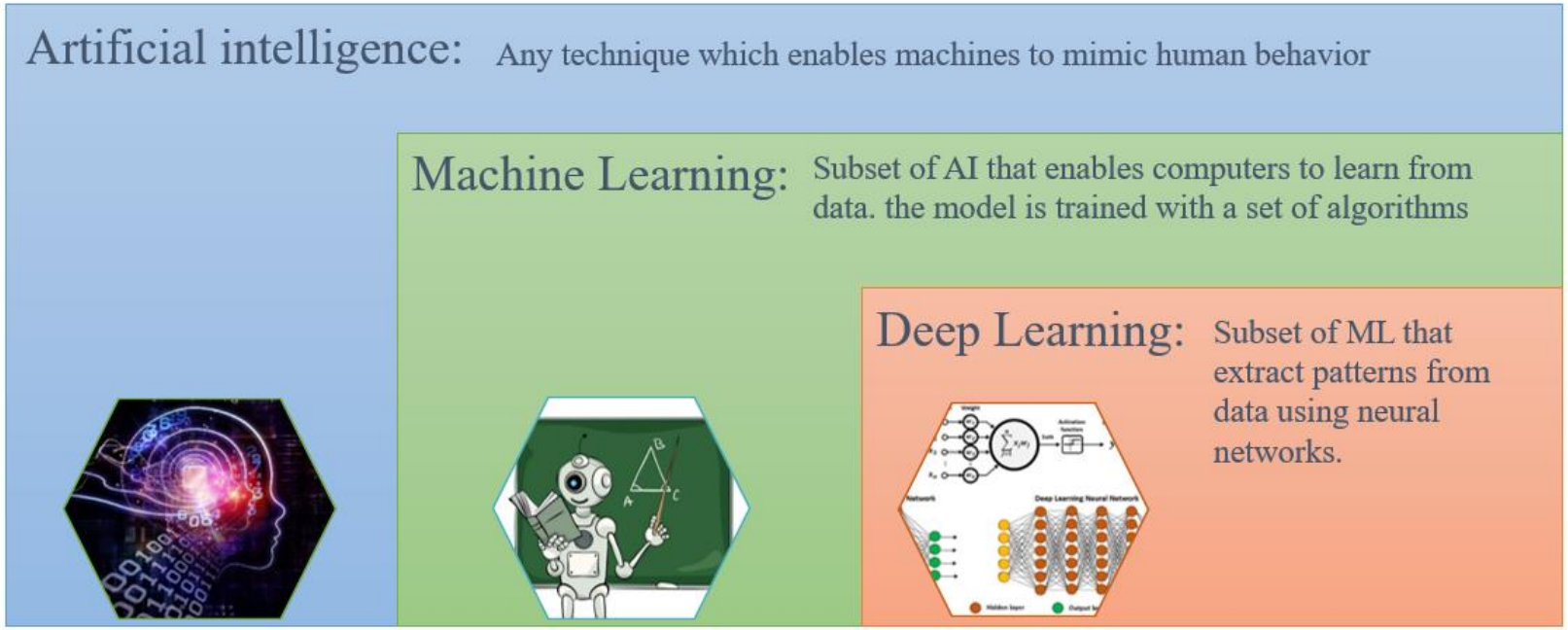
Module 5 – Part I
Machine Learning Fundamentals (review)



Road map!

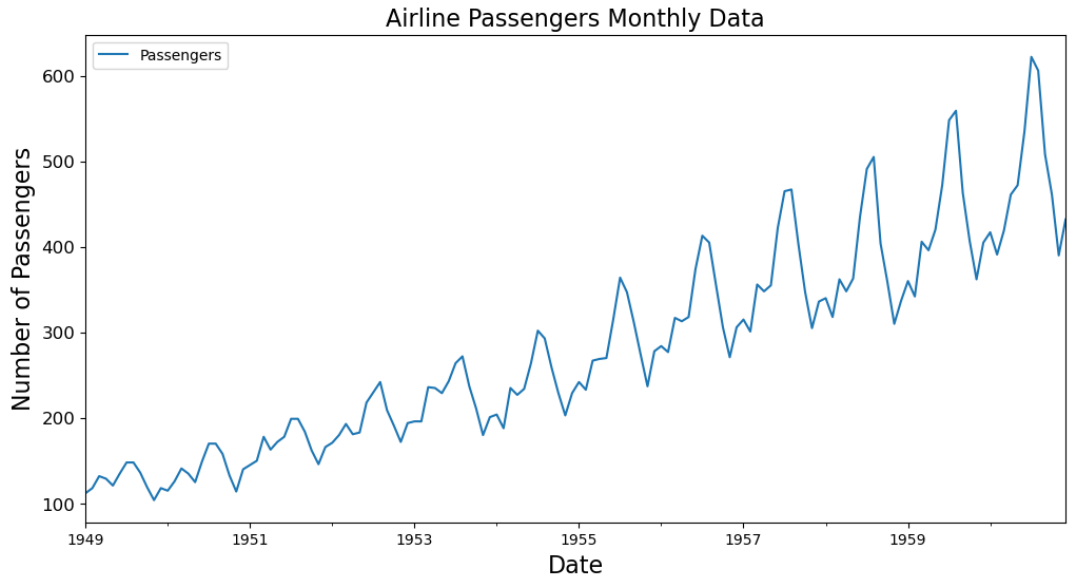
- Module 1- Introduction to Deep Forecasting
- Module 2- Setting up Deep Forecasting Environment
- Module 3- Exponential Smoothing
- Module 4- ARIMA models
- Module 5- Machine Learning for Time series Forecasting
- Module 6- Deep Neural Networks
- Module 7- Deep Sequence Modeling (RNN, LSTM)
- Module 8- Prophet and Neural Prophet

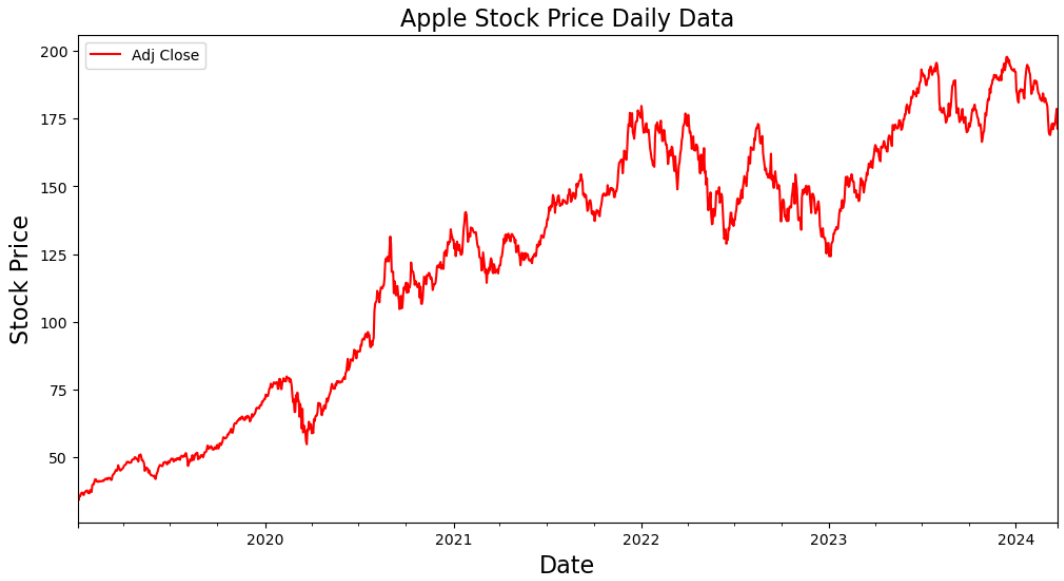
Model Comparison

Aspect	Econometric Models	Machine Learning (ML)	Deep Learning (DL)
Feature Engineering	Requires explicit modeling of seasonality and trend	Captures complex patterns with less need for manual engineering	Often automates feature engineering
Model Complexity	**Lower**; focuses on data generation process	**Moderate**; can handle non-linear interactions	**High**; suited for complex and high-dimensional data
Interpretability	High; interpretable parameters, statistical tests	Moderate; provides feature importance	Low; considered a 'black box' approach
Computational Intensity	Generally lower	Varies; dependent on model complexity and data size	High; requires significant computational resources
Data Suitability	Works well when the underlying process is **well understood**	Effective for structured datasets with **complex relationships**	Ideal for large datasets, including **unstructured** data
Core Models	ARIMA, Exponential Smoothing (ETS)	Random Forest, Gradient Boosting	RNNs, LSTMs, CNNs

Pre-processing the data for machine learning

- How to convert time series problems into machine learning problems?





Single-Output (one-step ahead)

Input Features (X)				Single-Output (y)
Lag 3	Lag 2	Lag 1	Lag 0	Lead 1
y_1	y_2	y_3	y_4	y_5
y_2	y_3	y_4	y_5	y_6
y_3	y_4	y_5	y_6	y_7
y_4	y_5	y_6	y_7	y_8
y_5	y_6	y_7	y_8	y_9
y_6	y_7	y_8	y_9	y_{10}
y_7	y_8	y_9	y_{10}	y_{11}
y_8	y_9	y_{10}	y_{11}	y_{12}
y_9	y_{10}	y_{11}	y_{12}	y_{13}
y_{10}	y_{11}	y_{12}	y_{13}	y_{14}

y_t: Actuals
y_t: Predictions

Single-Output (multiple-step ahead)

Input Features (X)				Single-Output (y)
Lag 3	Lag 2	Lag 1	Lag 0	Lead 1
y_1	y_2	y_3	y_4	y_5
y_2	y_3	y_4	y_5	y_6
y_3	y_4	y_5	y_6	y_7
y_4	y_5	y_6	y_7	y_8
y_5	y_6	y_7	y_8	y_9
y_6	y_7	y_8	y_9	y_{10}
y_7	y_8	y_9	y_{10}	y_{11}
y_8	y_9	y_{10}	y_{11}	y_{12}
y_9	y_{10}	y_{11}	y_{12}	y_{13}
y_{10}	y_{11}	y_{12}	y_{13}	y_{14}

y_t: Actuals
y_t: Predictions

Multi-Output

Input Features (X)				Multi-Output (Y)		
Lag 3	Lag 2	Lag 1	Lag 0	Lead 1	Lead 2	Lead 3
y_1	y_2	y_3	y_4	y_5	y_6	y_7
y_2	y_3	y_4	y_5	y_6	y_7	y_8
y_3	y_4	y_5	y_6	y_7	y_8	y_9
y_4	y_5	y_6	y_7	y_8	y_9	y_{10}
y_5	y_6	y_7	y_8	y_9	y_{10}	y_{11}
y_6	y_7	y_8	y_9	y_{10}	y_{11}	y_{12}
y_7	y_8	y_9	y_{10}	y_{11}	y_{12}	y_{13}
y_8	y_9	y_{10}	y_{11}	y_{12}	y_{13}	y_{14}
y_9	y_{10}	y_{11}	y_{12}	y_{13}	y_{14}	y_{15}
y_{10}	y_{11}	y_{12}	y_{13}	y_{14}	y_{15}	y_{16}

y_t: Actuals
y_t: Predictions

Machine Learning Fundamentals

- ML vs traditional programming
- Types of ML
- The Model
- Evaluation metrics
- Bias-Variance tradeoff, overfitting
- Train, Test, Validation
- Resampling methods
- Cost Function
- Solvers/learners (GD, SGD)
- How do machines actually learn?

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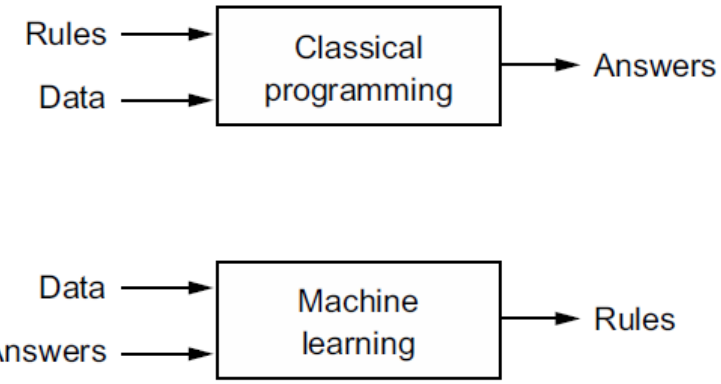
What is Machine Learning?

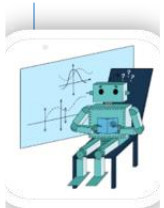
- A machine learning system is **trained** (with algorithms) rather than explicitly **programmed**.
- Machine Learning is a subset of AI that enables computers to learn from data.
- ML involves automated detection of meaningful patterns in data and apply the pattern to make predictions on unseen data! The purpose is to generalize.
- This is done by minimizing the loss on the training data.
- The goal is to maximize the performance on the unseen data.



Types of Machine Learning

Supervised

- Regression
- Classification

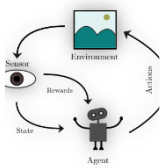


Unsupervised

- Clustering
- Anomaly detection
- Dimensionality reduction

Semi-supervised

Self-supervised



Reinforcement Learning

The Model

$$y = f(X, \theta) + \epsilon = f(X_1, X_2 \ \dots, X_m, \theta_1, \theta_2, \dots, \theta_k) + \epsilon$$

y : response, dependent variables, output, Target

X: predictors, independent variables, input, Features

θ: estimates, specifications, Parameters

✓ It is all about estimating f by $\hat{f}$ for two purposes:

1) Inference (interpretable ML)

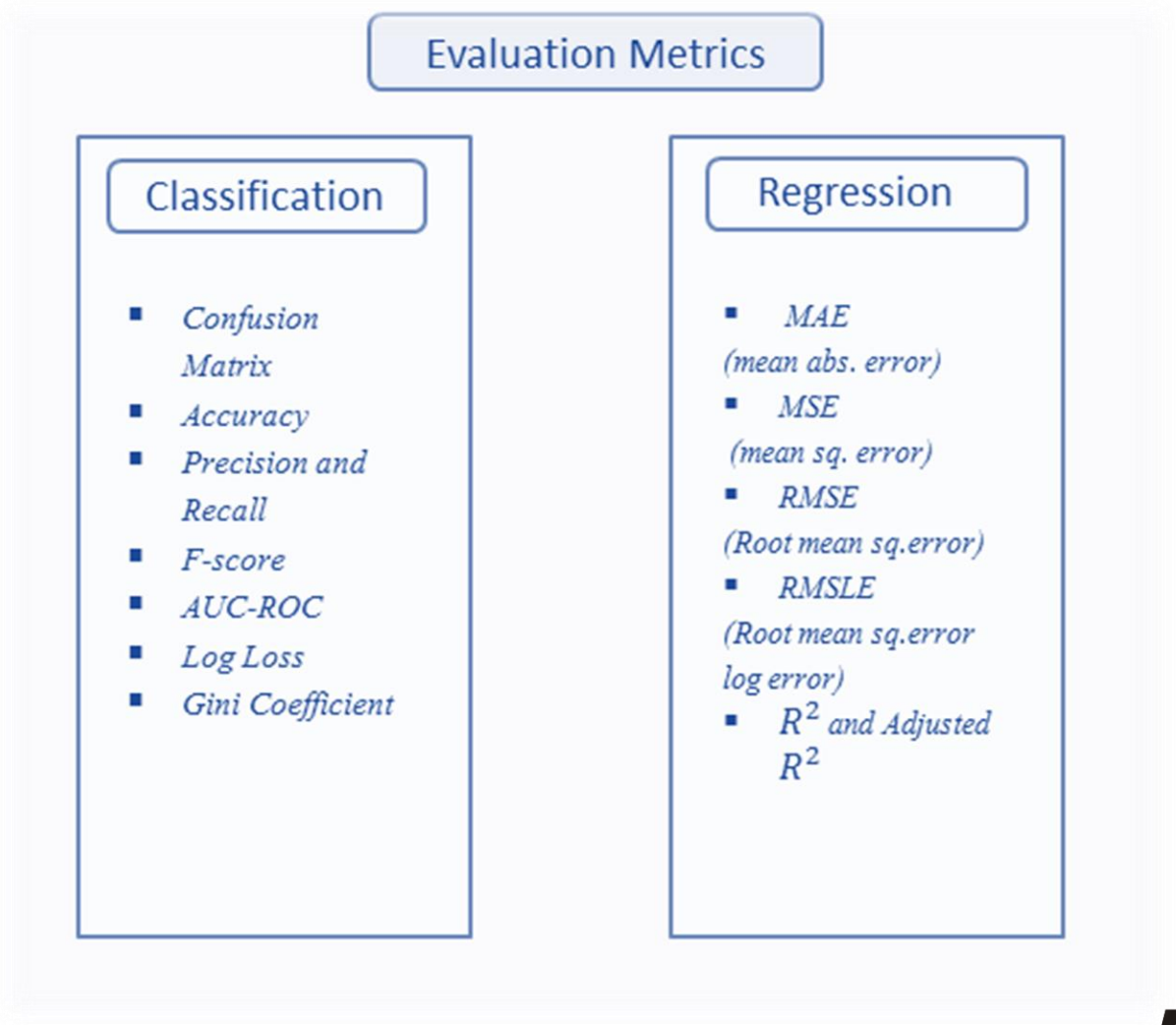
2) Prediction

Evaluation metrics

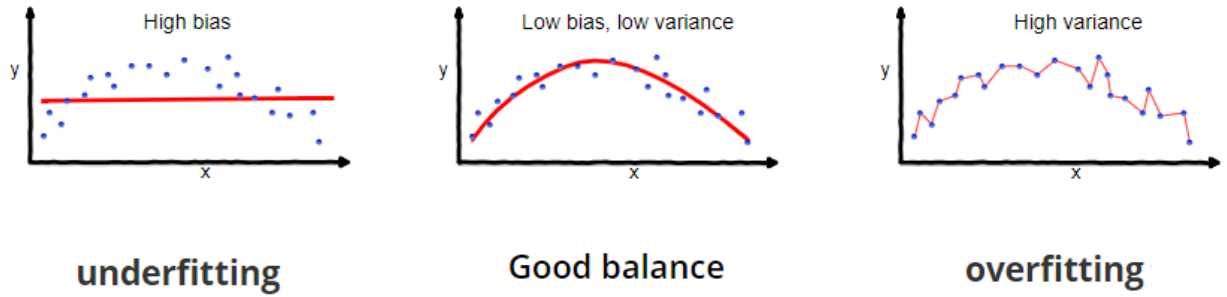
In general, we want to compare how close are the predictions to the actual numbers in the test set.

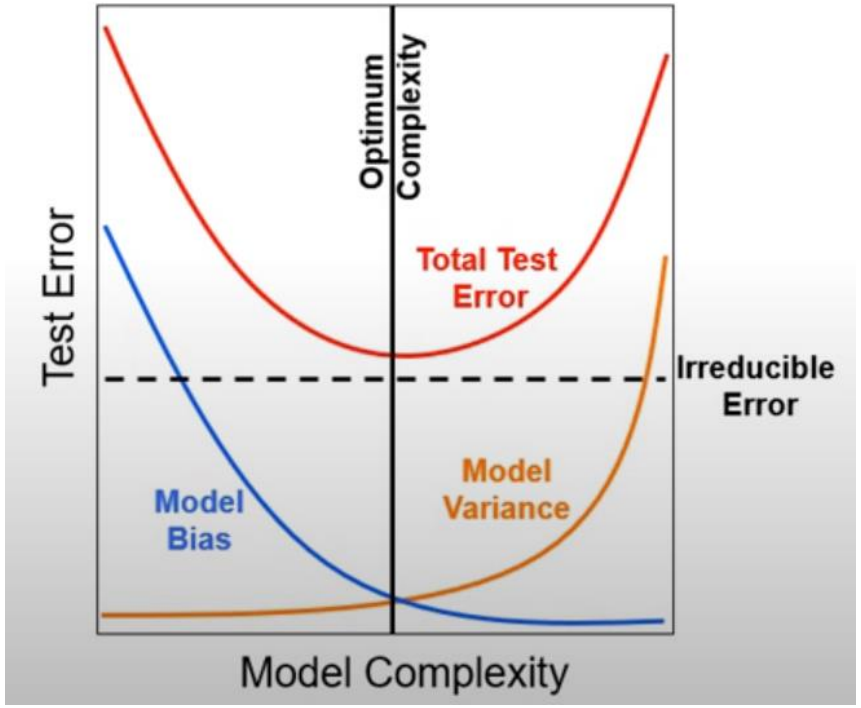
This is typically assessed using

- MSE for quantitative response
- Misclassification rate for qualitative response



Representations of the bias-variance tradeoff



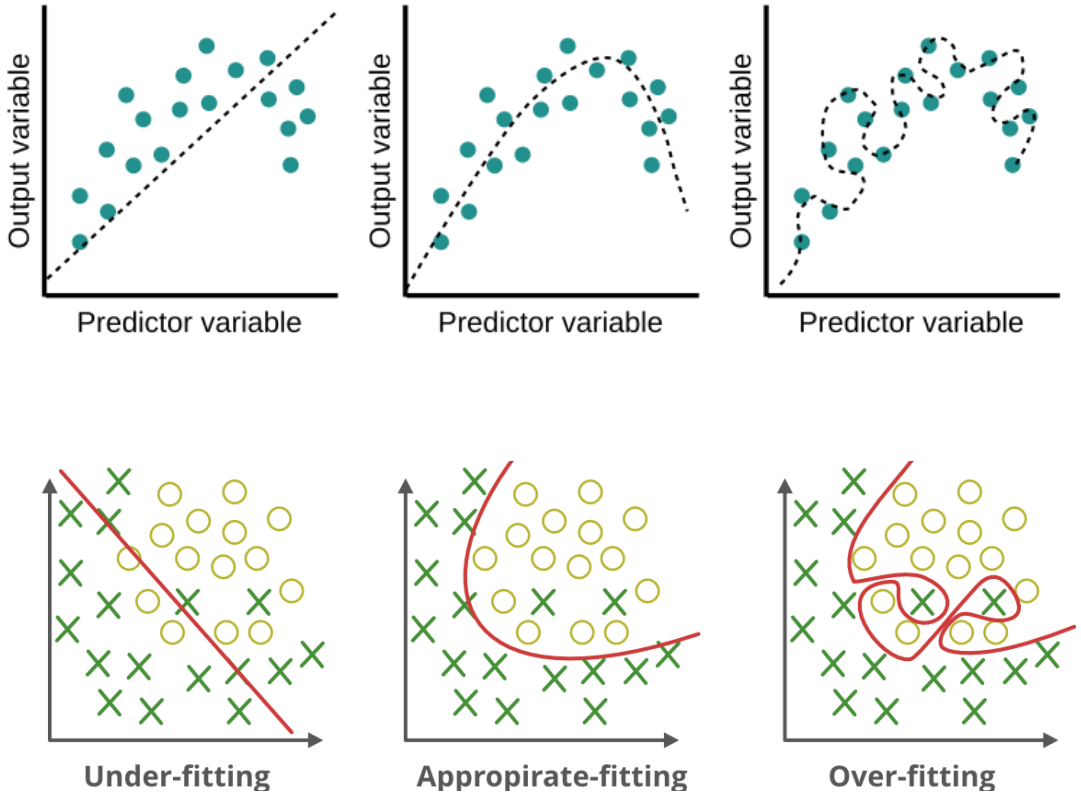


Optimization
Vs
Generalization

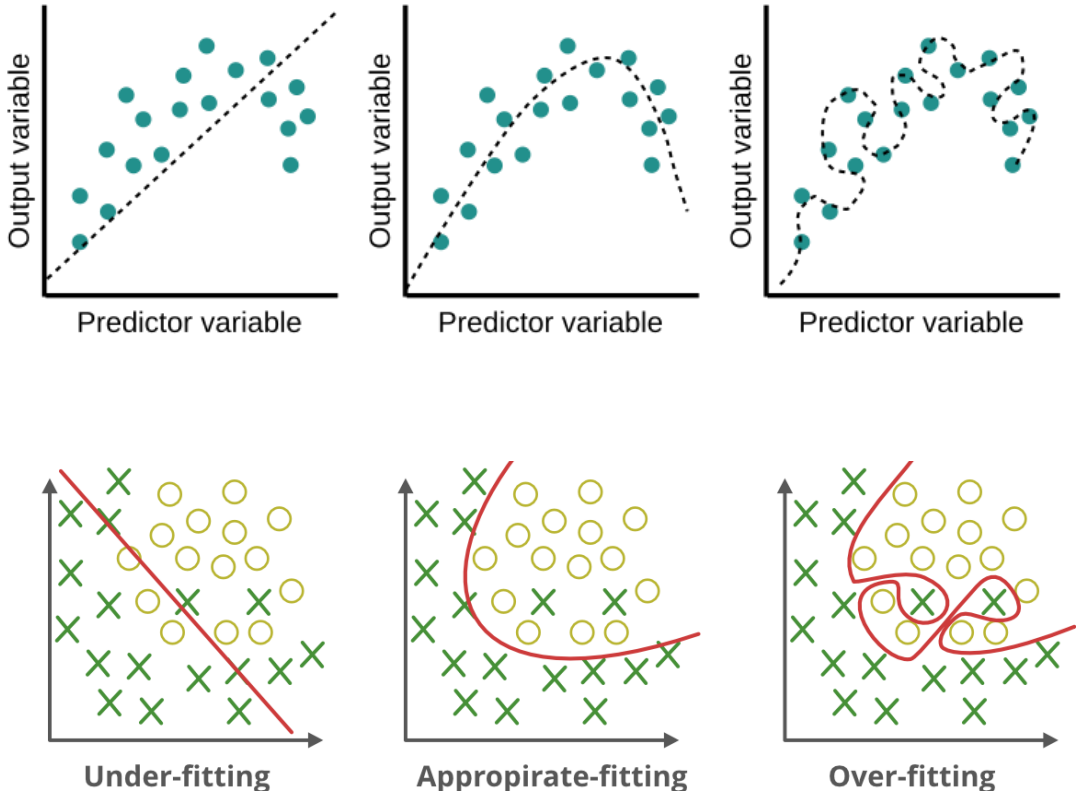
Overfitting

Overfitting happens when the fitted algorithm does not generalize well to new data:

- The model fits the training data too well while not predicts well in the new data
- The model fits the noise (ϵ) in training data (finds a pattern that does not exist)
- The algorithm has simply memorized the data, rather than learned from it!
- The model is too complex!



Overfitting



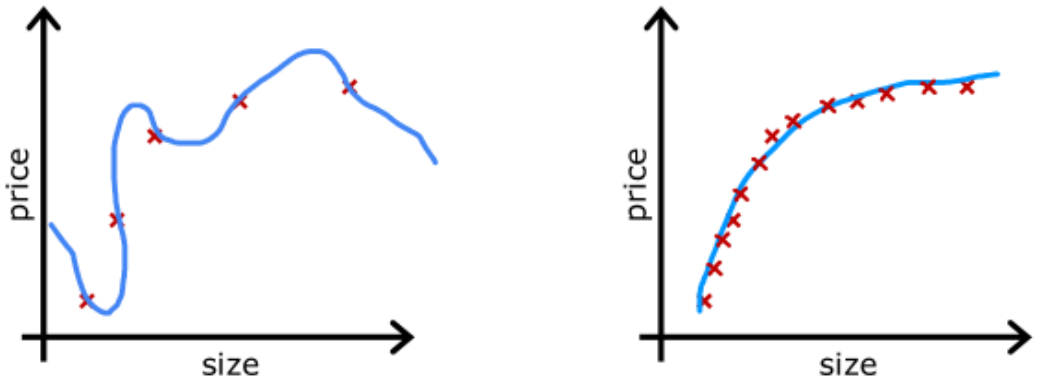
Mitigate overfitting

The main techniques used to mitigate overfitting risk in a model construction are:

1) Collect more data (Can reduce bias AND variance)

2) Complexity reduction (regularization, feature selection)

3) Cross validation (estimate the performance in test set)

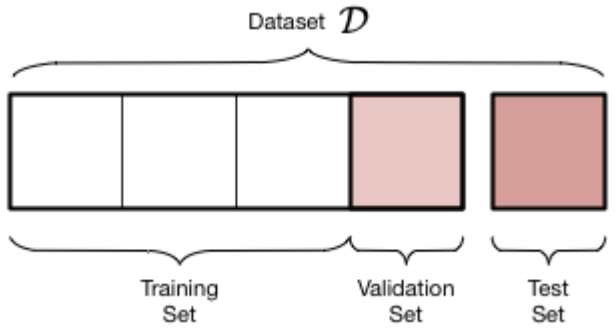


With more training example

Partitioning of the dataset

The data set is typically divided into three non-overlapping samples:

1) Training set: to train the model
2) Validation set: to validate and tune the model
3) Test set: to test the model's ability to predict well on new data (generalize)

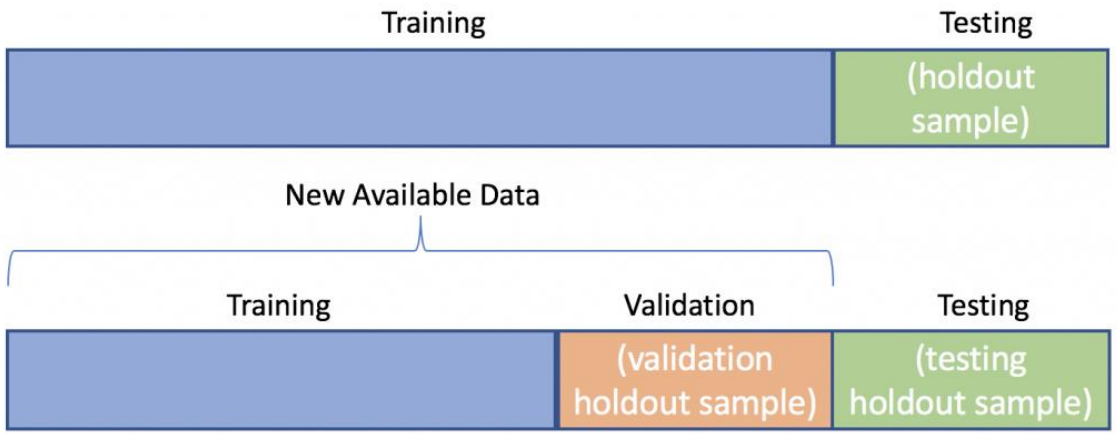


To be valid and useful, any supervised machine learning model must generalize well beyond the training data.

Large dataset is needed! But what if we don't have it?

Resampling methods

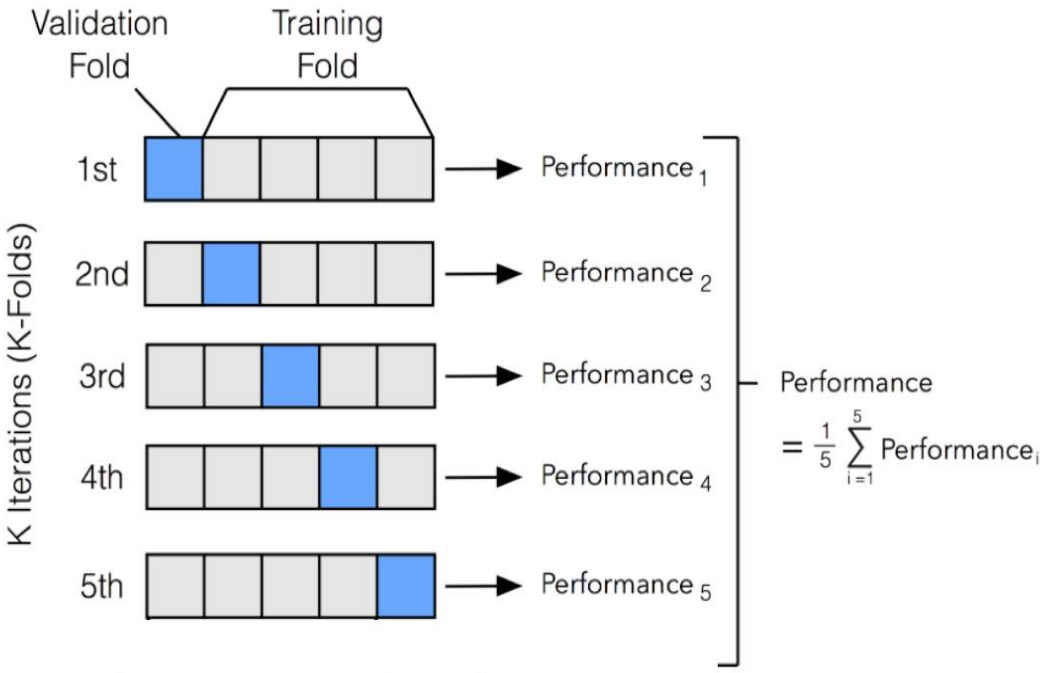
- Sometimes we cannot afford to split the data in three because the algorithm may not learn anything from a small training dataset!
- Small validation set is also problematic because we cannot tune the hyperparameters properly! Unstable model performance in validation set!
- Solution: combining the training and validation sets and use cross validation!



K-fold Cross Validation

1) Divide the training data into K roughly equal-sized non-overlapping groups. Leave out k^{th} fold and fit the model to the other $k-1$ folds. Finally, obtain predictions for the left-out k^{th} fold.

2) This is done in turn for each part k and then the results are combined.



Why do we use Cross Validation?

Cross validation is mainly used for two purposes:

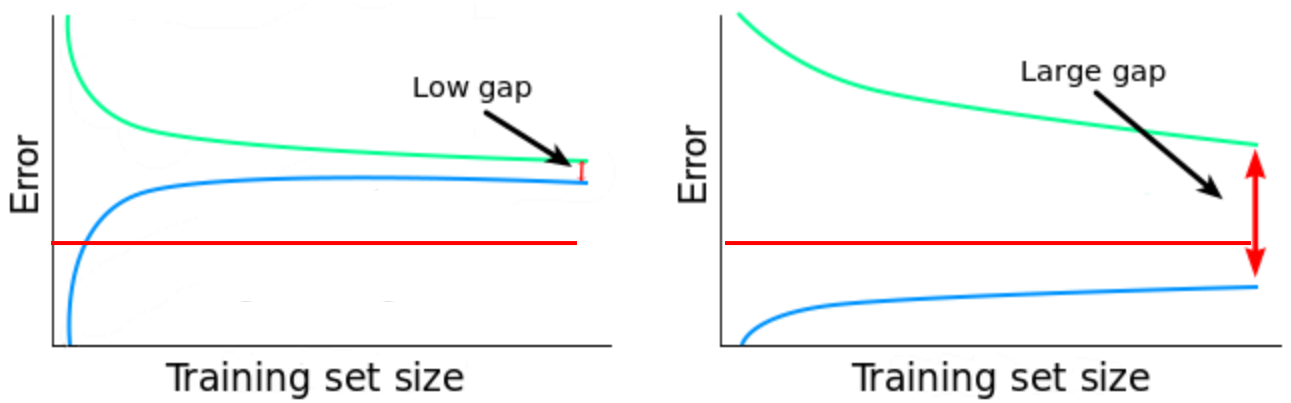
1. Model architecture selection (optimization vs generalization)
2. Estimation of model performance in the test set

- After selecting the best model architecture, we estimate the generalization error using the test set.
- Different model comparison is based on test set performance!

The Learning Curve: Do we need to collect more data?

- A learning curve is a plot that shows the relationship between the amount of training data and the performance of a machine learning model.
- It is used to diagnose whether a model has high bias, high variance, or is just right.

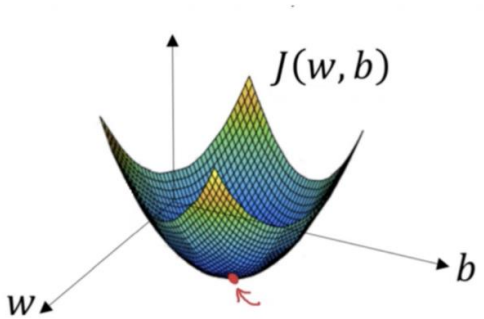
-- Training score
-- Cross validation score
-- Benchmark performance
(common sense performance)



How do Machines Learn?

Terminology

- Learning: Finding the model weights (parameters' values)
- Cost Function: Tells us "how good" our model is at making predictions for a given set of parameters.
- The cost function has its own curve and its own gradients. The slope of this curve tells us how to update our parameters to make the model more accurate.
- The two most frequently used optimization algorithms when the cost function is continuous and differentiable are Gradient Descent (GD) and Stochastic GD.



Solvers (learners)!

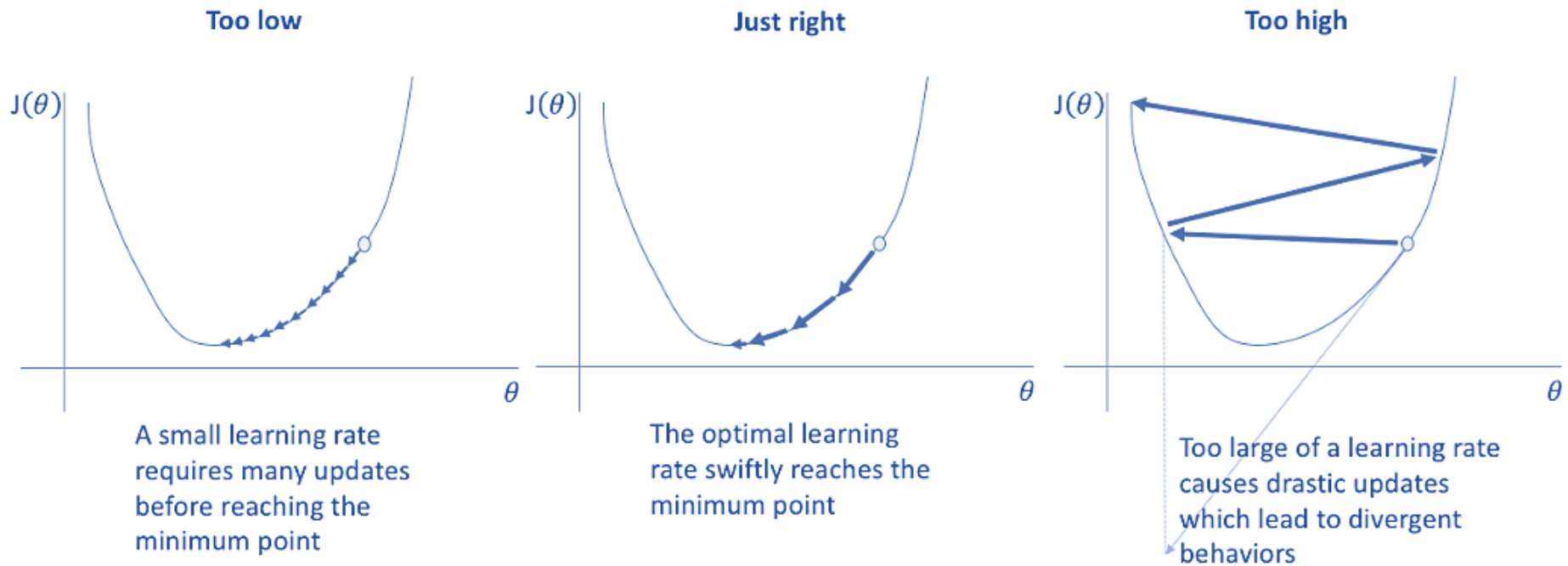
- Gradient Descent: is an iterative optimization algorithm for finding the minimum of a function.
- We starts at some random point and take steps proportional to the negative of the gradient of the function at the current point.

$$\theta_j := \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta)$$

- θ_j is the model's j^{th} parameter
- α is the learning rate
- $J(\theta)$ is the cost function (which is differentiable)

Choice of learning rate

- If α is too small, gradient descent can be slow
- If α is too large, the gradient descent can even **diverge**.



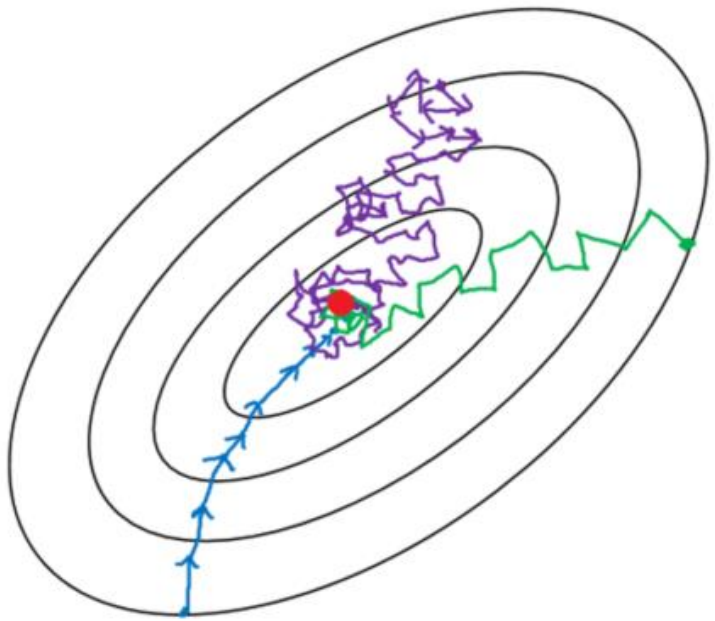
Beyond Gradient Descent?

Disadvantages of gradient descent:

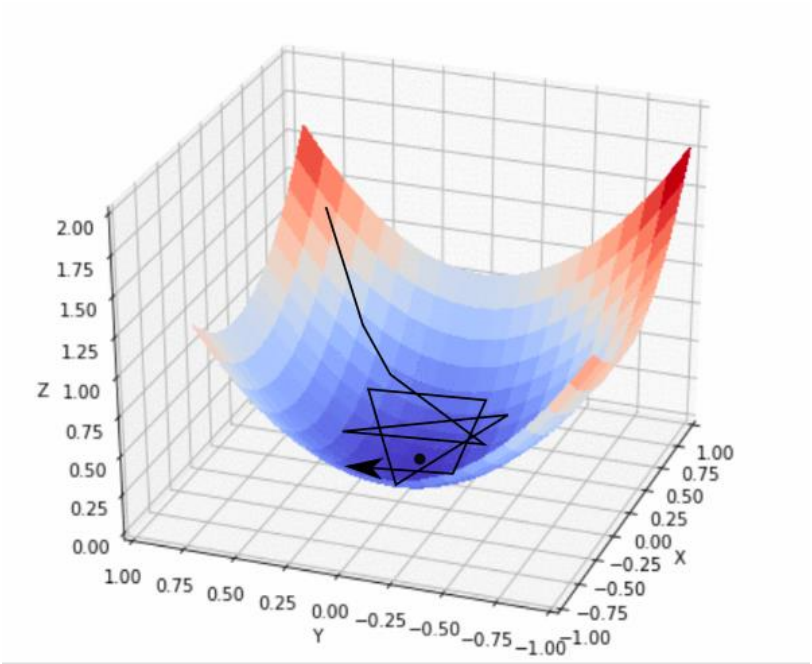
- Single batch: use the entire training set to update parameters!
- Sensitive to the choice of the learning rate
- Slow for large datasets

(Minibatch) Stochastic Gradient Descent: is a version of the algorithm that speeds up the computation by approximating the gradient using smaller batches (subsets) of the training data. SGD itself has various "upgrades".

SGD vs GD

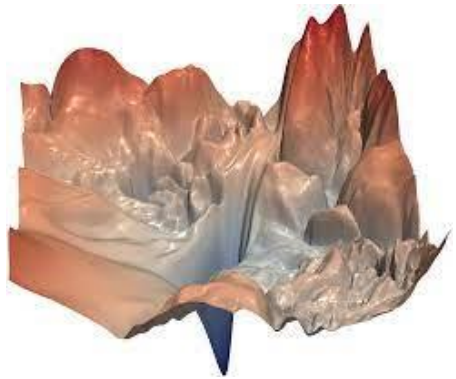


Batch gradient descent
Mini-batch gradient Descent
Stochastic gradient descent



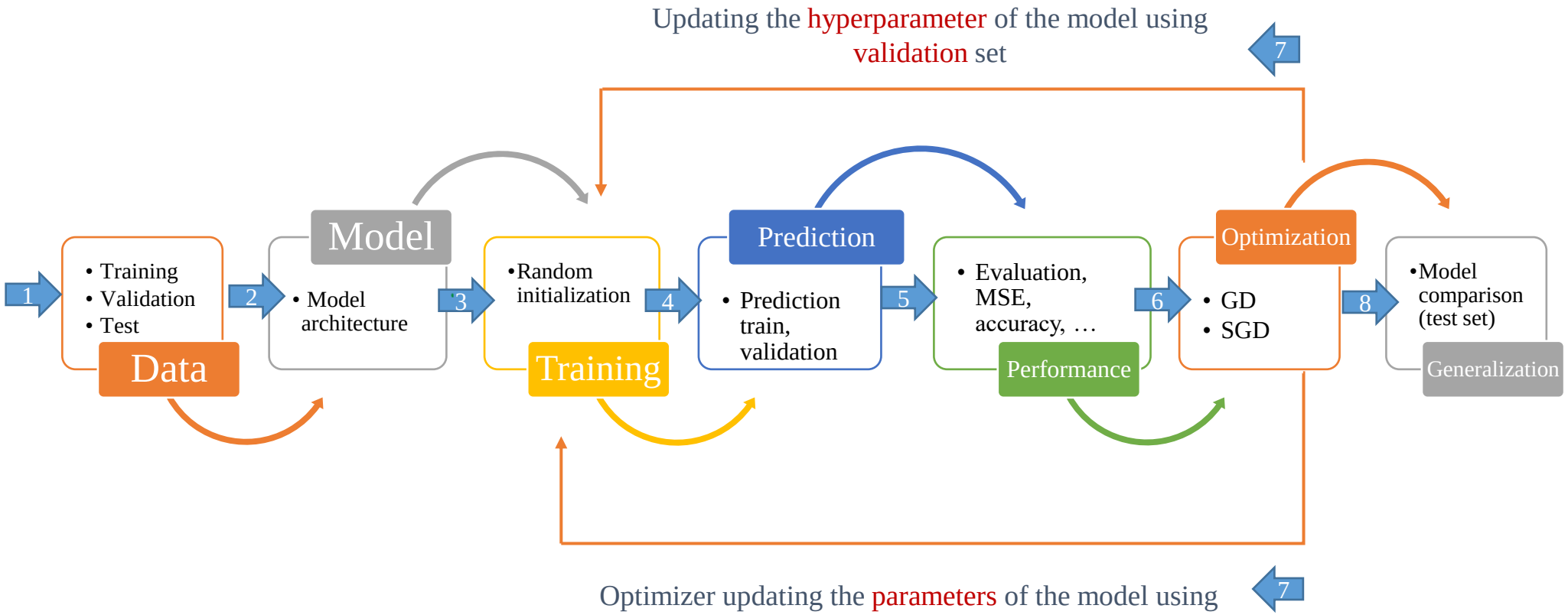
Beyond SGD?

- Loss functions can be difficult to optimize!
- *Visualizing the loss landscape of neural nets*, Li et all, 2018



- Solution: Designing an adaptive learning rate that can adapt to the loss landscape.
- Rather than just looking at the current gradient, consider the previous weight updates.
- This is called, momentum!
- Examples: Adam, Adadelta, Adagrad, RMSProp!

How do machines actually learn?



Module 5 – Part II
Machine Learning Boosting models

The modern machine learning landscape

- From 2016 to 2020, the entire machine learning and data science industry has been dominated by these two approaches:
  1. Deep learning
  2. Gradient boosted trees

- Most practitioners of deep learning use Keras, often in combination with its parent framework TensorFlow.
- This means you'll need to be familiar with Scikit-learn, XGBoost, and Keras

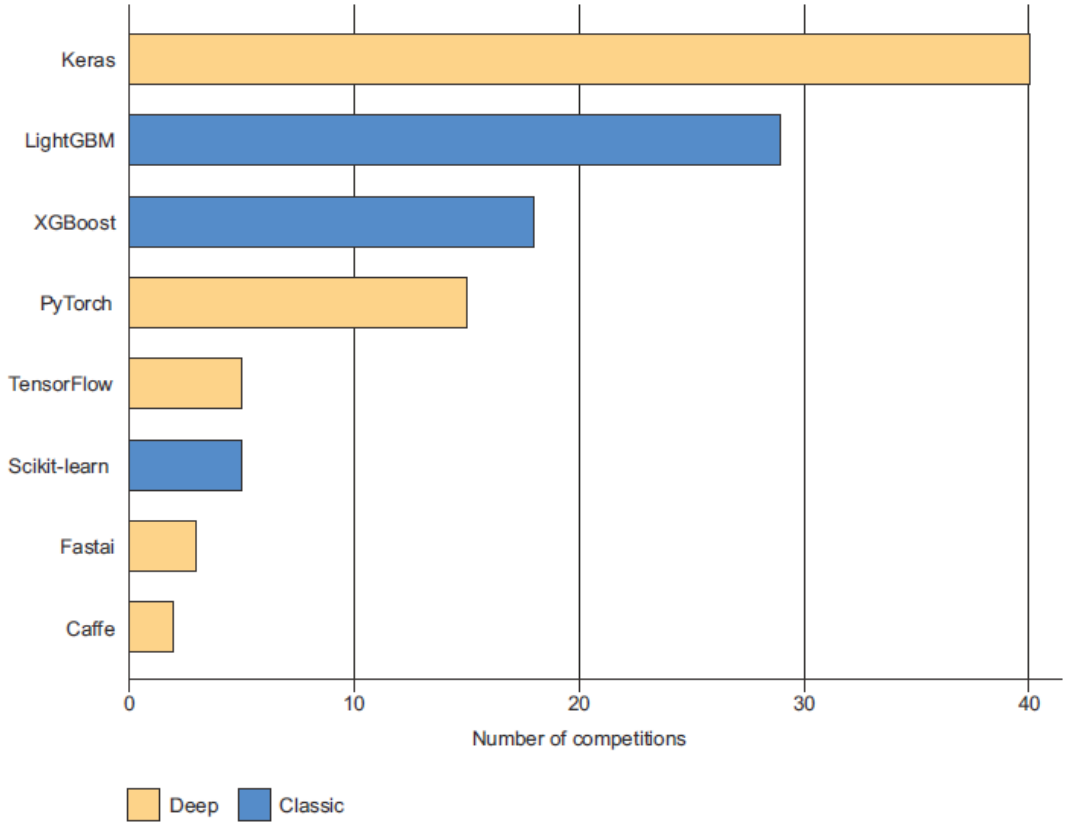
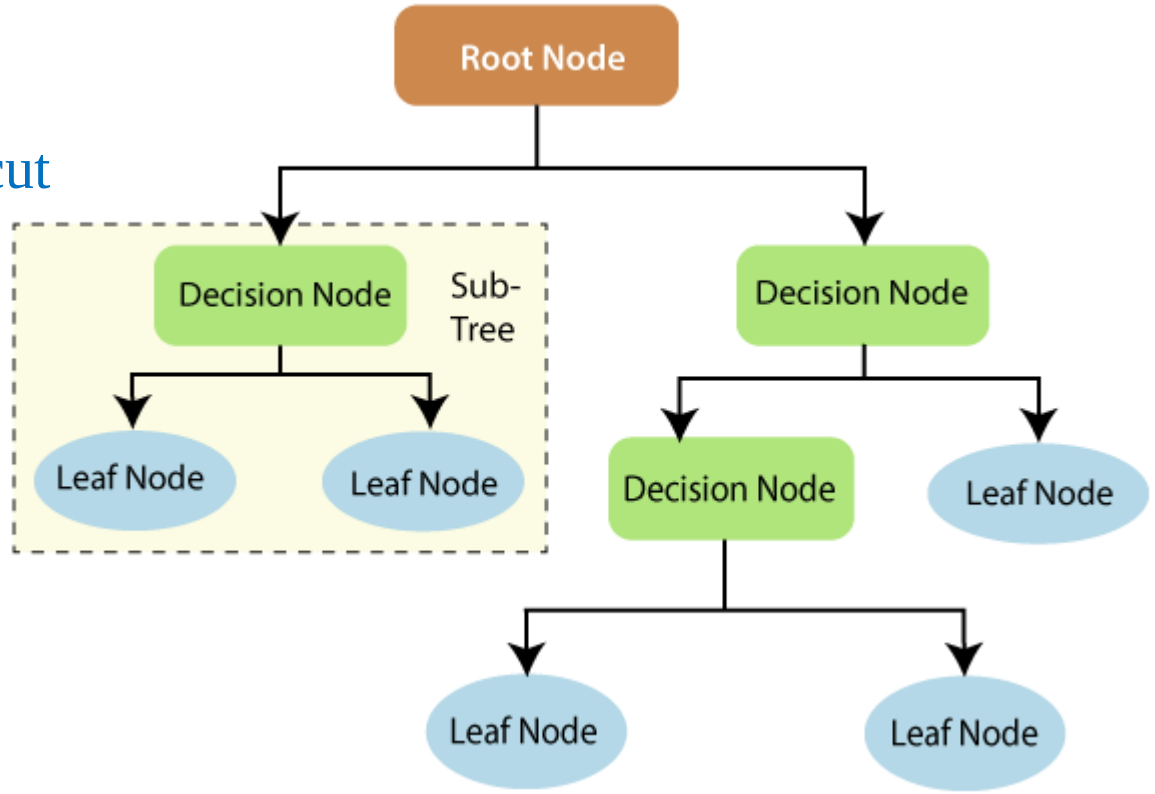


Figure 1.12 Machine learning tools used by top teams on Kaggle

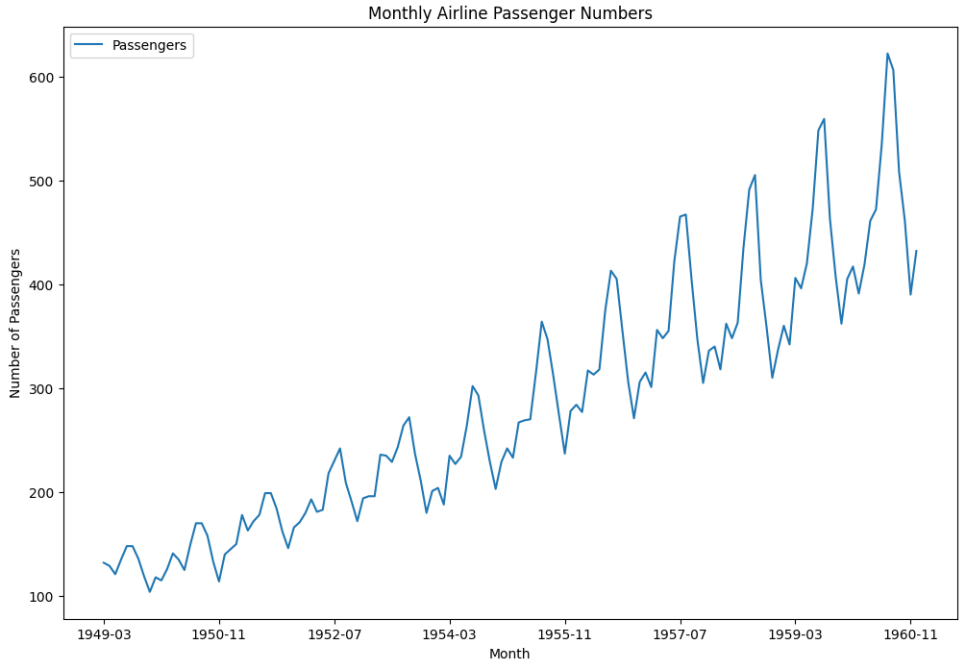
Decision Trees Fundamental questions

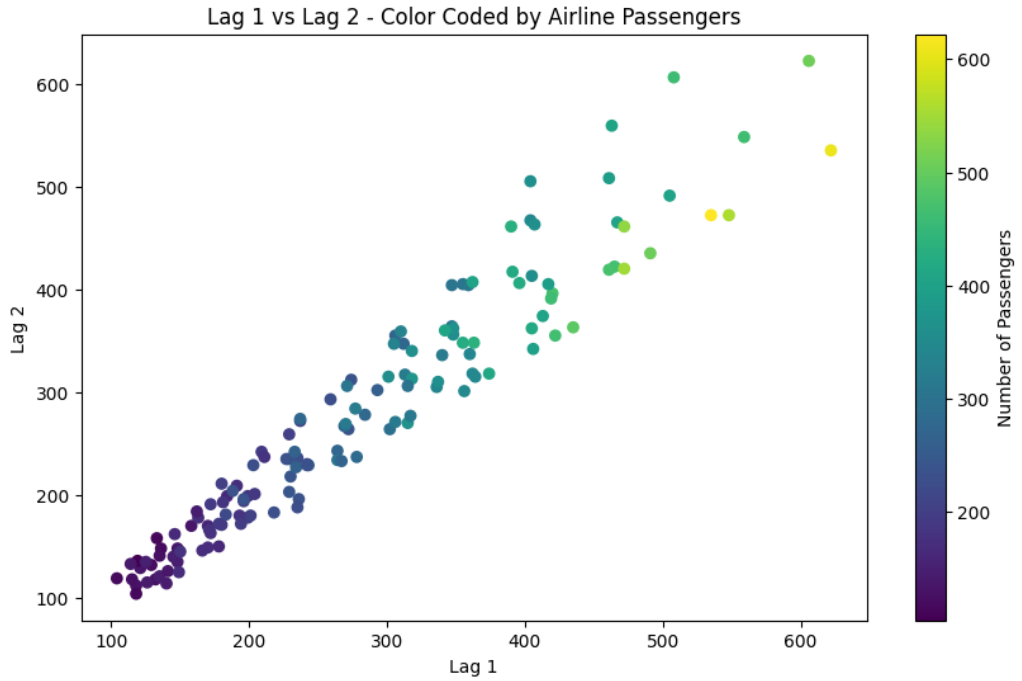
- Four fundamental questions to be answered:

1) How to sample the data for splitting?
2) How to split the samples, What feature and cut off to start with?
3) How to grow a tree?
4) How to combine trees?



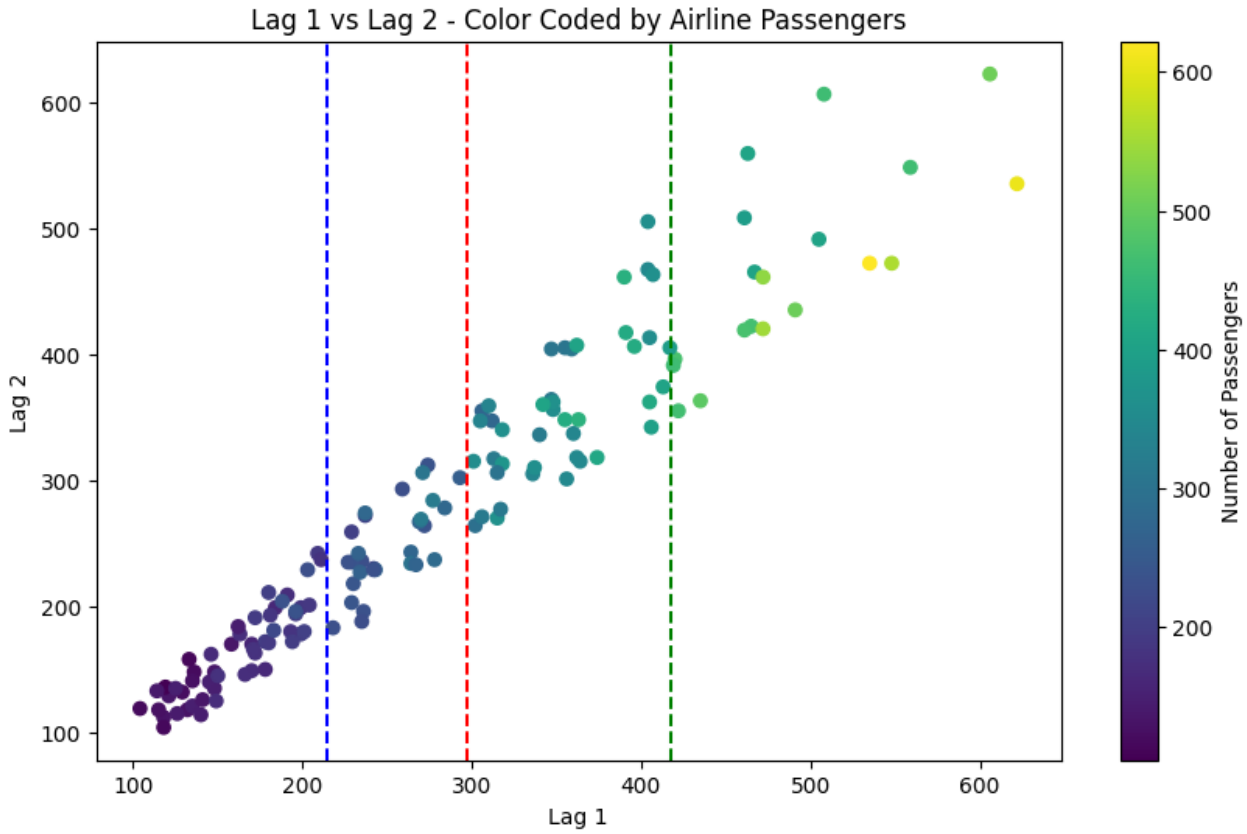
Decision Tree TS regression (Intuition)

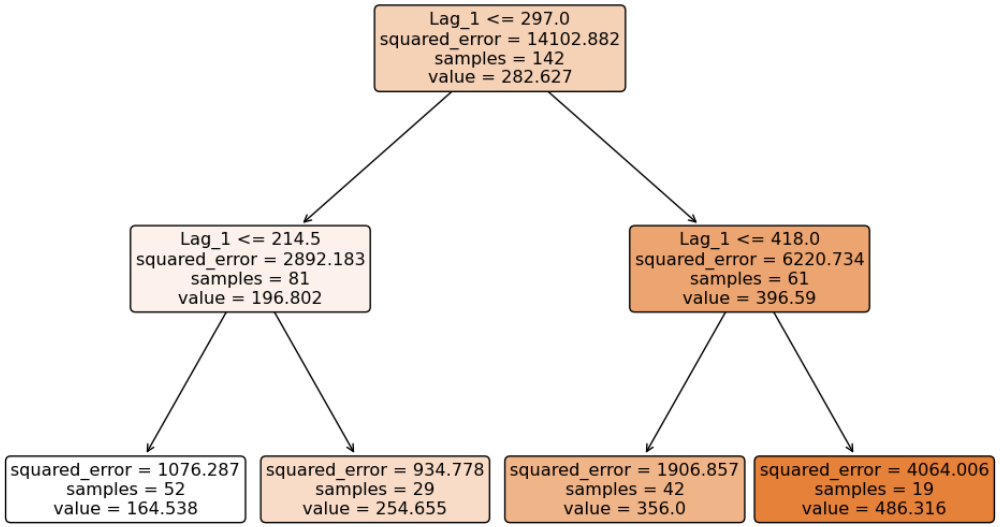




Month	Passengers	Lag_1	Lag_2
1949-01	112	NaN	NaN
1949-02	118	112.0	NaN
1949-03	132	118.0	112.0
1949-04	129	132.0	118.0
1949-05	121	129.0	132.0

Decision Tree TS regression (Intuition)





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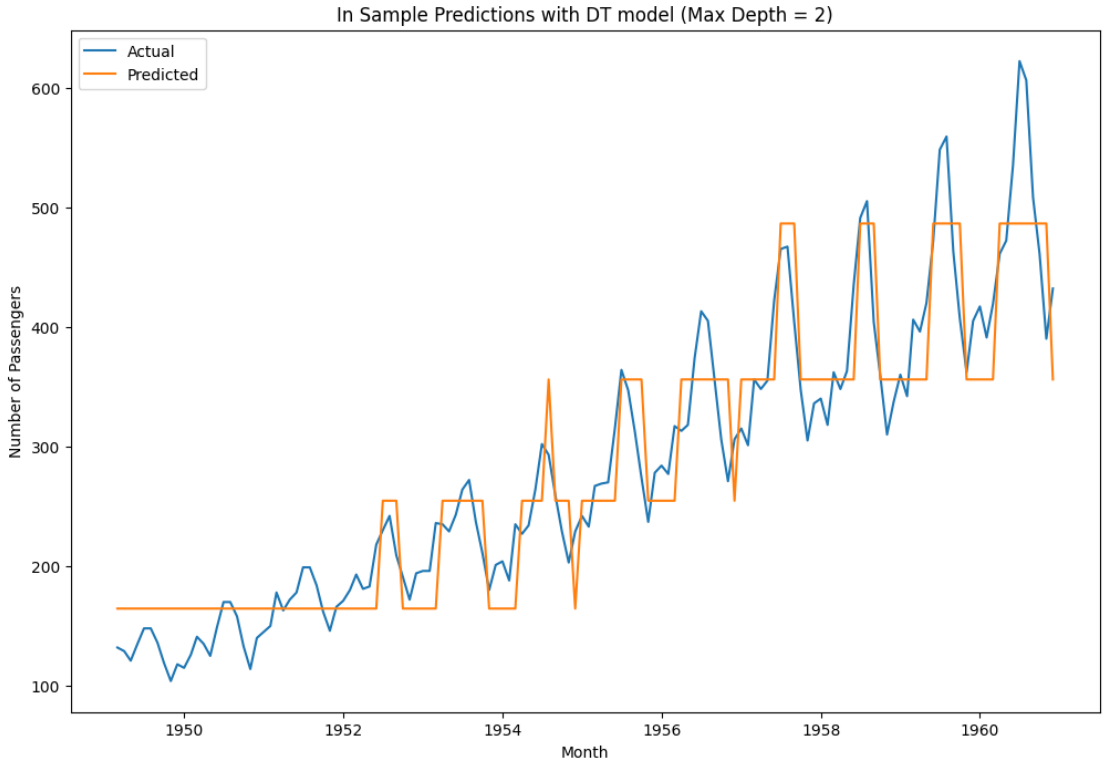
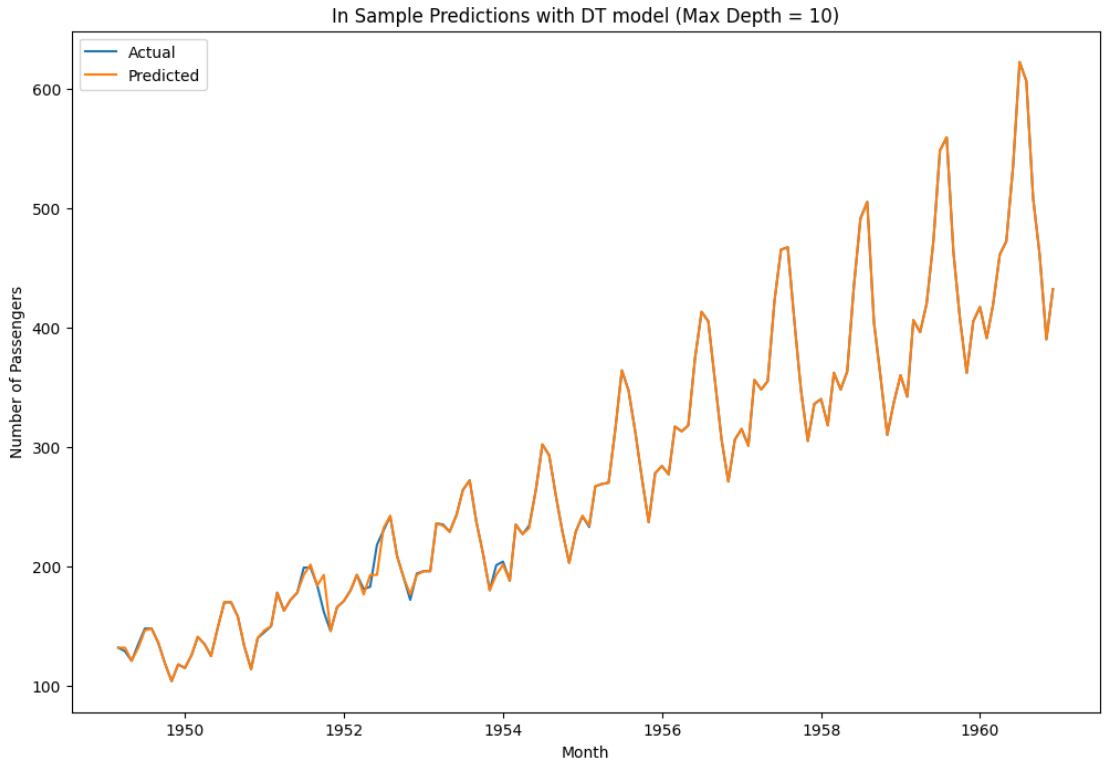
Decision Tree TS regression (Intuition)





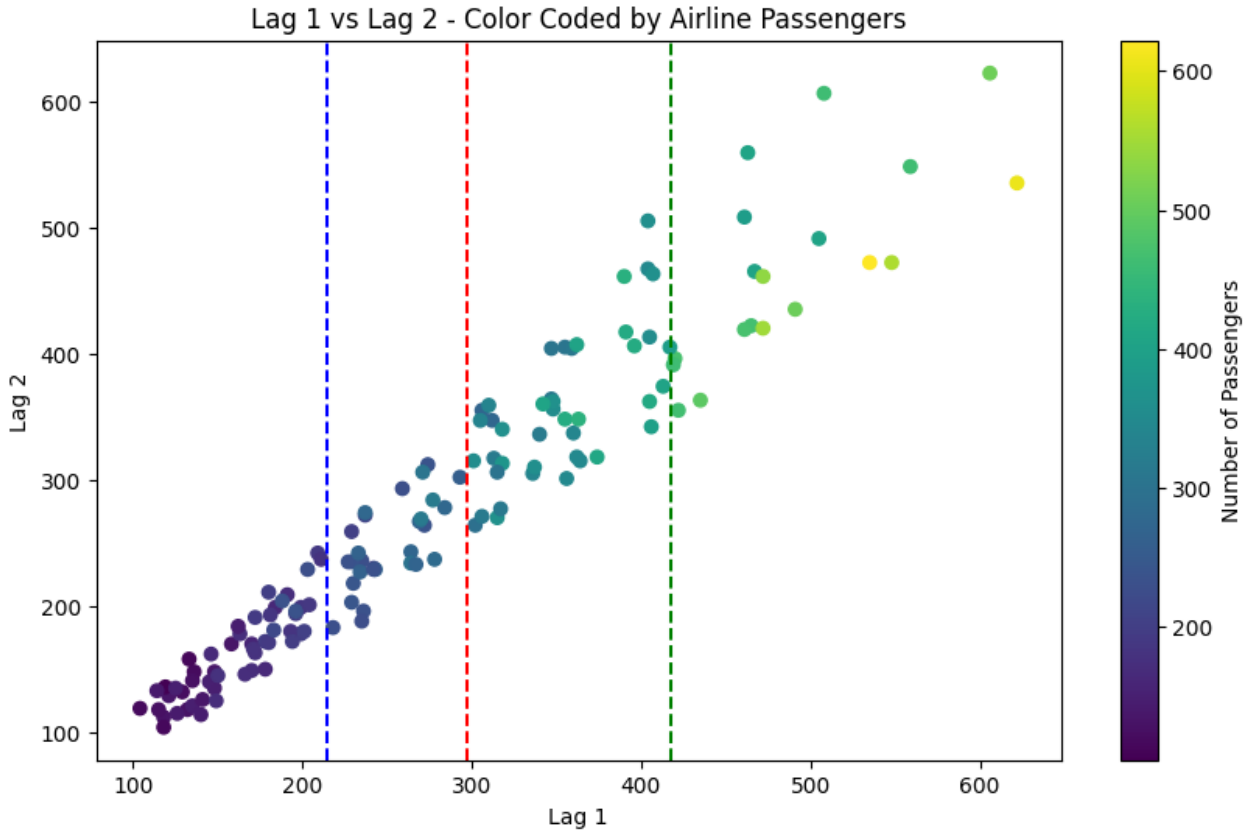
What feature and cut off to start with?

- Which feature and cut off adds the most information gain (minimum impurity)?

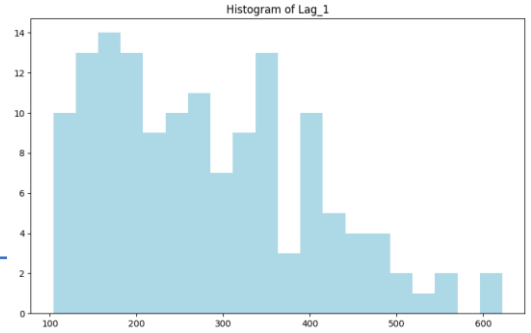
- Regression trees: MSE
- Classification trees:
  1. Error rate
  2. Entropy
  3. Gini Index

Control how a Decision Tree decides to split the data

$$\sum_{j=1}^{J} \sum_{i \in R_j} (y_i - \hat{y}_{R_j})^2$$



How to sample the data for splitting?

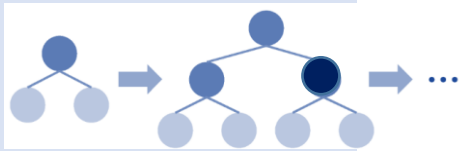
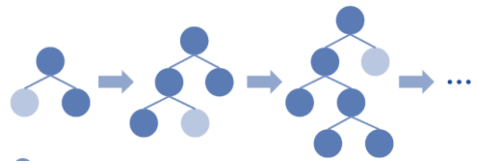
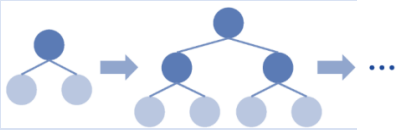


Method	Description
Pre-sorted Naive	Sorts all data for each feature to evaluate every possible split point. Data is pre-sorted to expedite split evaluation. + Simple and accurate - Computationally intensive
Histogram-Based	Bins continuous feature values into discrete intervals (histograms) to reduce the number of potential split points evaluated. + Reduces computational load - May miss optimal splits within bins
GOSS (Gradient-based One-Side Sampling) for Gradient Boosting models only	Focuses on samples with large gradients (errors) by retaining them and under-sampling those with small gradients. Adjusts sample weights accordingly. + Reduces computational cost - Adds complexity to the implementation.

How to Split the Samples? (What Features and Cutoffs to Start With)

Method	Description
Greedy	At each node, selects the feature and cutoff that provide the greatest immediate reduction in the loss function (e.g., MSE). Decisions are made based solely on local optimization without considering future splits. + Simple and computationally efficient - May not lead to the globally optimal tree
Non-Greedy	Considers the global impact of splits by evaluating future nodes or using global optimization techniques. Methods include optimal decision trees, lookahead splits, evolutionary algorithms, Bayesian trees, and etc. + More accurate and generalizable models by avoiding local optima - Computationally intensive and complex

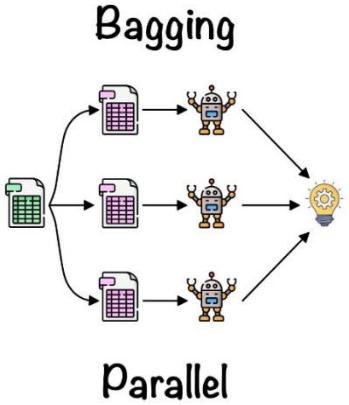
How to grow a tree?

Algorithm	Description	
Depth-Wise Level-Wise	This strategy grows the tree level by level (one level at a time), all nodes are expanded simultaneously before moving to the next level. This results in a balanced tree structure.	
Leaf-wise	This strategy, rather than growing by levels, focuses on expanding the tree by adding nodes to the leaves, specifically those that result in the highest decrease in impurity or error. This can lead to a more unbalanced tree but potentially more efficient learning.	
Symmetric	This strategy attempts to maintain balance not just in the depth of the tree but also in how the features are split, aiming for a tree that grows evenly across all paths. This results in faster compute.	

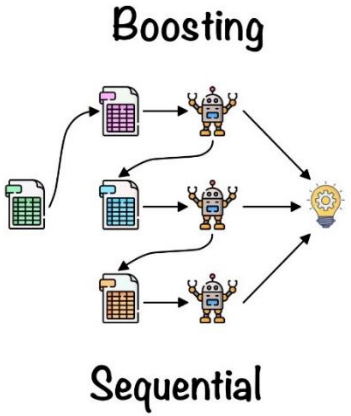
All the methods, repeatedly split the data along the feature with the highest information gain and process continues until a stopping criterion is met (max depth, min samples at nodes, etc)

How to combine trees?

- Bagging consists of creating many "copies" of the training data at the same time (each copy is slightly different from another) and then apply the weak learner to each copy to obtain multiple weak models and then combine them.
- In bagging, the bootstrapped trees are independent from each other.



- Boosting consists of using the "original" training data and iteratively (sequentially) creating multiple models by using a weak learner. Each new model tries to "fix" the errors which previous models make.
- In boosting, each tree is grown using information from previous tree.



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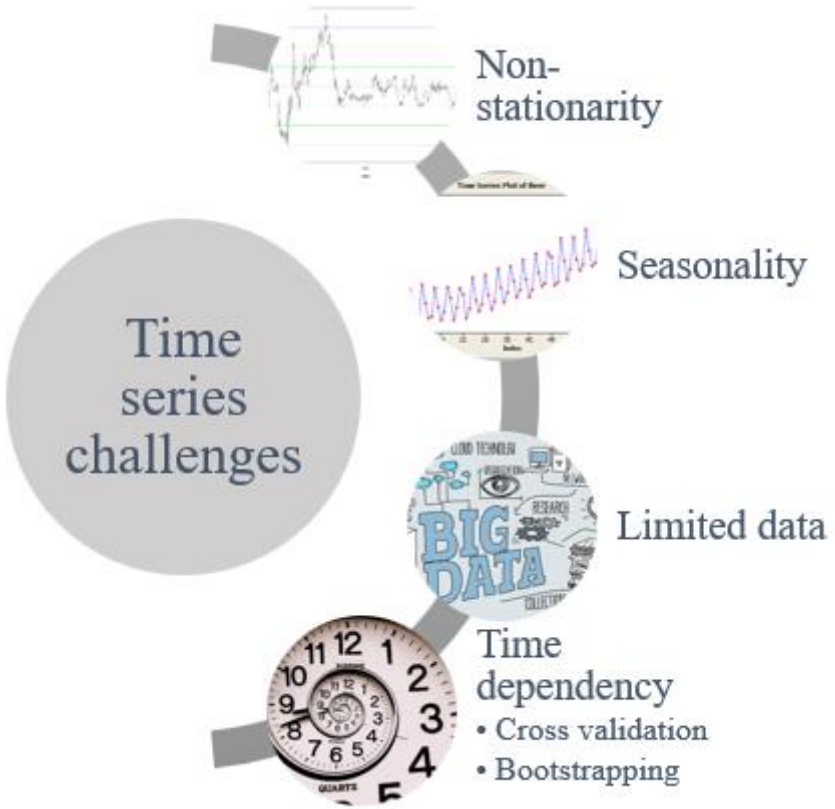
Decision-Tree based models

Aspect	Decision Tree (DT)	Random Forest (RF)	XGBoost	CatBoost	LightGBM
1- Sampling Process	Naïve	Naïve	Histogram-based	Feature Binning (Quantization)	GOSS
2. Splitting Method	Greedy	Greedy	Greedy	Greedy	Greedy
3. Tree Growth Strategy	Depth-wise	Depth-wise	Depth-wise (Leaf-wise)	Symmetric	Leaf-wise
4. Combining Trees	Not applicable	Bagging	Boosting	Boosting	Boosting

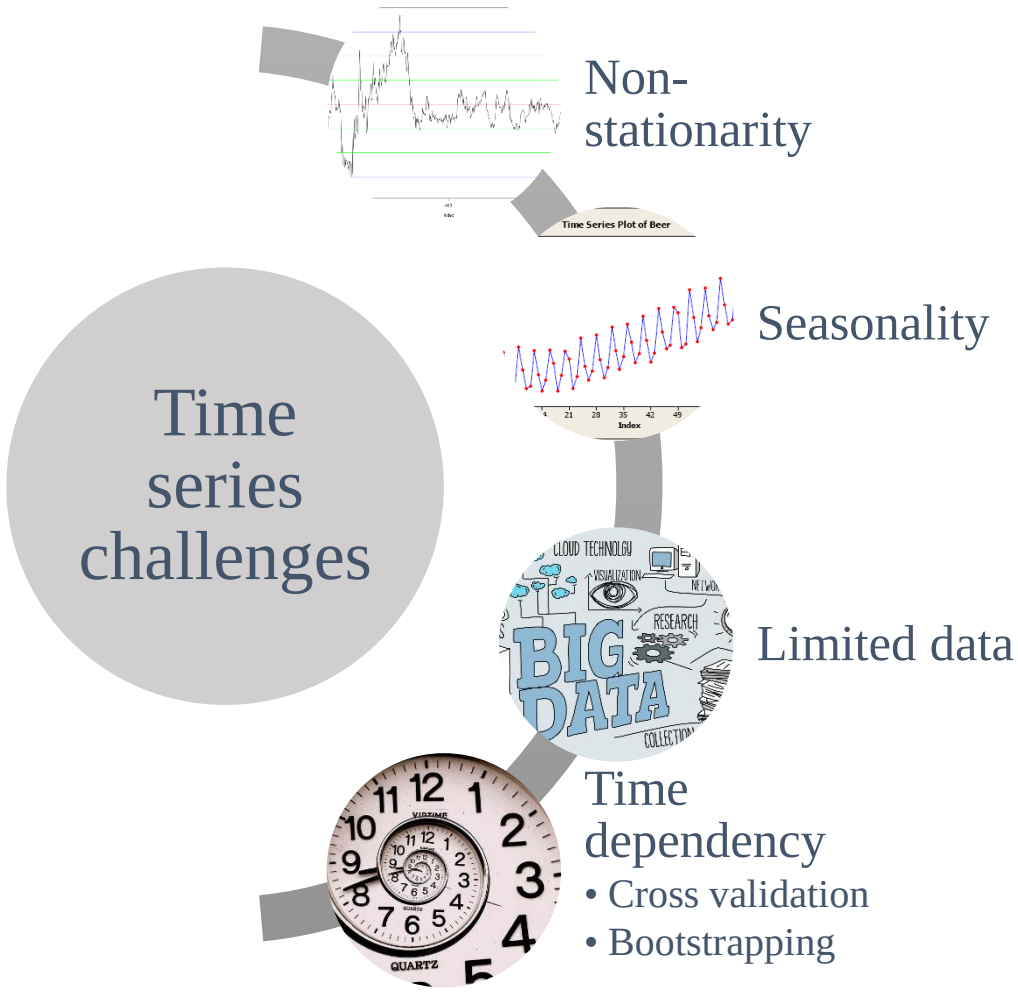
Cost functions and minimization methods

Model	Cost Function(s)	Minimization Method(s)
Decision Tree	Gini Impurity, Entropy, MSE, MAE, …	Greedy recursive splitting
Random Forest	Gini Impurity, Entropy, MSE, MAE, …	Not directly optimized (aggregation of base trees)
XGBoost	Customizable (often: loss function + regularization terms)	Gradient Boosting
LightGBM	Customizable (often: loss function + regularization terms)	Gradient Boosting (with specialized techniques)
CatBoost	Customizable (often: loss function + regularization terms)	Gradient Boosting (with ordered boosting)

Module 5 – Part III
Challenges in Time Series Machine Learning

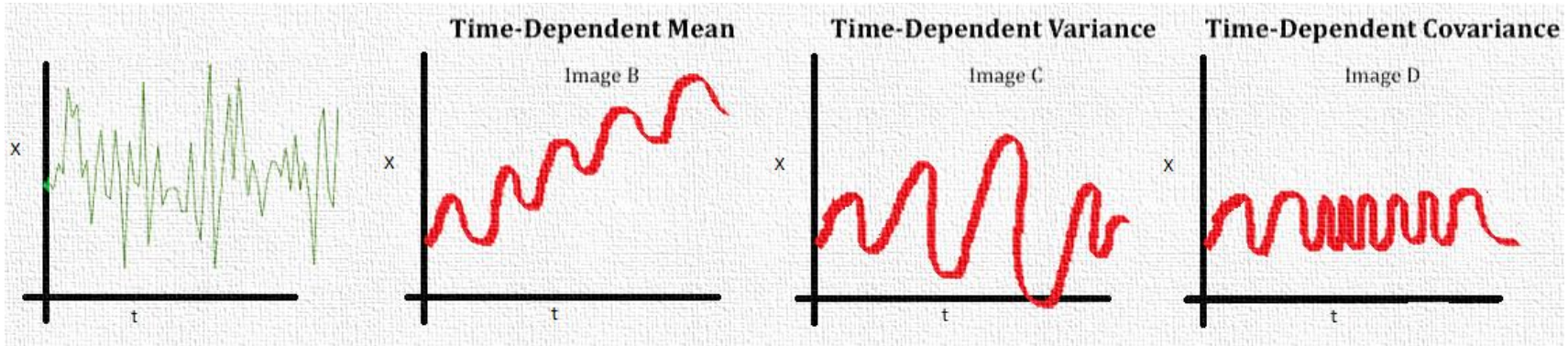


Challenges in Time Series Machine Learning



Stationarity

- Stationary vs Non-Stationary Data. What makes a data set Stationary?
- In a stationary timeseries, the statistical properties do not depend on the time



- Data with trend and seasonality are NOT stationary!

Time Series Cross Validation

- With time series data, we cannot shuffle the data! TS data is not IID.
- We also need to avoid data leakage!

- The main time series CV methods are:
  1) Purged K-Fold CV
  2) Walk forward rolling / expanding window
  3) Combinatorial purged CV

Purged K-Fold CV

- Leakage takes place when the training set contains information that also appears in the testing set.
- Leakage will enhance the model performance
- Solution: Purging and Embargoing

- Purged K-Fold CV: Adding purging and embargoing whenever we produce a train/test split in K-Fold CV.

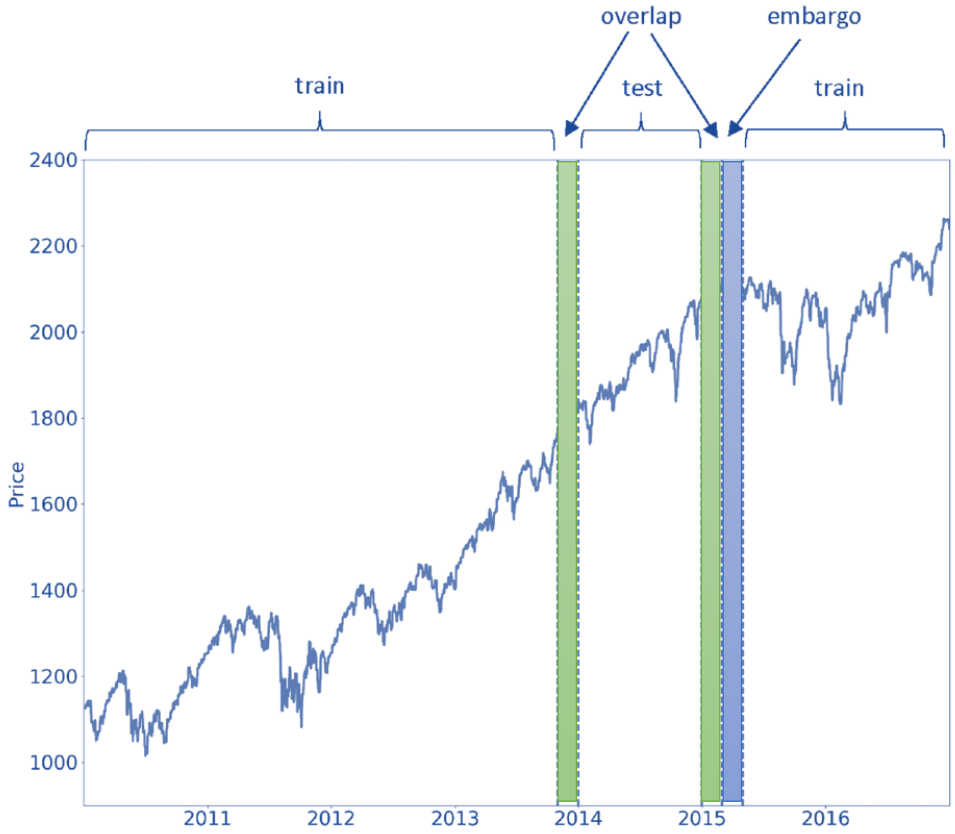
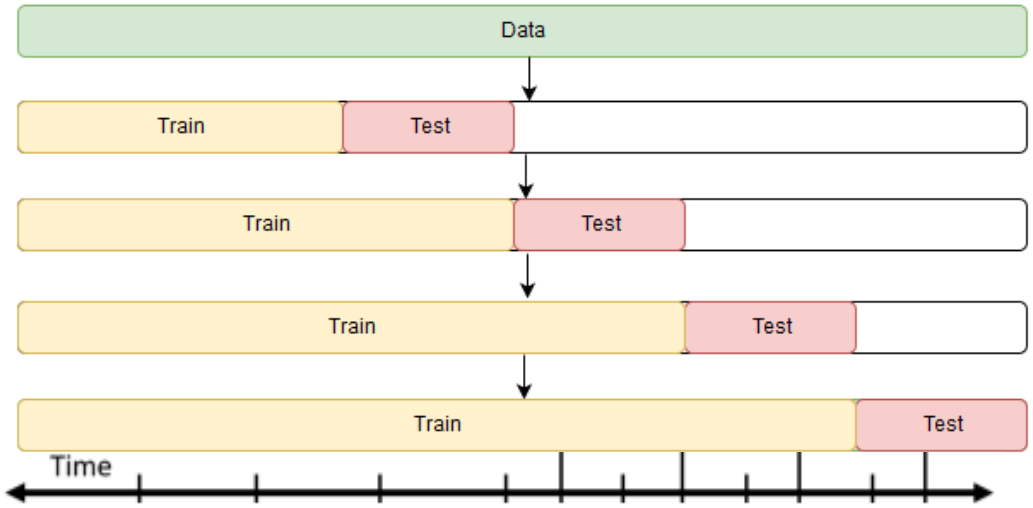


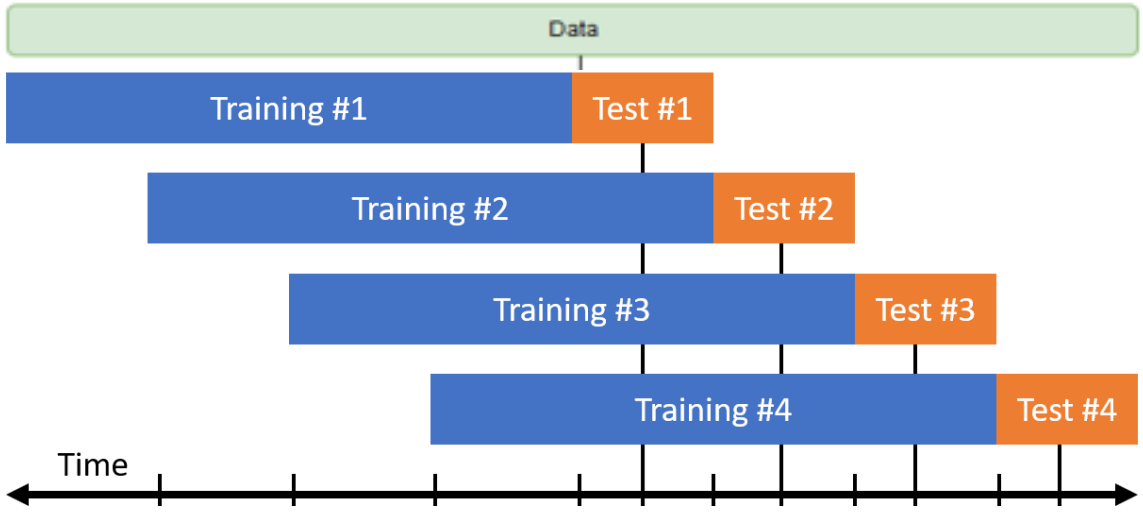
FIGURE 7.3 Embargo of post-test train observations

Walk Forward Cross Validation

Walk forward cross validation
Expanding windows

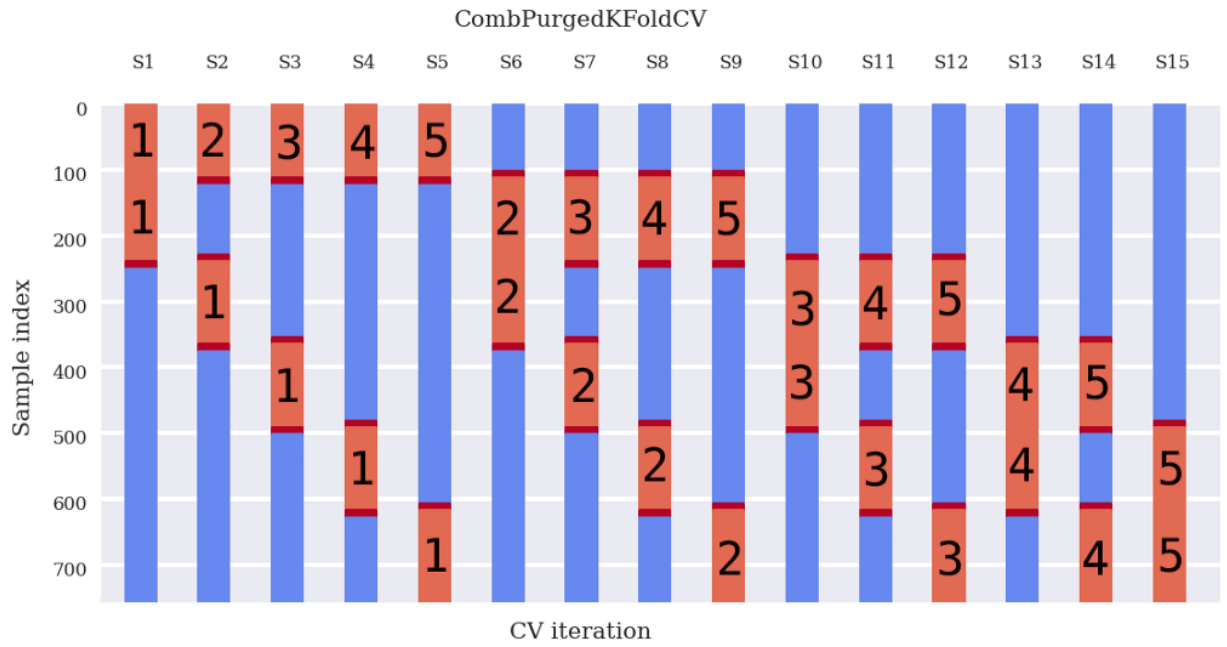


Walk forward cross validation
Rolling windows



Combinatorial Purged Cross Validation (CPCV)

- The goal is to generate multiple unique back-test path that span the entire data set.
- In each path, we can look at the model's OOS performance for the entire time period.

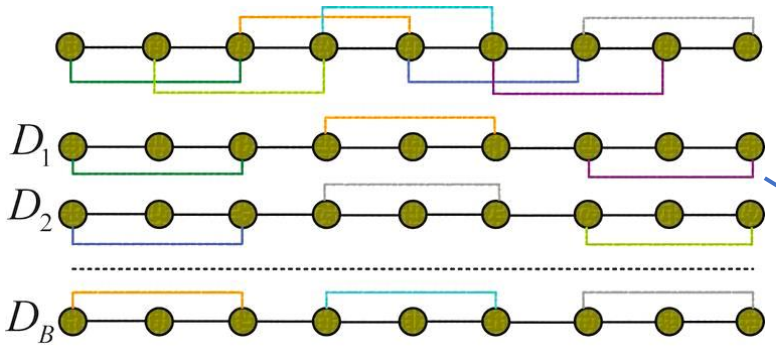


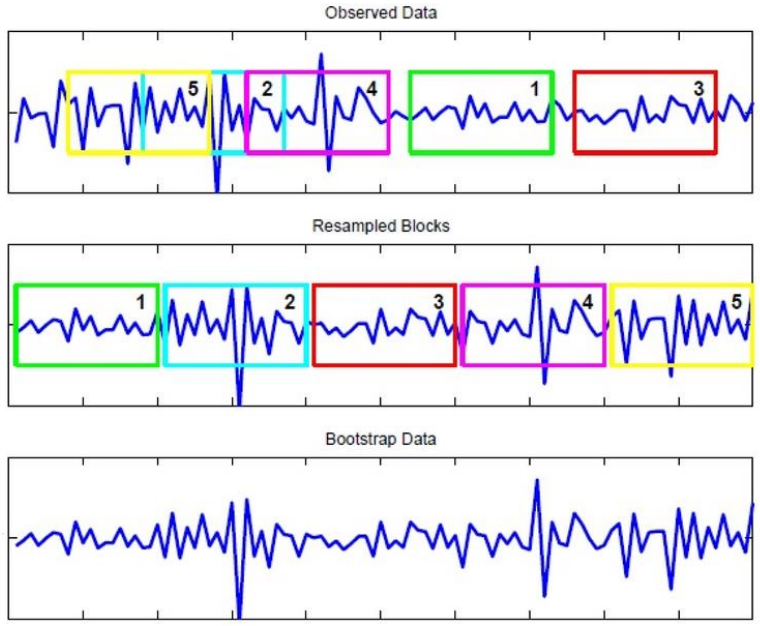
Time Series Bootstrapping

- IID bootstrapping (random sample with replacement) does not work for time series data with temporal dependency.
- Time series Bootstrapping methods:
  - Parametric (based on models with iid residuals and resampling from residuals. Example: ARIMA bootstrap)
  - Non-parametric block bootstrap (data is directly resampled. Assumption: blocks can be samples so that they are approximately iid)
    - Moving Block Bootstrap (MBB)
    - Circular Block Bootstrap (CBB)
    - Stationary Bootstrap (SB)

Moving Block Bootstrap (MBB)

- Moving Block Bootstrap, samples overlapping fixed size blocks of m consecutive observations.
- Blocks starts at indices 1, … , T-m+1

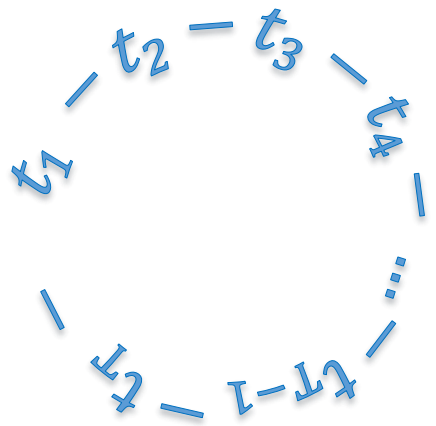




Circular Block Bootstrap (CBB)

- CBB is a simple extension of MBB which assumes the data live on a circle so that $y_{T+1} = y_1$, $y_{T+2} = y_2$, etc.

- CBB has better finite sample properties since all data points get sampled with equal probability.



Stationary Bootstrap (SB)

- In SB, the block size is no longer fixed.
- Chooses an average block size of m rather than an exact block size.
- Popularity of SB stems from difficulty in determining optimal m
- Once applied to stationary data, the resampled pseudo time series by SB are stationary. This is not the case for MBB and CBB.

Road map!

- ✓ Module 1- Introduction to Deep Forecasting
- ✓ Module 2- Setting up Deep Forecasting Environment
- ✓ Module 3- Exponential Smoothing
- ✓ Module 4- ARIMA models
- ✓ Module 5- Machine Learning for Time series Forecasting
- Module 6- Deep Neural Networks
- Module 7- Deep Sequence Modeling (RNN, LSTM)
- Module 8- Prophet and Neural Prophet