- Overview of all registered models, their versions at Staging and Production
- Search by name, tags, etc.
- Model-based ACLs

Full lineage from deployed models to training code / data



Registered Models > clemens-power-forecasting-model > Version 11

Registered At: 2020-11-04 14:25:10
Creator: clemens.mewald@databricks.com
Stage: Production
Last Modified: 2020-12-06 16:51:41
Source Run: keras

/Users/clemens.mewald@databricks.com/_MLflow Dem... > keras

Date: 2020-09-03 20:54:54
Source: MLflow Model Registry example (multi framework)
User: clemens.mewald@databricks.com
Duration: 16.3s
Status: FINISHED

You are viewing a notebook revision from **Sep 3 2020, 20:55 PM PDT** that created the highlighted run. Exit

Notes: first trial
Test for overfit: yes
Test on golden dataset: no

Cmd 10

```
def train_scikit_model(X, y):
  from sklearn.ensemble import RandomForestRegressor
  import mlflow.sklearn
```

- Full lineage from Model Version to
  - Run that produced the model
  - Notebook that produced the run
  - Exact revision history of the notebook that produced the run

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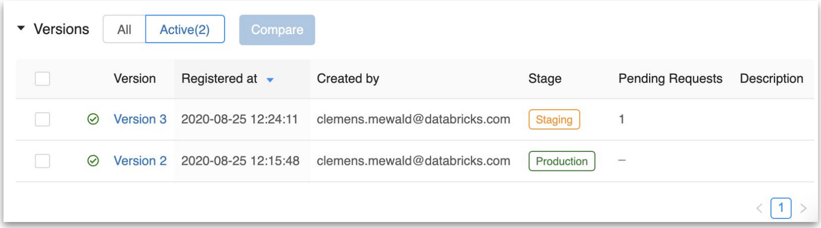
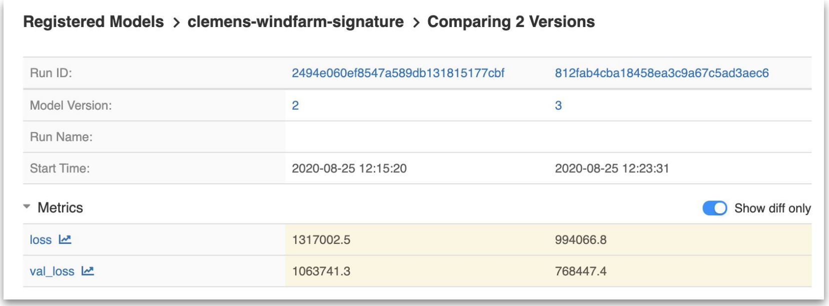
Version Control and Visibility into Deployment Process

Versioning of ML artifacts



□		Version	Registered at	Created by	Stage	Pending Requests	Description
□	✓	Version 3	2020-08-25 12:24:11	clemens.mewald@databricks.com	Staging	1	
□	✓	Version 2	2020-08-25 12:15:48	clemens.mewald@databricks.com	Production	–	



Registered Models > clemens-windfarm-signature > Comparing 2 Versions

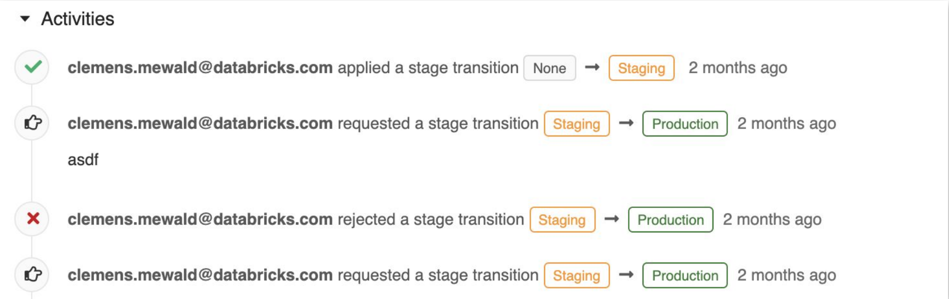
Run ID:	2494e060ef8547a589db131815177cbf	812fab4cba18458ea3c9a67c5ad3aec6
Model Version:	2	3
Run Name:		
Start Time:	2020-08-25 12:15:20	2020-08-25 12:23:31

Metrics — Show diff only

loss	1317002.5	994066.8
val_loss	1063741.3	768447.4

- Overview of active model versions and their deployment stage
- Comparison of versions and their logged metrics, parameters, etc.

Visibility and auditability of the deployment process



Activities

- ✓ **clemens.mewald@databricks.com** applied a stage transition None → Staging 2 months ago
- **clemens.mewald@databricks.com** requested a stage transition Staging → Production 2 months ago

  asdf
- ✗ **clemens.mewald@databricks.com** rejected a stage transition Staging → Production 2 months ago
- **clemens.mewald@databricks.com** requested a stage transition Staging → Production 2 months ago

- Audit log of stage transitions and requests per model

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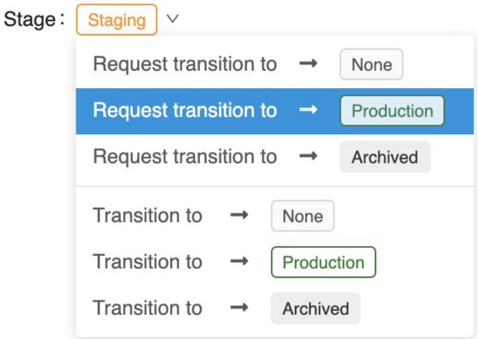
Review Processes and CI/CD Integration

Manual review process



Stage : Staging

Request transition to → None

Request transition to → Production

Request transition to → Archived

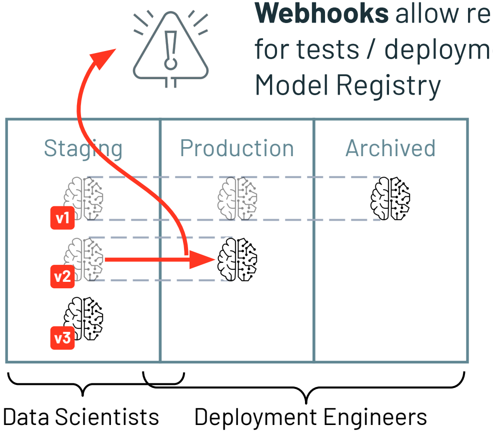
Transition to → None

Transition to → Production

Transition to → Archived

- Stage-based Access Controls
- Request and approval workflow for stage transitions

Automation through CI/CD integration



Webhooks allow registering of callbacks (e.g. for tests / deployment) on events in the Model Registry

- Webhooks for events like model creation, version creation, transition request, etc.
- Mechanisms to store results / metadata through Tags and Comments

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MLFLOW MODEL REGISTRY DEMO

MLFLOW LAB

Decision Trees

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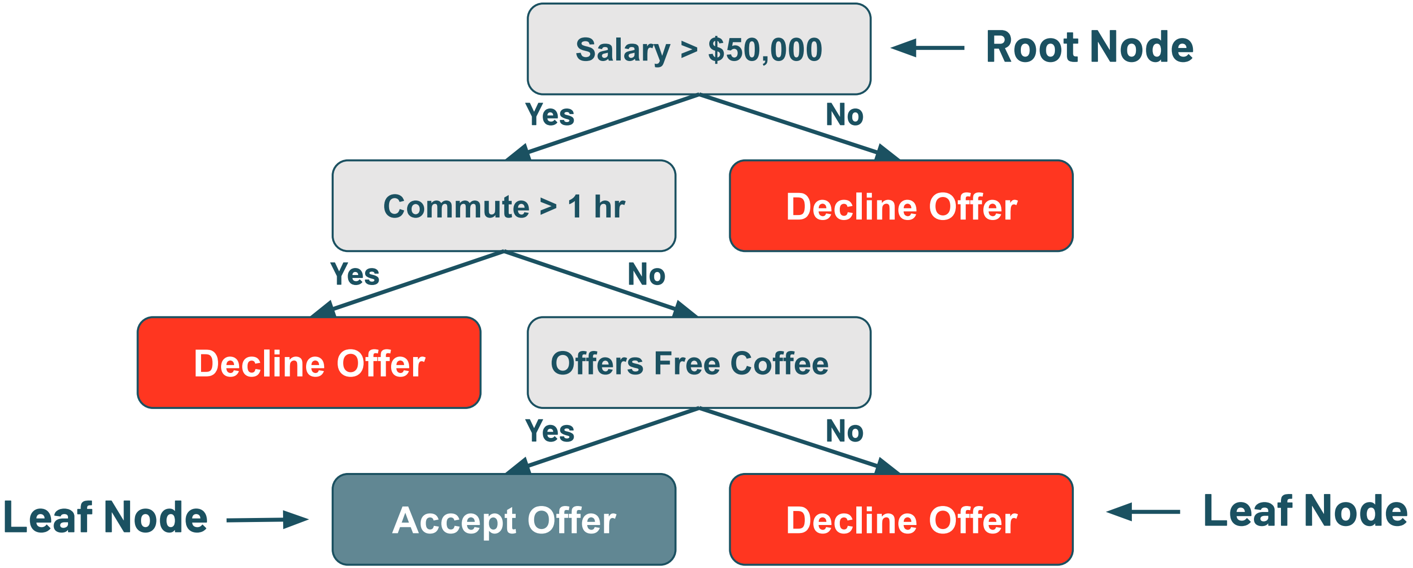
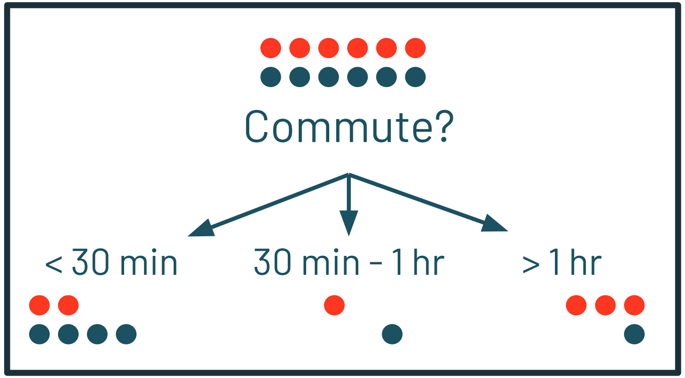
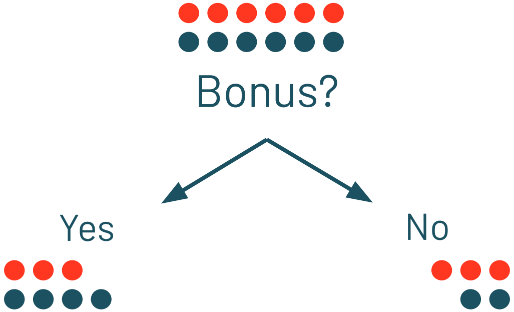
Decision Making



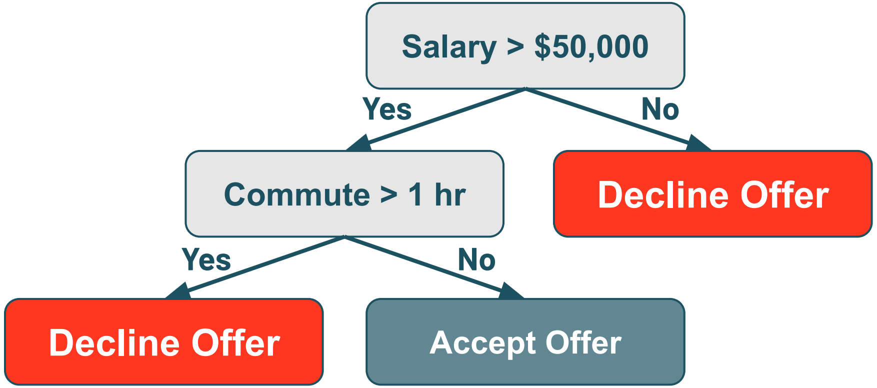
Determining Splits

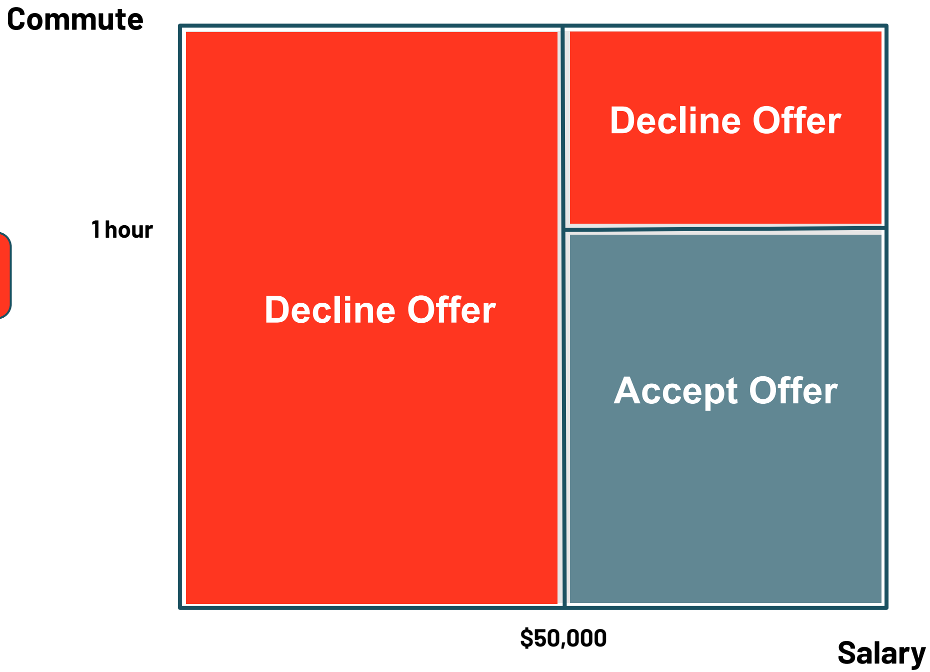




Commute is a better choice because it provides information about the classification.

Creating Decision Boundaries





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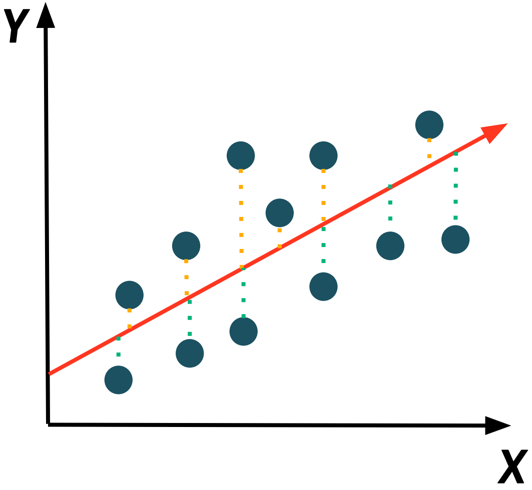
Lines vs. Boundaries

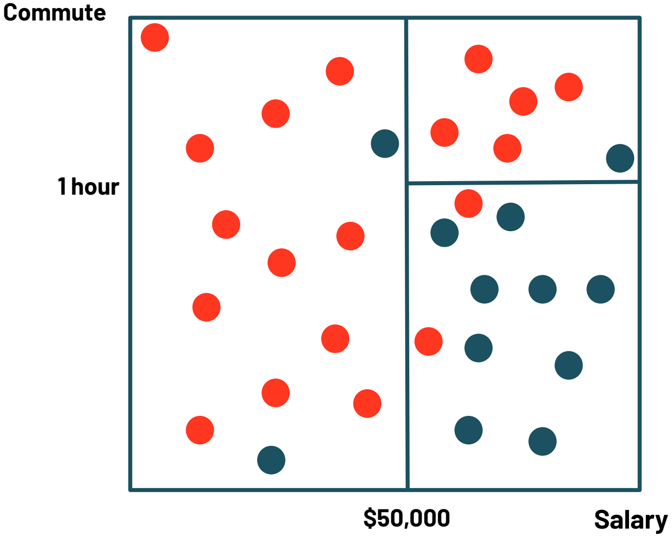
Linear Regression

- Lines through data
- Assumed linear relationship

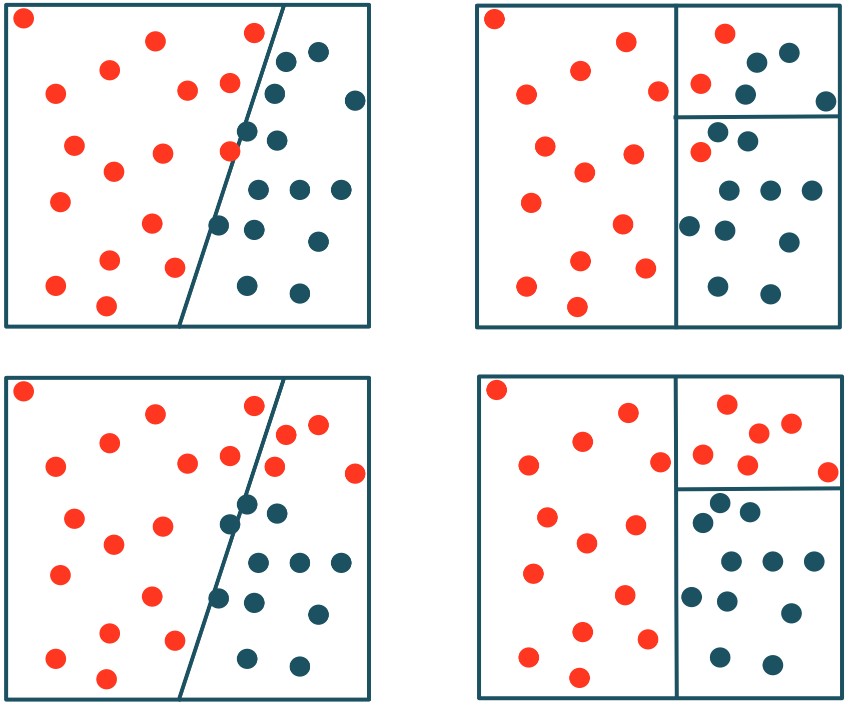


Decision Trees

- Boundaries instead of lines
- Learn complex relationships



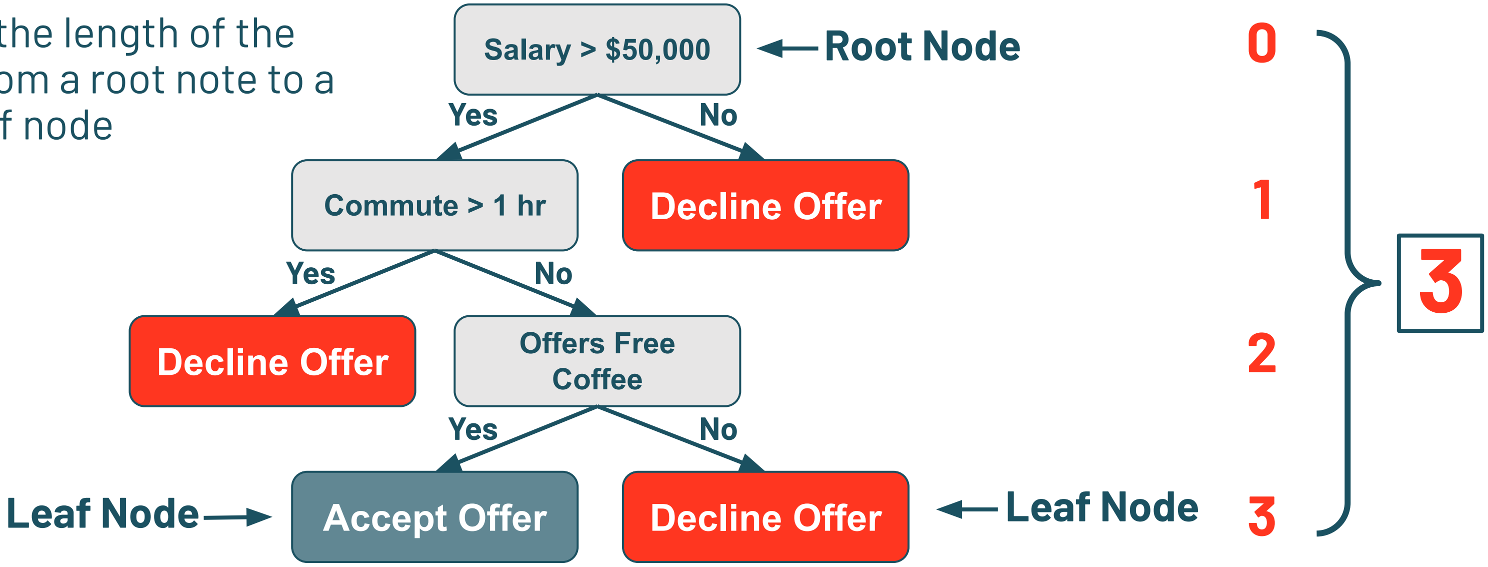
Linear Regression or Decision Tree?



It depends on the data...

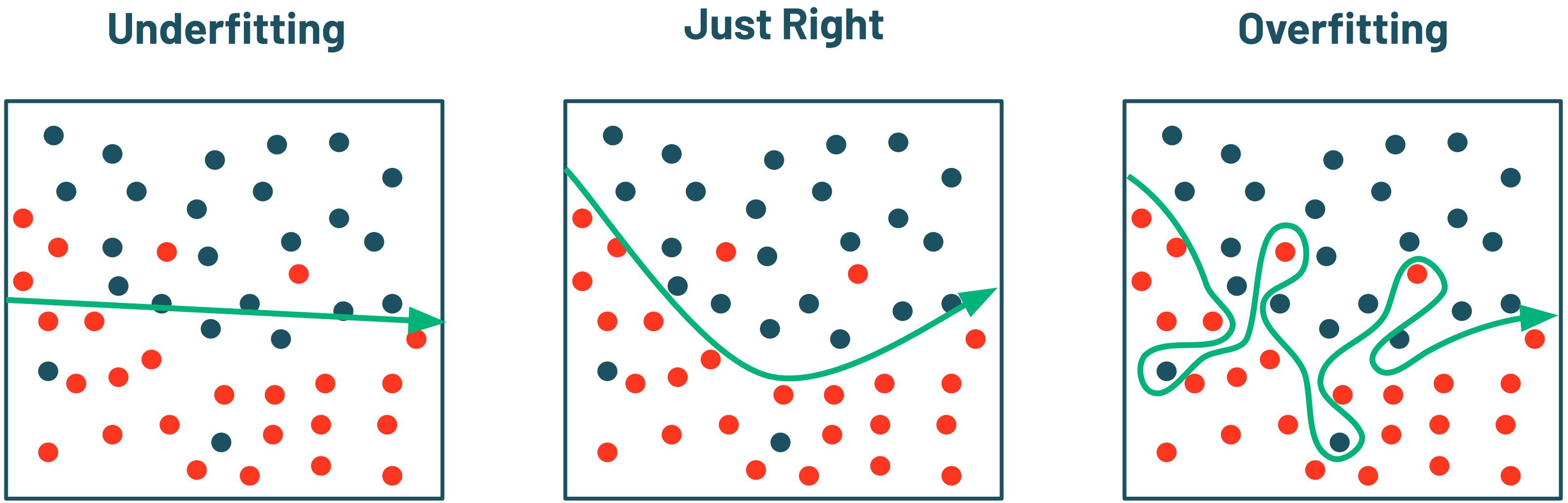
Tree Depth

Tree Depth: the length of the longest path from a root note to a leaf node



Note: shallow trees tend to **underfit**, and deep trees tend to **overfit**

Underfitting vs. Overfitting



Underfitting

Just Right

Overfitting

Additional Resource

R2D3 has an excellent visualization of how decision trees work.

DECISION TREE DEMO

Random Forests

Decision Trees

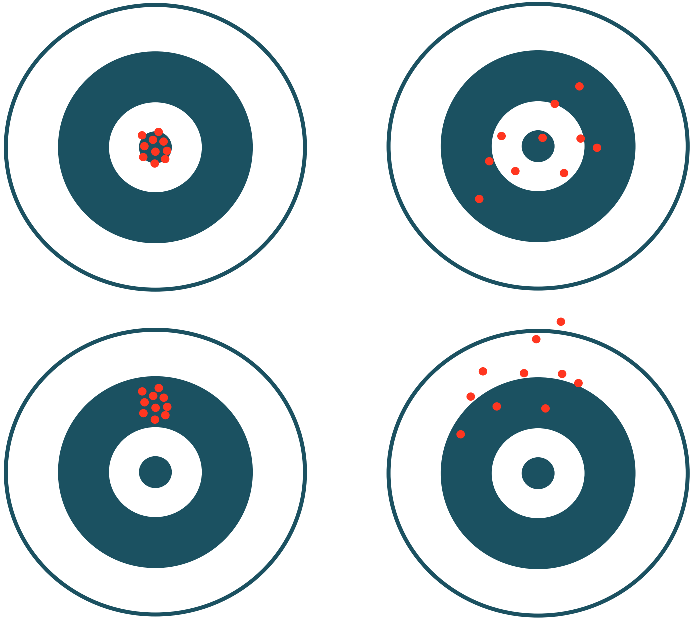
Pros

- Interpretable
- Simple
- Classification
- Regression
- Nonlinear relationships

Cons

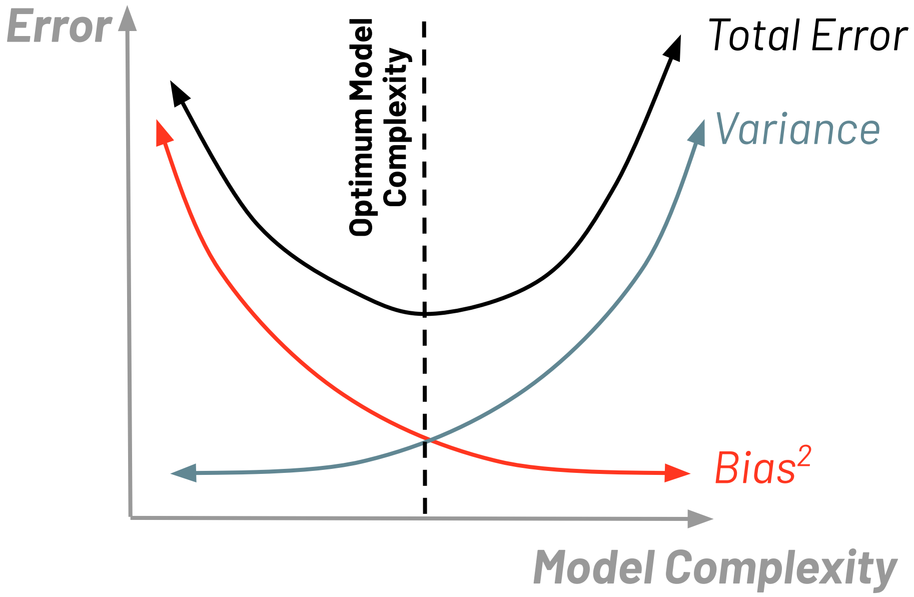
- Poor accuracy
- High variance

Bias vs. Variance



Bias-Variance Tradeoff

Error = Variance + Bias^2 + noise



- Reduce Bias
  - Build more complex models
- Reduce Variance
  - Use a lot of data
  - Build simple models
- What about the noise?

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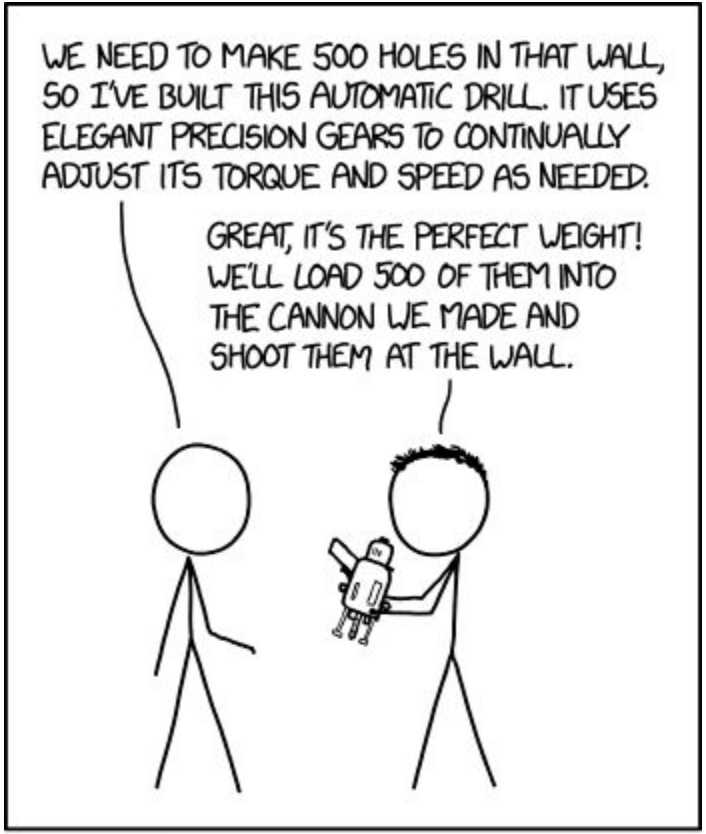

WE NEED TO MAKE 500 HOLES IN THAT WALL, SO I'VE BUILT THIS AUTOMATIC DRILL. IT USES ELEGANT PRECISION GEARS TO CONTINUALLY ADJUST ITS TORQUE AND SPEED AS NEEDED.
GREAT, IT'S THE PERFECT WEIGHT! WE'LL LOAD 500 OF THEM INTO THE CANNON WE MADE AND SHOOT THEM AT THE WALL.

HOW SOFTWARE DEVELOPMENT WORKS

https://www.explainxkcd.com/wiki/index.php/2021:_Software_Development

Building Five Hundred Decision Trees

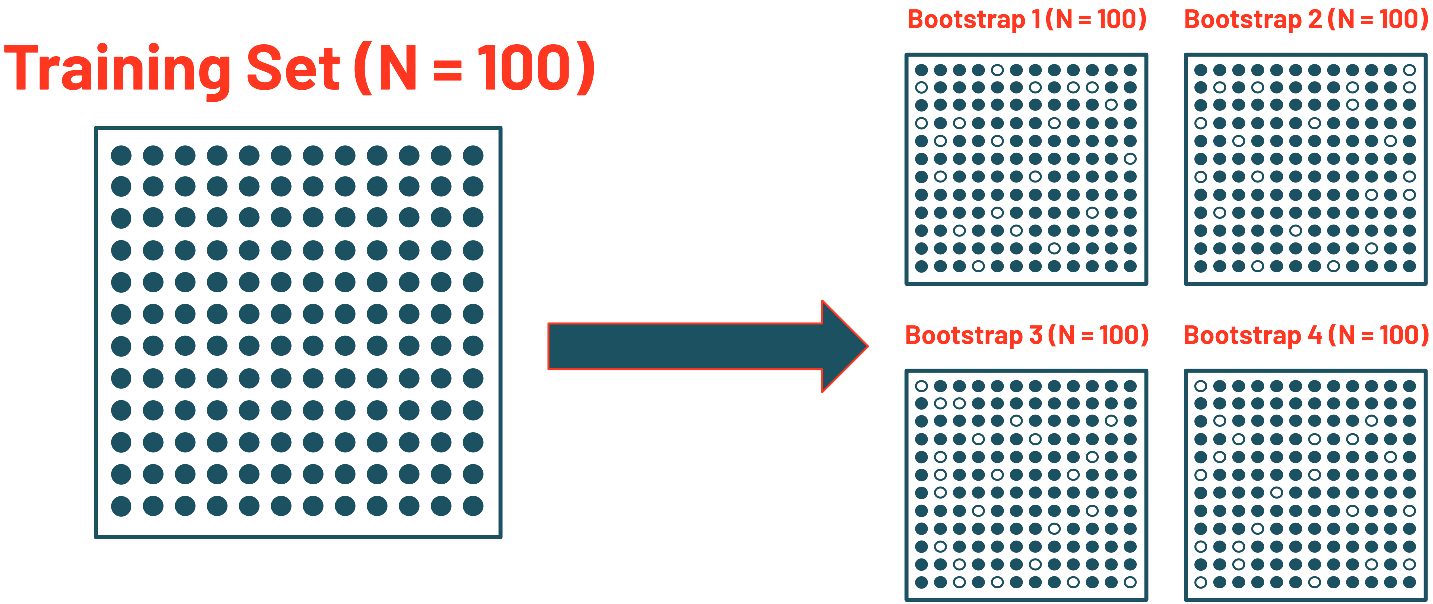
- Using more data reduces variance for one model
- Averaging more predictions reduces prediction variance
- But that would require more decision trees
- And we only have one training set ... or do we?

Bootstrap Sampling

A method for simulating *N* new datasets:

1. Take sample *with replacement* from original training set
2. Repeat *N* times

Bootstrap Visualization



Training Set (N = 100)

Bootstrap 1 (N = 100)

Bootstrap 2 (N = 100)

Bootstrap 3 (N = 100)

Bootstrap 4 (N = 100)

Why are some points in the bootstrapped samples not selected?

Training Set Coverage

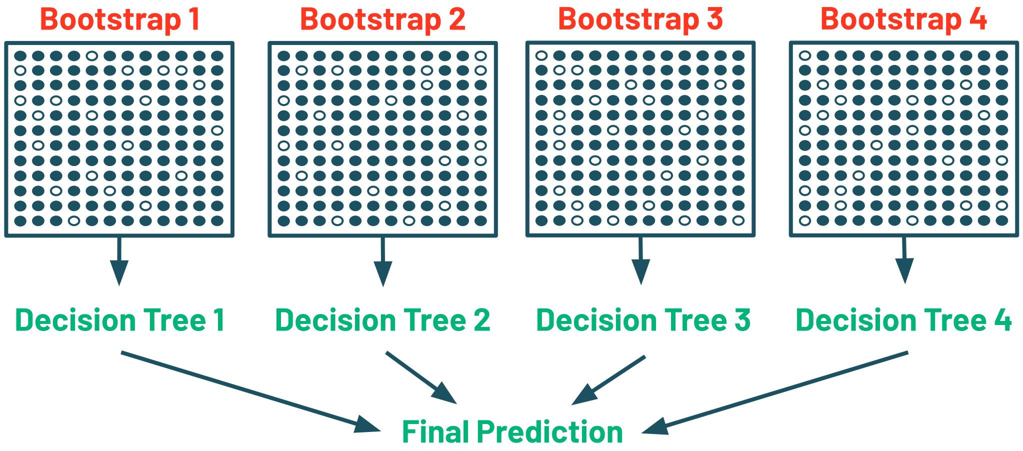
Assume we are bootstrapping *N* draws from a training set with *N* observations ...

- Probability of an element getting picked in *each draw* $\frac{1}{N}$
- Probability of an element *not* getting picked in *each draw*: $1 - \frac{1}{N}$
- Probability of an element *not* getting drawn in the entire *sample*: $(1 - \frac{1}{N})^N$

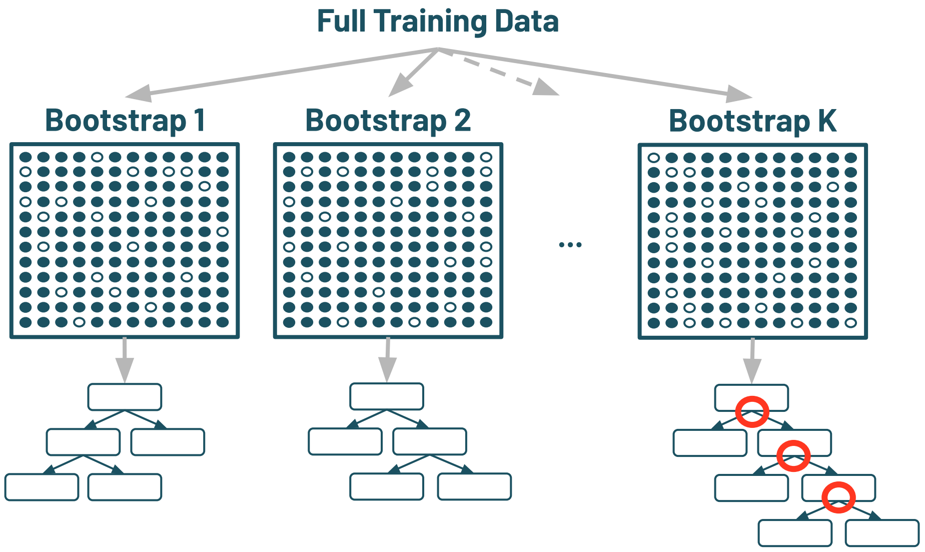
As $N \longrightarrow \infty$, the probability for each element of not getting picked in a sample approaches **0.368.**

Bootstrap Aggregating

- Train a tree on each of sample, and average the predictions
- This is bootstrap aggregating, commonly referred to as bagging



Random Forest Algorithm



At each split, a **subset of features** is considered to ensure each tree is different.

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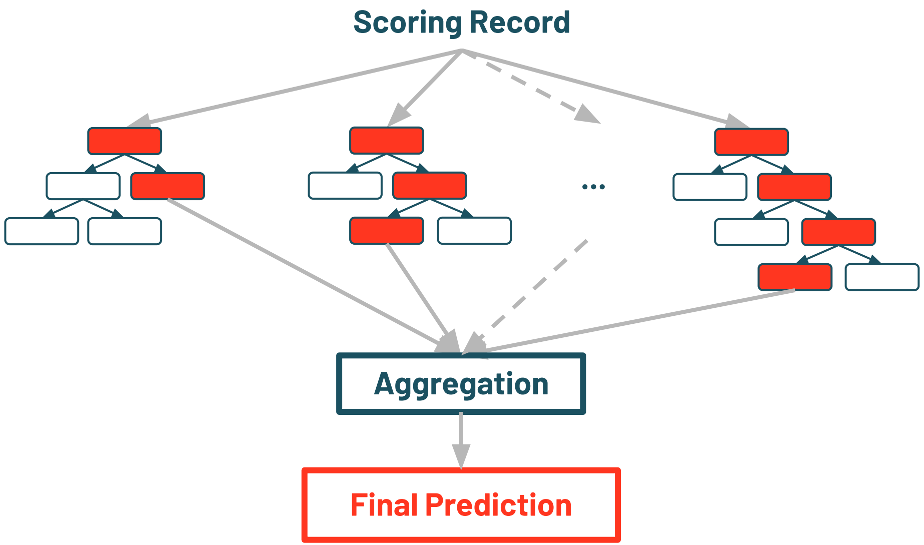
Random Forest Aggregation



- Majority-voting for classification
- Mean for regression

RANDOM FOREST DEMO

Hyperparameter Tuning

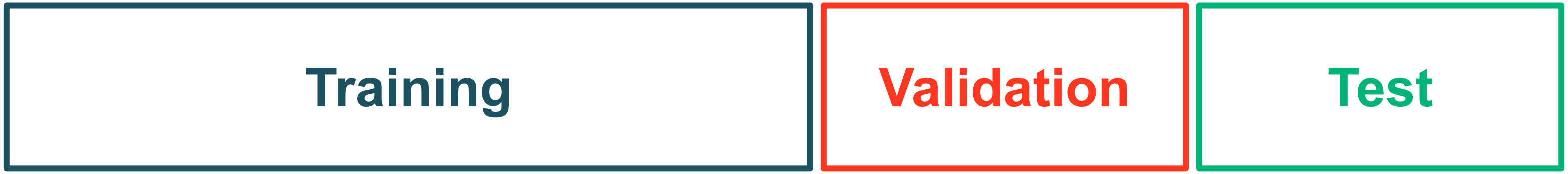
What is a Hyperparameter?

- Examples for Random Forest:
  - Tree depth
  - Number of trees
  - Number of features to consider

A parameter whose value is used to control the training process.

Selecting Hyperparameter Values

- Build a model for each hyperparameter value
- Evaluate each model to identify the optimal hyperparameter value
- What dataset should we use to train and evaluate?



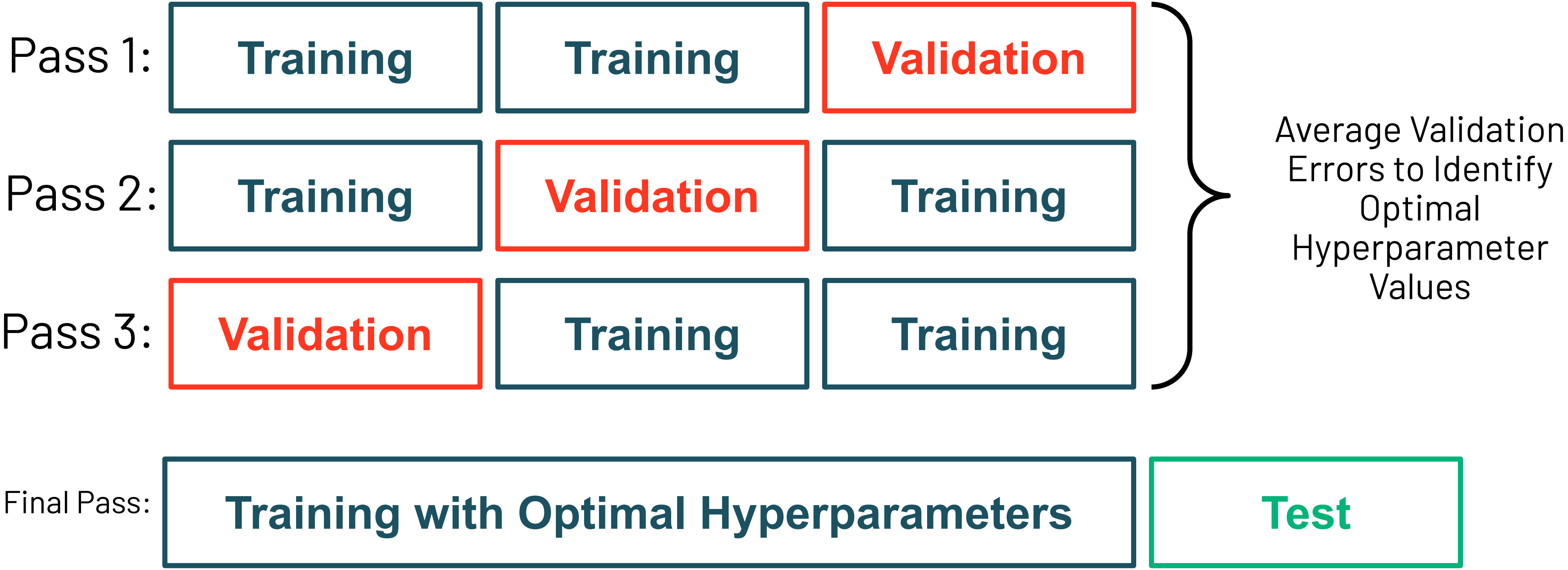
Training

Validation

Test

What if there isn't enough data to split
into three separate sets?

K-Fold Cross Validation



Pass 1:	Training	Training	Validation
Pass 2:	Training	Validation	Training
Pass 3:	Validation	Training	Training

Average Validation Errors to Identify Optimal Hyperparameter Values

Final Pass:	Training with Optimal Hyperparameters	Test

Optimizing Hyperparameter Values

Grid Search

- Train and validate every unique combination of hyperparameters

Tree Depth	Number of Trees
5	2
8	4

Tree Depth	Number of Trees
5	2
5	4
8	2
8	4

Question: With 3-fold cross validation, how many models will this build?

HYPERPARAMETER TUNING DEMO

HYPERPARAMETER TUNING LAB

Hyperparameter Tuning with HyperOpt

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Problems with Grid Search

- Exhaustive enumeration is expensive
- Manually determined search space
- Past information on good hyperparameters isn’t used
- So what do you do if…
  - You have a training budget
  - You have a non-parametric search space
  - You want to pick your hyperparameters based on past results

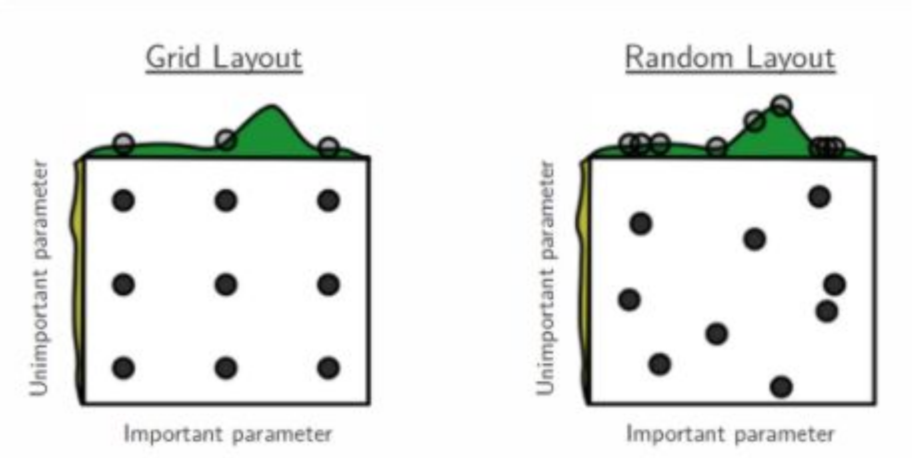
Hyperopt

- Open-source Python library
- Optimization over *awkward search spaces*
- Serial
- Parallel
- Spark integration
- Three core algorithms for optimization:
  - Random Search
  - Tree of Parzen Estimators (TPE)
  - Adaptive TPE

Paper

Optimizing Hyperparameter Values

Random Search



- Generally outperforms grid search
- Can struggle on some datasets (e.g. convex spaces)

Optimizing Hyperparameter Values

Tree of Parzen Estimators

- Meta-learner, Bayesian process
- Non-parametric densities
- Returns candidate hyperparameters based on best expected improvement
- Provide a range and distribution for continuous and discrete values
- Adaptive TPE better tunes the search space
  - Freezes hyperparameters
  - Tunes number of random trials before TPE

HYPEROPT DEMO

HYPEROPT LAB

MLlib Deployment Options

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Data Science vs. Data Engineering

- Data Science != Data Engineering
- Data Science
  - Scientific
  - Art
  - Business problems
  - Model mathematically
  - Optimize performance
- Data Engineering
  - Reliability
  - Scalability
  - Maintainability
  - SLAs

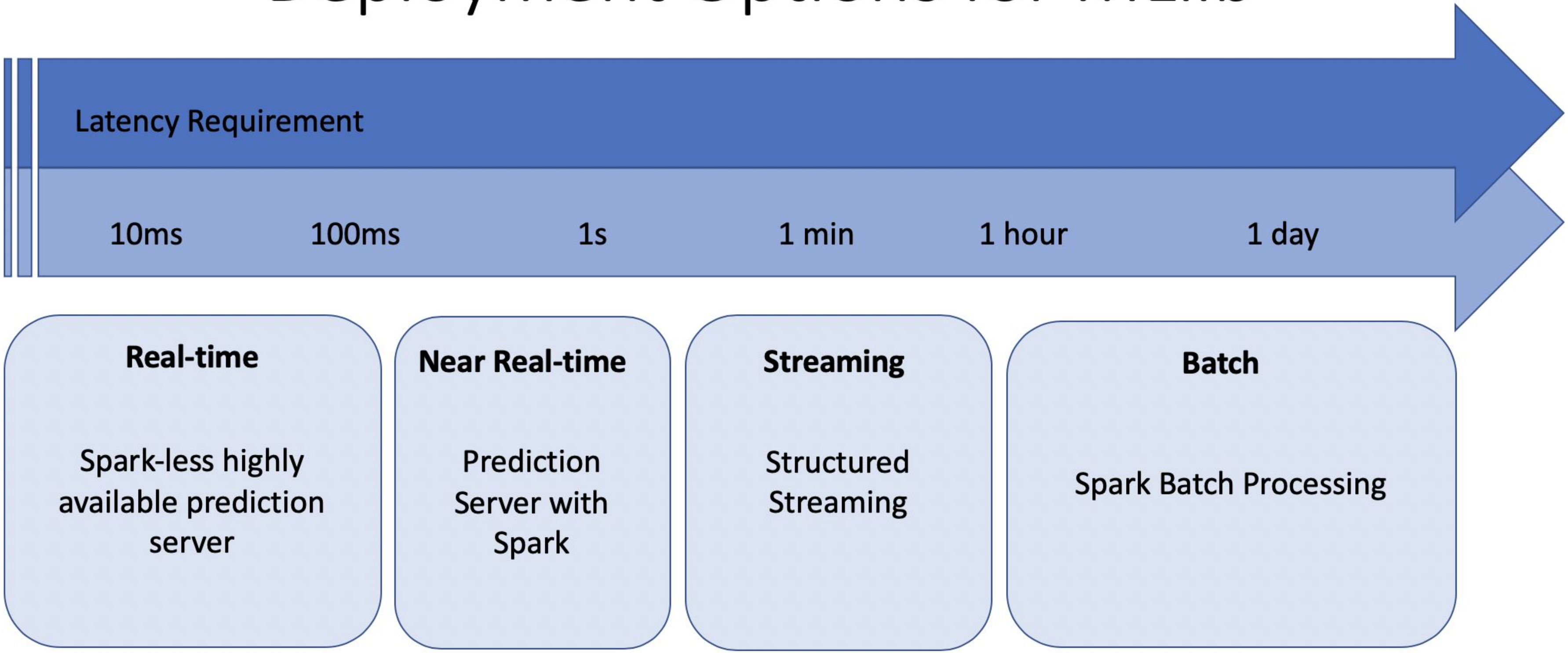
Model Operations (ModelOps)

- DevOps
  - Software development and IT operations
  - Manages deployments
  - CI/CD of features, patches, updates, and rollbacks
  - Agile vs. waterfall
- ModelOps
  - Data modeling and deployment operations
  - Java environments
  - Containers
  - Model performance monitoring

The Four ML Deployment Options

- Batch
  - 80-90 percent of deployments
  - Leverages databases and object storage
  - Fast retrieval of stored predictions
- Continuous/Streaming
  - 10-15 percent of deployments
  - Moderately fast scoring on new data
- Real-time
  - 5-10 percent of deployments
  - Usually using REST (Azure ML, SageMaker, containers)
- On-device

Deployment Options for MLlib



Latency Requirement

10ms 100ms 1s 1 min 1 hour 1 day

Real-time

Spark-less highly available prediction server

Near Real-time

Prediction Server with Spark

Streaming

Structured Streaming

Batch

Spark Batch Processing

ML DEPLOYMENT DEMO

Gradient Boosted Decision Trees

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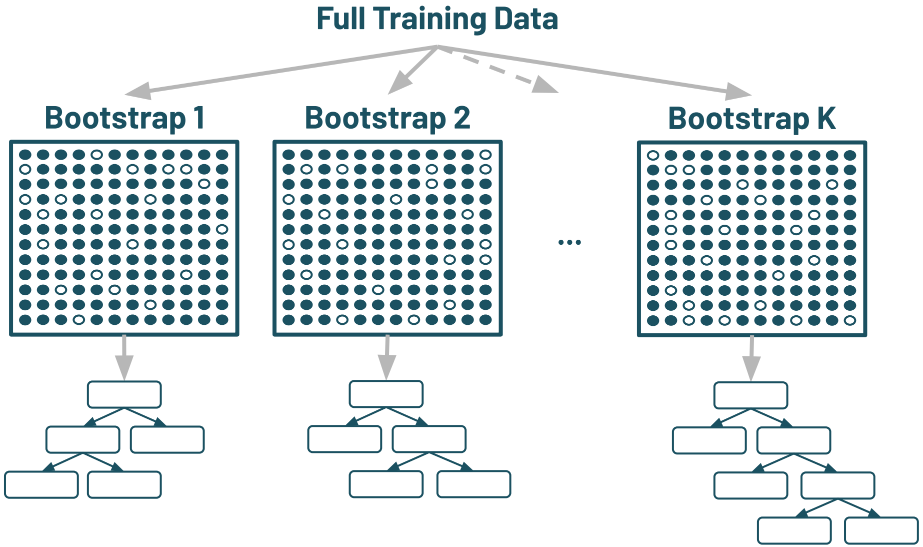
Decision Tree Ensembles

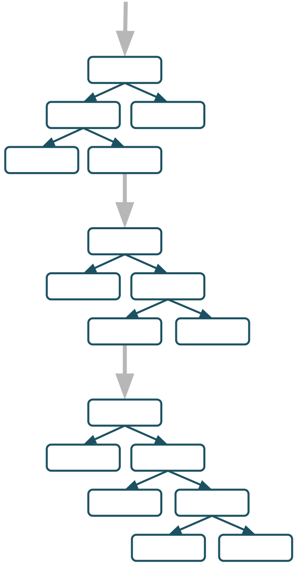
- Combine many decision trees
- Random Forest
  - Bagging
  - Independent trees
  - Results aggregated to a final prediction
- There are other methods of *ensembling* decision trees



Boosting

- Sequential (one tree at a time)
- Each tree learns from the last
- Sequence of trees is the final model

Full Training Data



Gradient Boosted Decision Trees

- Common boosted trees algorithm
- Fits each tree to the residuals of the previous tree
- On the first iteration, residuals are the actual label values

Model 1

Y	Prediction	Residual
40	35	5
60	67	-7
30	28	2
33	32	1

Model 2

Y	Prediction	Residual
5	3	2
-7	-4	-3
2	3	-1
1	0	1

Final Prediction

Y	Prediction
40	38
60	63
30	31
33	32

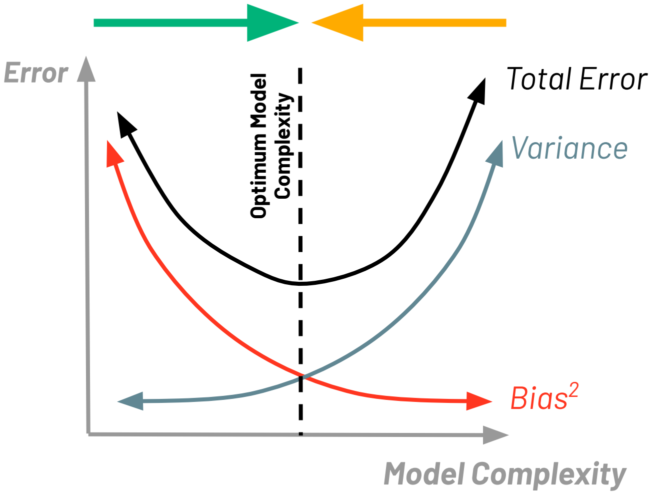
Boosting vs. Bagging

GBDT

- Starts with high bias, low variance
- Works right

RF

- Starts with high variance, low bias
- Works left



Gradient Boosted Decision Trees Implementations

- Spark ML
  - Built into Spark
  - Utilizes Spark’s existing decision tree implementation
- XGBoost
  - Designed and built specifically for gradient boosted trees
  - Regularized to prevent overfitting
  - Highly parallel
  - Works nicely with Spark in Scala

XGBOOST DEMO

Appendix

Electives

The following electives are also available:

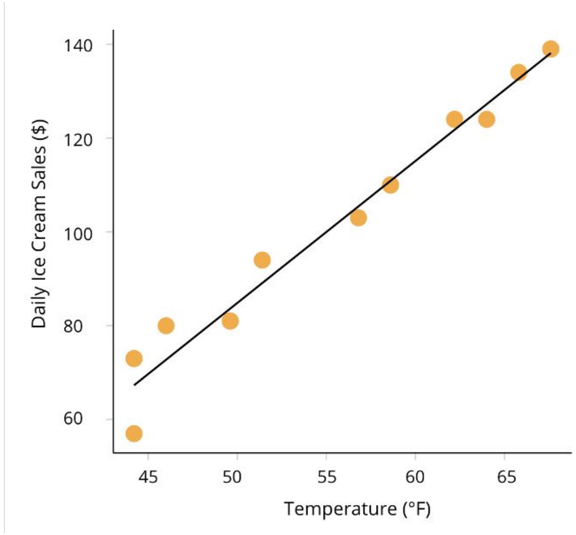
- Machine Learning Algorithms and Applications
  - **K-Means**
  - **Logistic Regression Lab**
  - **Time Series Forecasting**
  - **Isolation Forests for Outlier and Fraud Detection**
  - **Collaborative Filtering for Recommendation Systems Lab**
- Tools
  - **Joblib**
- Other
  - **Databricks Best Practices**

Logistic Regression

Types of Supervised Learning

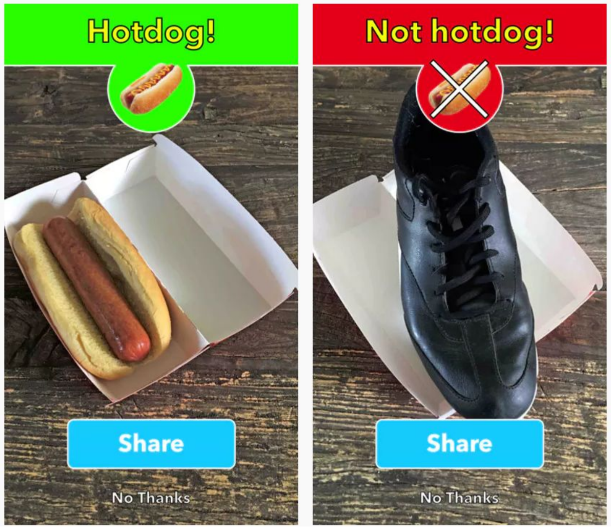
Regression

- Predicting a continuous output



Classification

- Predicting a categorical/discrete output



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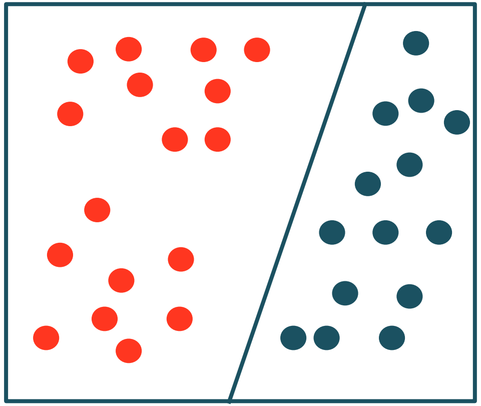
Types of Classification

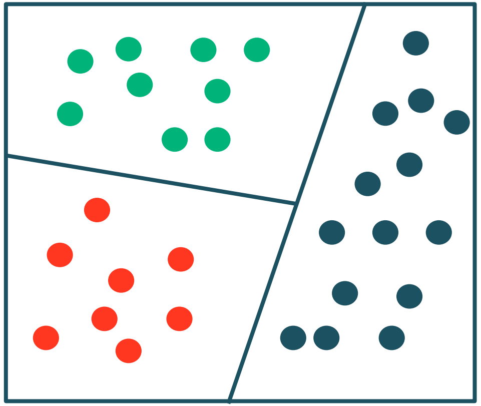
Binary Classification

Two label classes



Multiclass Classification

Three or more label classes



Model output is commonly the **probability** of a record belonging to **each of the classes**.

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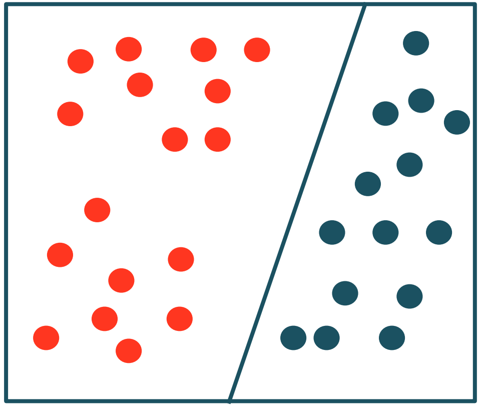
Binary Classification

Binary Classification

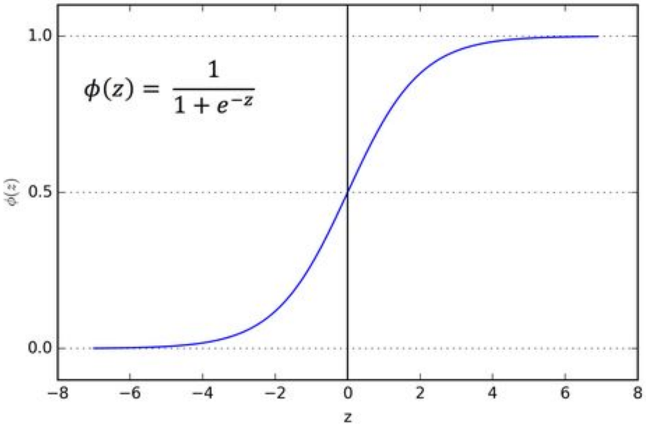
Two label classes



- Outputs:
  - Probability that the record is **Red** given a set of features
  - Probability that the record is **Blue** given a set of features
- Reminders:
  - Probabilities are bounded between 0 and 1
  - And linear regression returns any real number

Bounding Binary Classification Probabilities

How can we keep model outputs between 0 and 1?



- Logistic Function:
  - Large positive inputs → 1
  - Large negative inputs → 0

Converting Probabilities to Classes

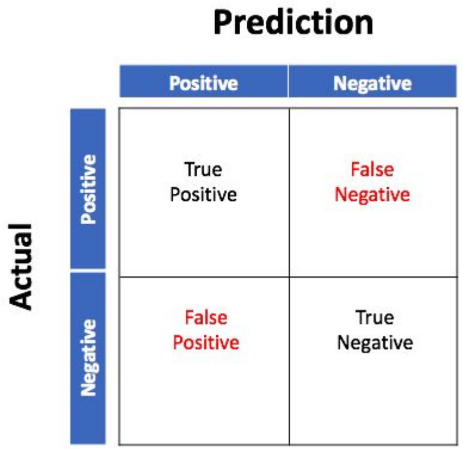
- In binary classification, the class probabilities are directly complementary
- So let's set our **Red** class equal to 1, and our **Blue** class equal to 0
- The model output is $\mathbf{P}[y = 1 \mid x]$ where x represents the features

But we need **class** predictions, not **probability** predictions

- Set a threshold on the probability predictions
  - $\mathbf{P}[y = 1 \mid x] < 0.5 \rightarrow y = 0$
  - $\mathbf{P}[y = 1 \mid x] \geq 0.5 \rightarrow y = 1$

Evaluating Binary Classification Models

- How can the model be wrong?
  - Type I Error: False Positive
  - Type II Error: False Negative
- Representing these errors with a **confusion matrix**.



		Prediction	
		Positive	Negative
Actual	Positive	True Positive	False Negative
	Negative	False Positive	True Negative

Binary Classification Metrics

Accuracy

$$\frac{TP + TN}{TP + FP + TN + FN}$$

Precision

$$\frac{TP}{TP + FP}$$

Recall

$$\frac{TP}{TP + FN}$$

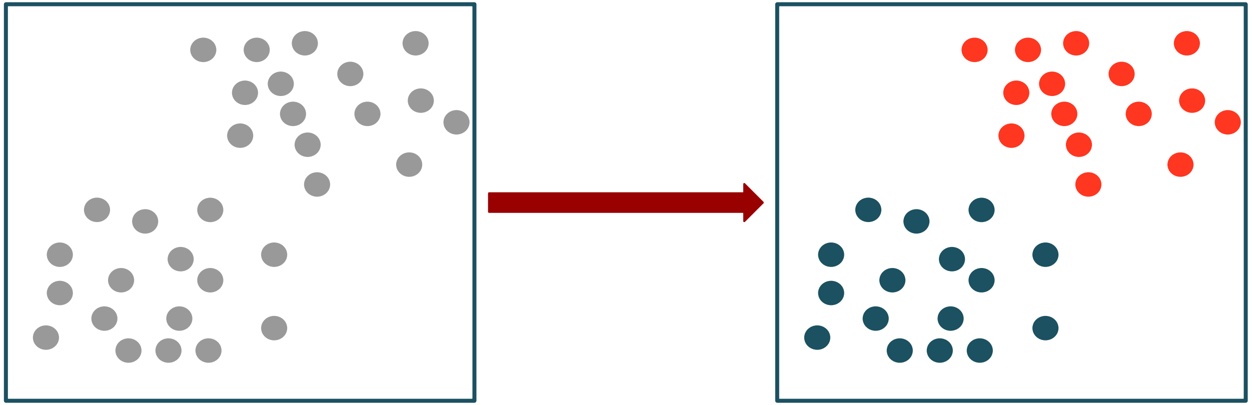
F1

$$\frac{2 \times Precision \times Recall}{Precision + Recall}$$

K-Means

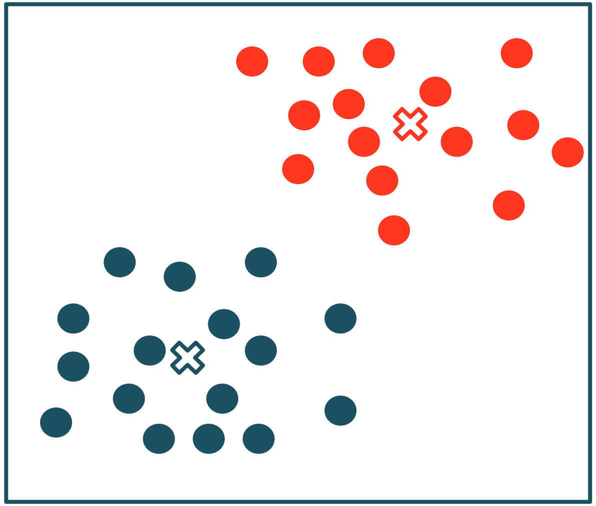
Clustering

- Unsupervised learning
- Unlabeled data (no known function output)
- Categorize records based on features



K-Means Clustering

- Most common clustering algorithm
- Number of clusters, *K*, is manually chosen
- Each cluster has a centroid
- Objective of minimizing the total distance between all of the points and their assigned centroid



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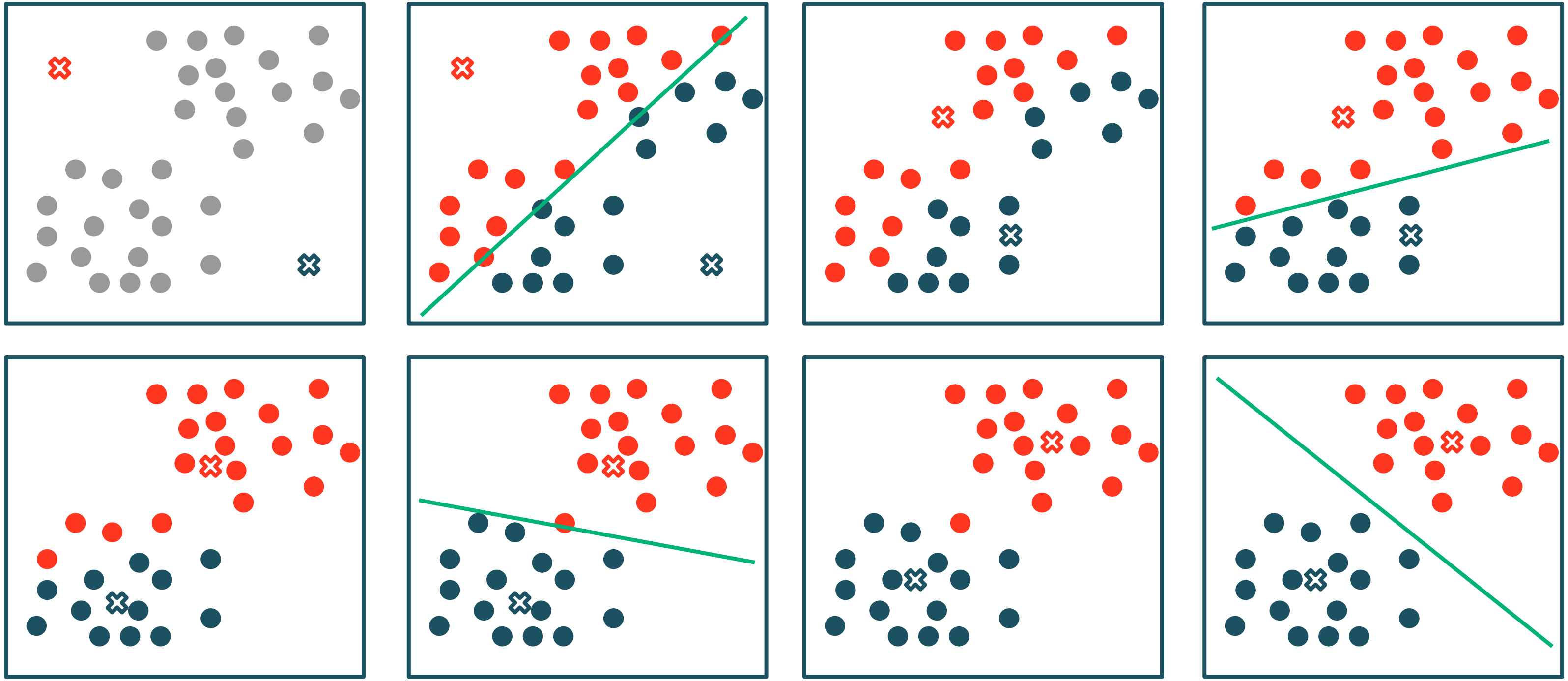
K-Means Algorithm

- **Step 1:** Randomly create centroids for *k* clusters
- Repeat until convergence/stopping criteria:
    - **Step 2:** Assign each data point to the cluster with the closest centroid
    - **Step 3:** Move the cluster centroids to the average location of their assigned data points

Visualizing K-Means



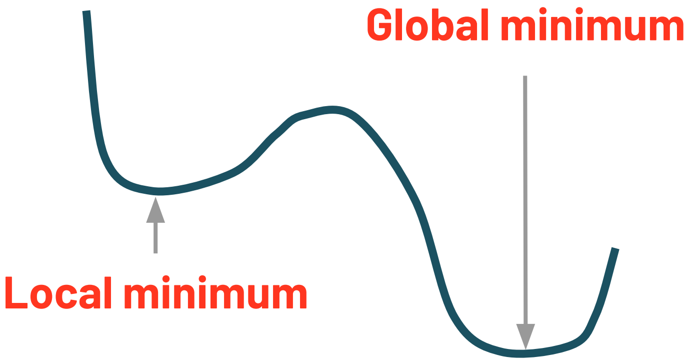
Choosing the Number of Clusters

- *K* is a hyperparameter
- Methods of identifying the optimal *K*
  - Prior knowledge
  - Visualizing data
  - Elbow method for within-cluster distance

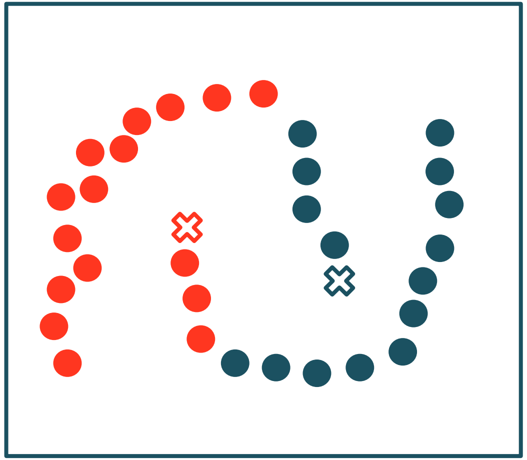
Note: Error will always decrease as *K* increases, unless a penalty is imposed.

Issues with K-Means

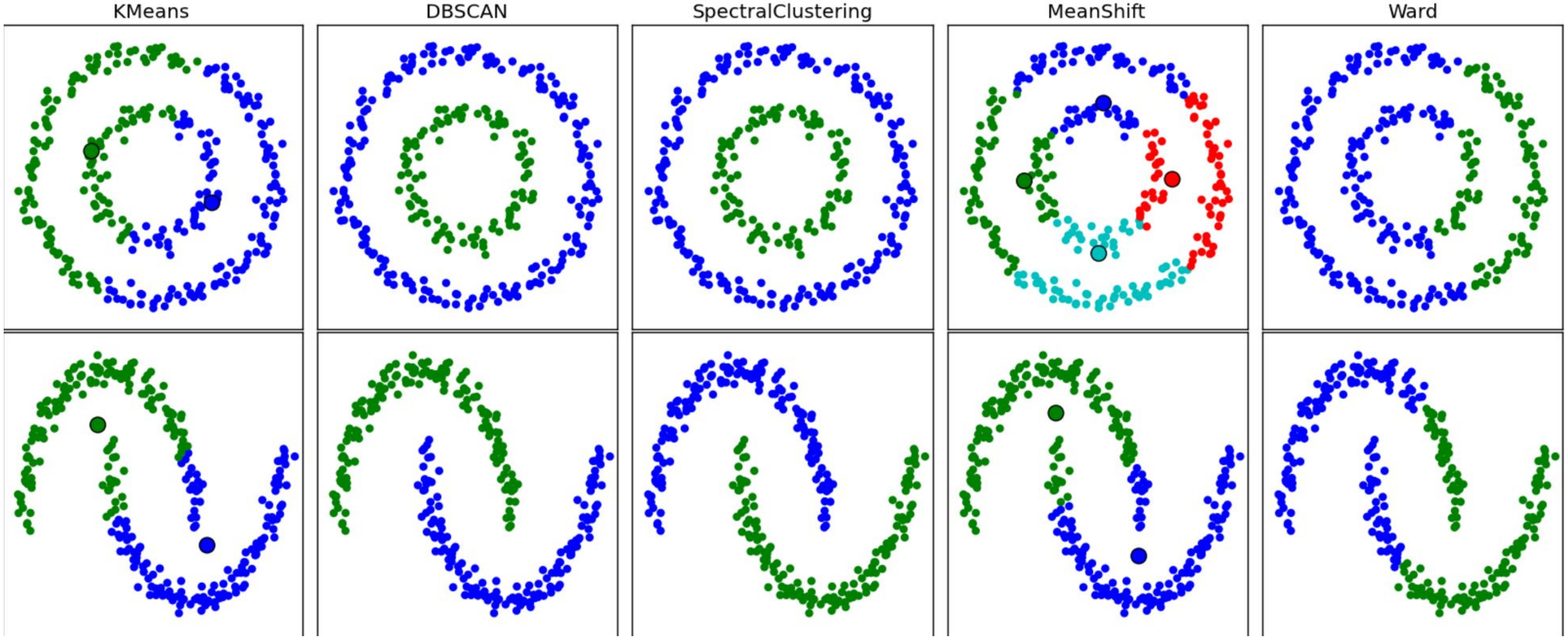
Local optima vs. global optima



Straight-line distance



Other Clustering Techniques



Collaborative Filtering

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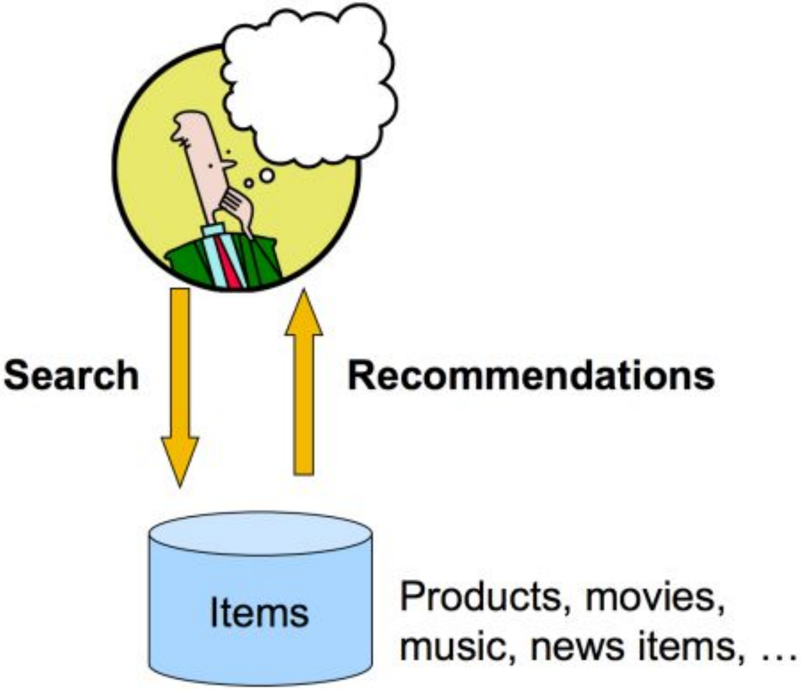
Recommendation Systems



Search

Recommendations

Items

Products, movies, music, news items, …

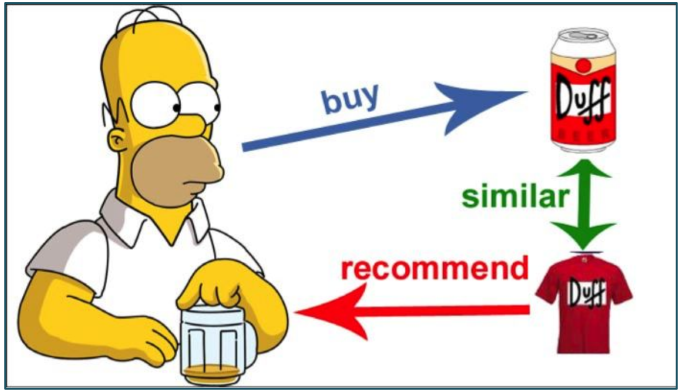
Naive Approaches to Recommendation

- Hand-curated
- Aggregates

Question: What are problems with these approaches?

Content-based Recommendation

- Idea: Recommend items to a customer that are *similar* to other items the customer liked
- Creates a profile for each user or product
  - User: demographic info, ratings, etc.
  - Item: genre, flavor, brand, actor list, etc.



Content-based Recommendation

- Advantages
  - No need for data from other users
  - New item recommendations
- Disadvantages
  - Cold-start problem
  - Determining appropriate features
  - Implicit information

Collaborative Filtering

- Idea: Make recommendations for one customer (filtering) by collecting and analyzing the interests of many users (collaboration)
- Advantages over content-based recommendation
  - Relies only on past user behavior (no profile creation)
  - Domain independent
  - Generally more accurate
- Disadvantages
  - Extremely susceptible to cold-start problem (user and item)

Types of Collaborative Filtering

- **Neighborhood Methods:** Compute relationships between items or users
  - Computationally expensive
  - Not empirically as good
- **Latent Factor Models:** Explain the ratings by characterizing items and users by small number of inferred factors
  - Matrix factorization
  - Characterizes both items and users by vectors of factors from item-rating pattern
  - Explicit feedback: sparse matrix
  - Scalable

Latent Factor Approach

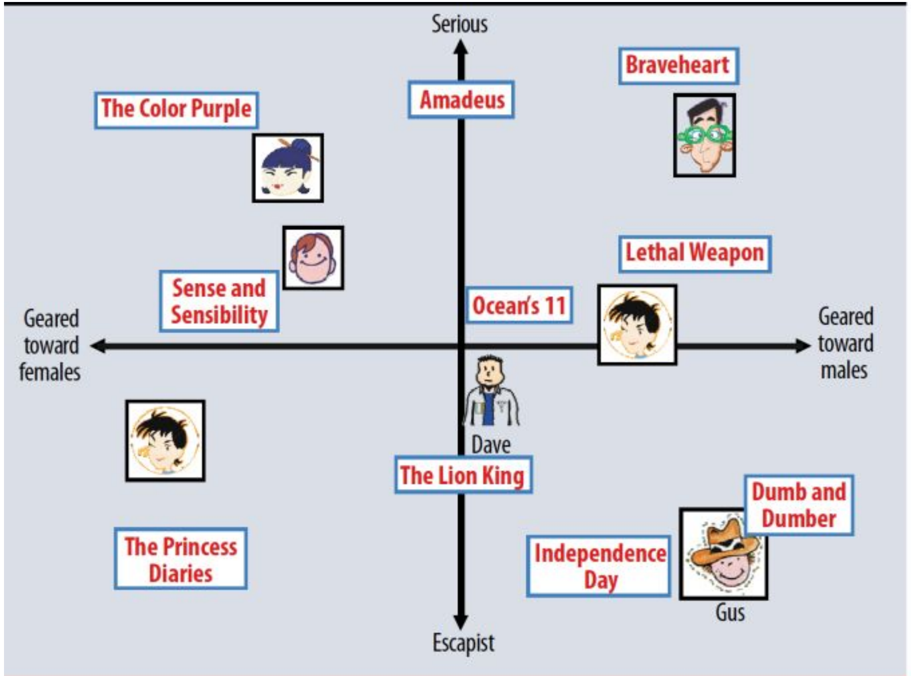
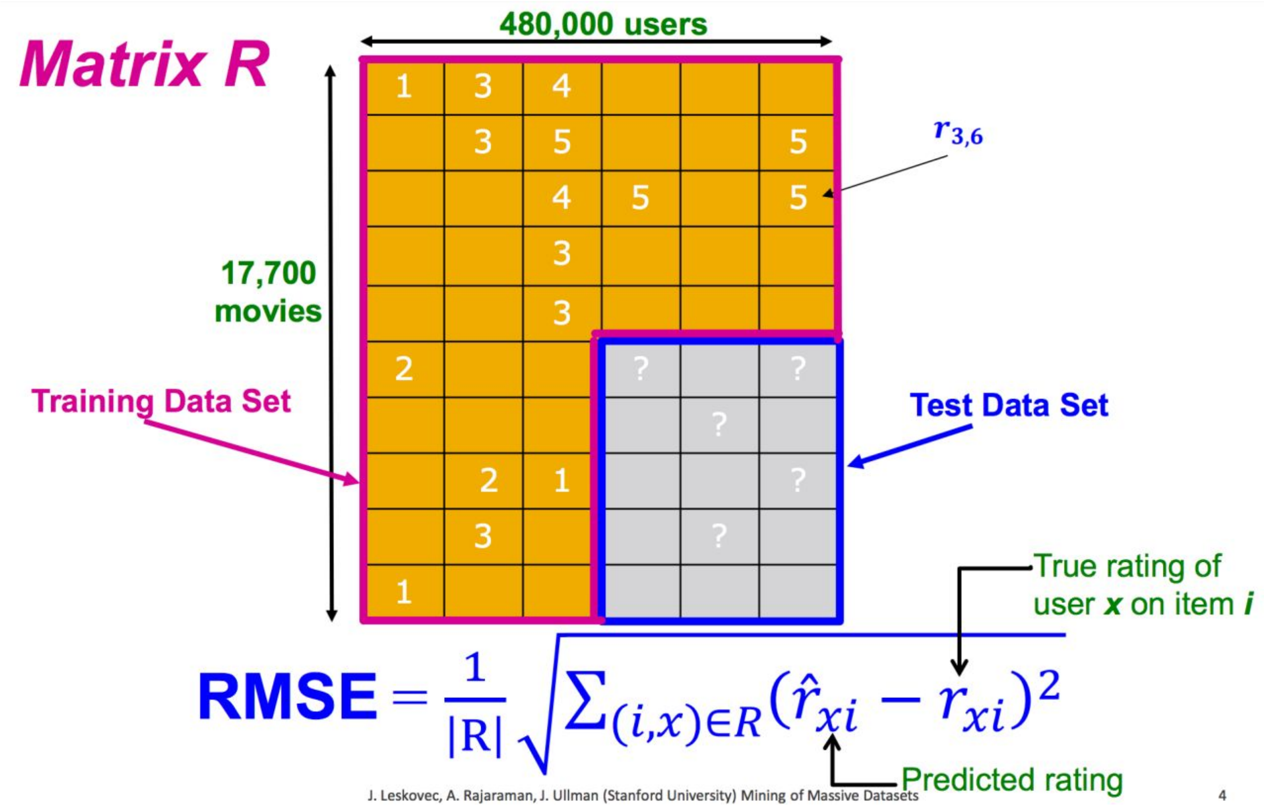


Figure 2. A simplified illustration of the latent factor approach, which characterizes both users and movies using two axes—male versus female and serious versus escapist.

Ratings Matrix



Matrix R

480,000 users

17,700 movies

1	3	4			
	3	5			5
		4	5		5
		3			
		3			
2			?		?
				?	
	2	1			?
	3			?	
1					

$r_{3,6}$

Training Data Set

Test Data Set

$$\textbf{RMSE} = \frac{1}{|\mathrm{R}|}\sqrt{\sum_{(i,x)\in R}(\hat{r}_{xi} - r_{xi})^2}$$

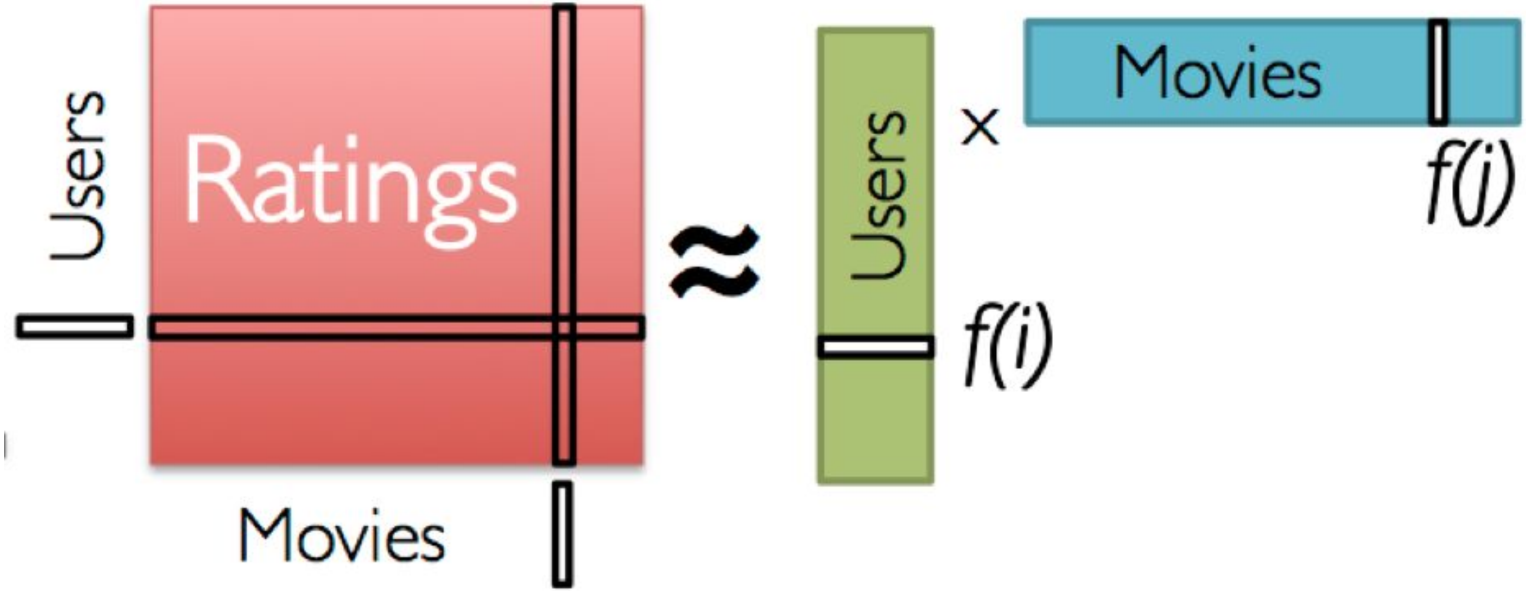
True rating of user ***x*** on item ***i***

Predicted rating

J. Leskovec, A. Rajaraman, J. Ullman (Stanford University) Mining of Massive Datasets

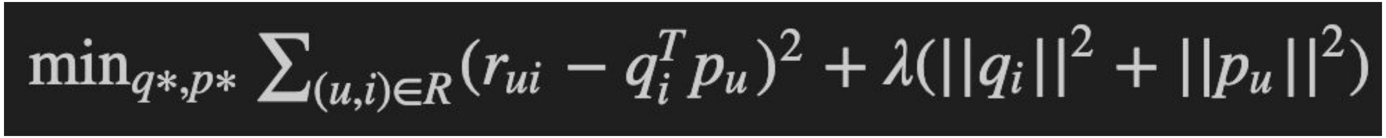
4

Matrix Factorization



Alternating Least Squares

- **Step 1:** Randomly initialize user and movie factors
- **Step 2:** Repeat the following
  1. Fix the movie factors, and optimize user factors
  2. Fix the user factors, and optimize movie factors



$$\min_{q*,p*} \sum_{(u,i)\in R} (r_{ui} - q_i^T p_u)^2 + \lambda(||q_i||^2 + ||p_u||^2)$$

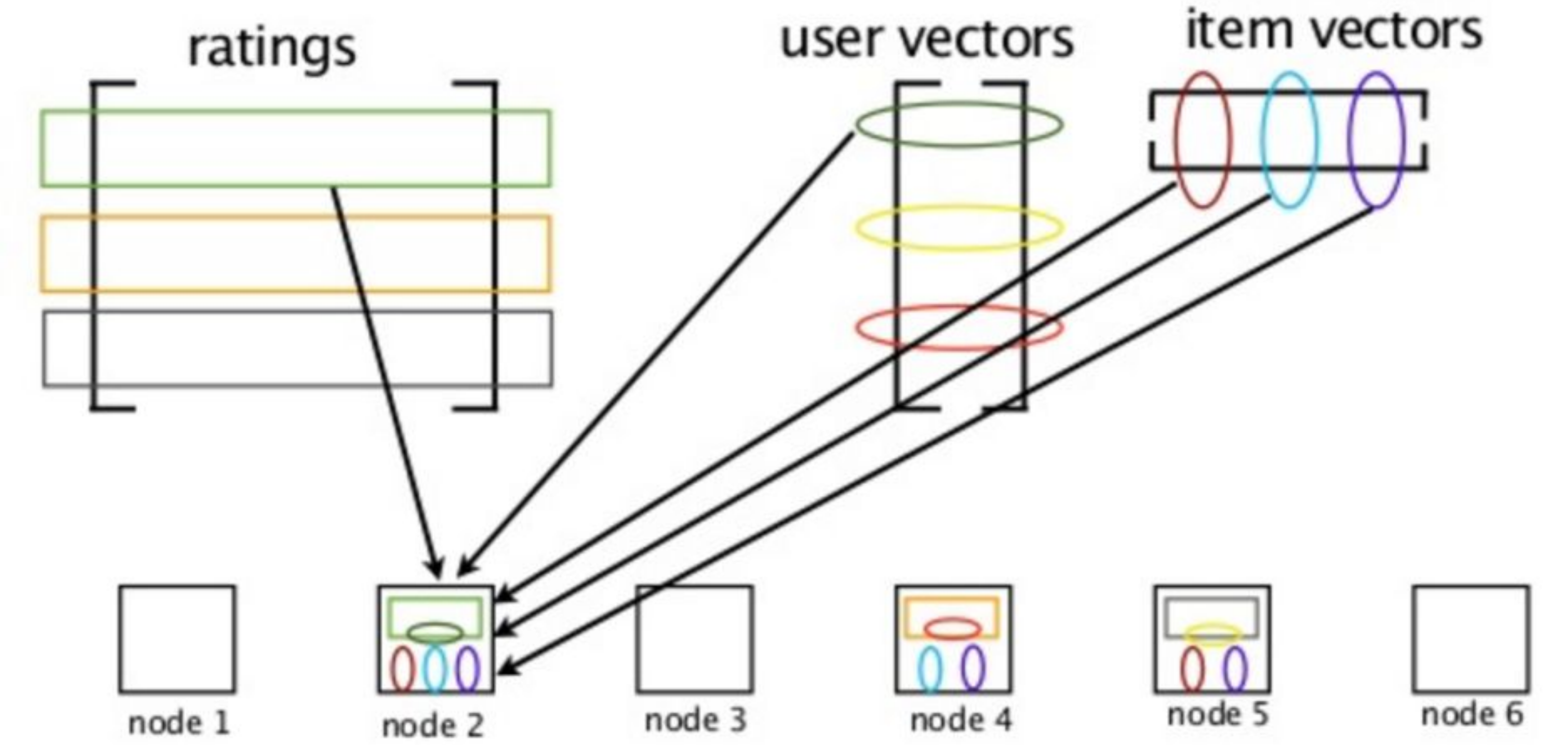
Why not SVD?

- The matrix is too sparse
- Imputation can be inaccurate
- Imputation can be expensive

Distributed ALS Implementation

- Naive approach
  - Broadcast R, U, and V
  - Problems?
  - R is large, and it's duplicating copies for each worker
- Better approach
  - Distribute R and broadcast U and V
  - Problems?
  - U and V might be large, too, and we're still duplicating copies
- Best approach
  - Join ALS

Join ALS


ratings
user vectors
item vectors
node 1
node 2
node 3
node 4
node 5
node 6

Blocked Join ALS

- Spark implements a smarter version of Join ALS
- Limits data shuffling
- ALS is a distributed model (i.e. stored across executors)