

Module 5 – Part I

Machine Learning Fundamentals (review)

Artificial intelligence: Any technique which enables machines to mimic human behavior



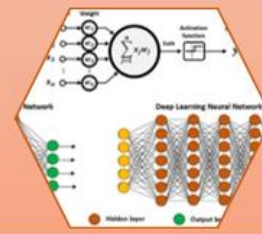
1950's

Machine Learning: Subset of AI that enables computers to learn from data. the model is trained with a set of algorithms



1980's

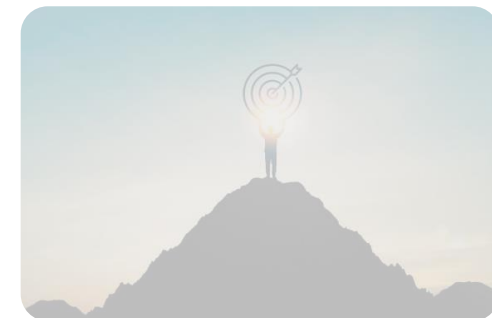
Deep Learning: Subset of ML that extract patterns from data using neural networks.



2010's

➔ 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



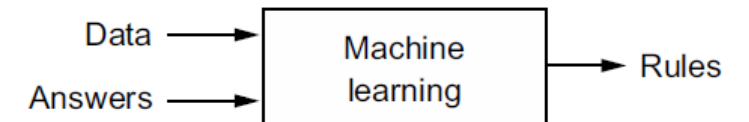
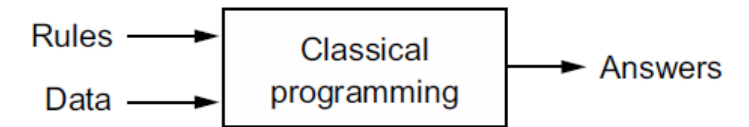
➔ Machine Learning Fundamentals

- 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?



➔ 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.

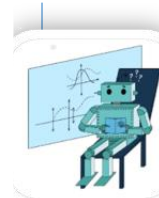


→ Types of Machine Learning



Supervised

- Regression
- Classification



Unsupervised

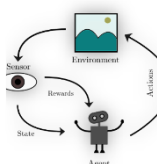
- Clustering
- Anomaly detection
- Dimensionality reduction



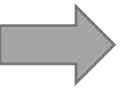
Semi-supervised



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

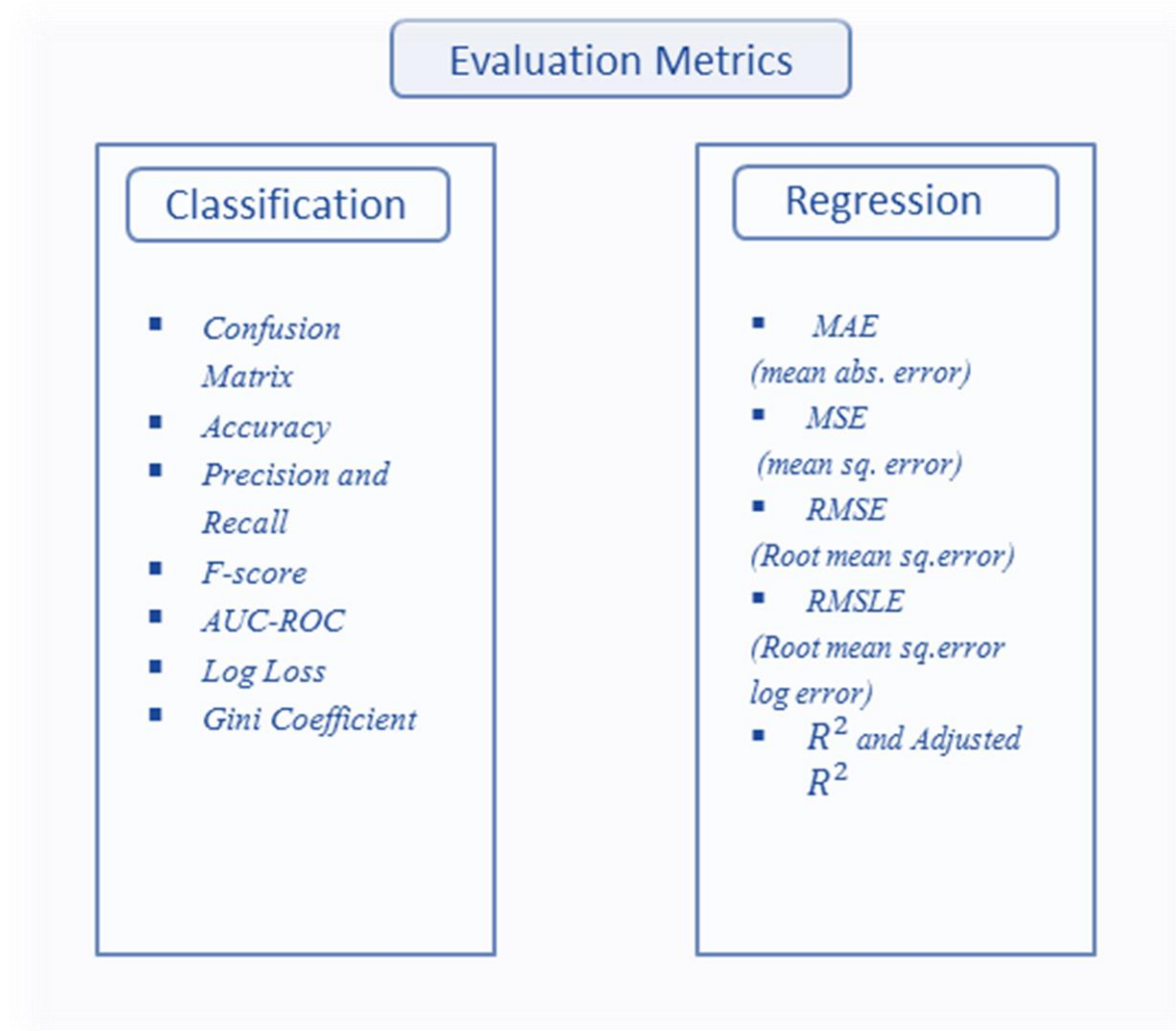


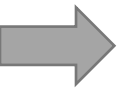
Evaluation metrics

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

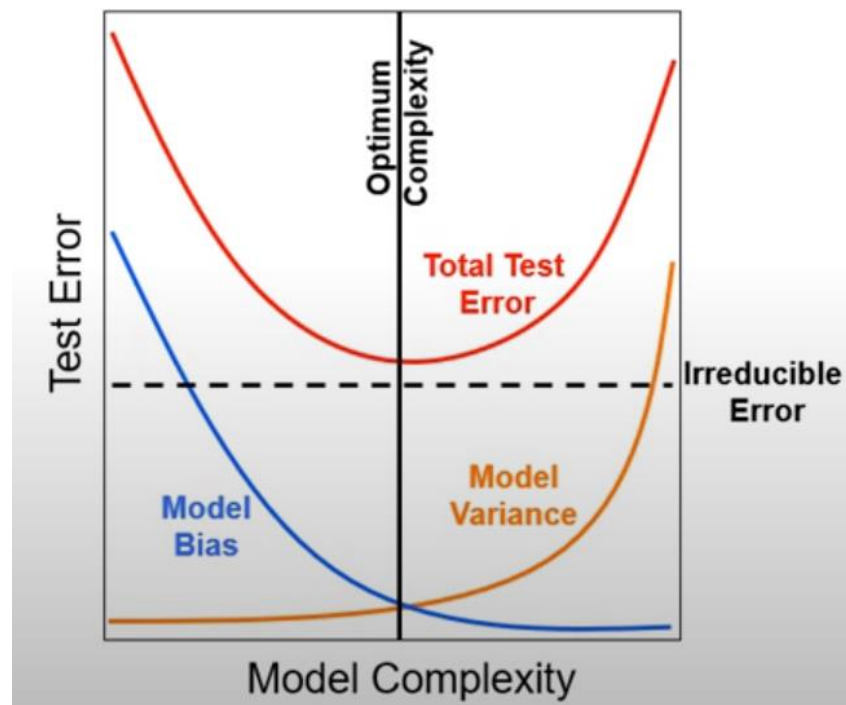
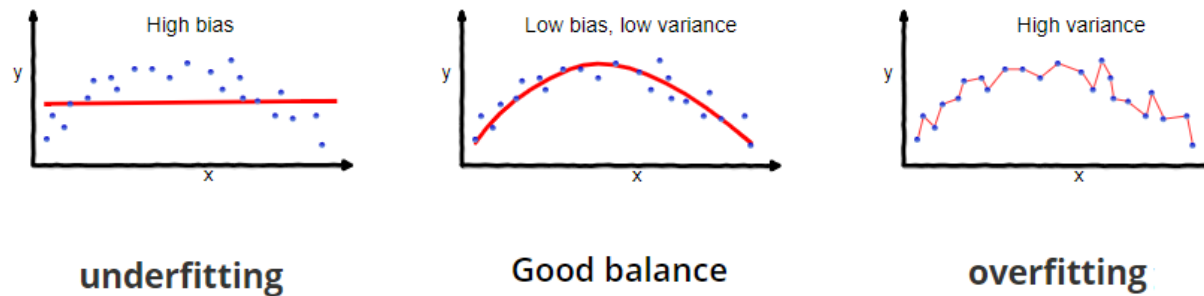
This is typically assessed using

- MSE for **quantitative** response
- Misclassification rate for **qualitative** response

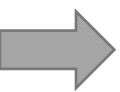




Representations of the bias-variance tradeoff



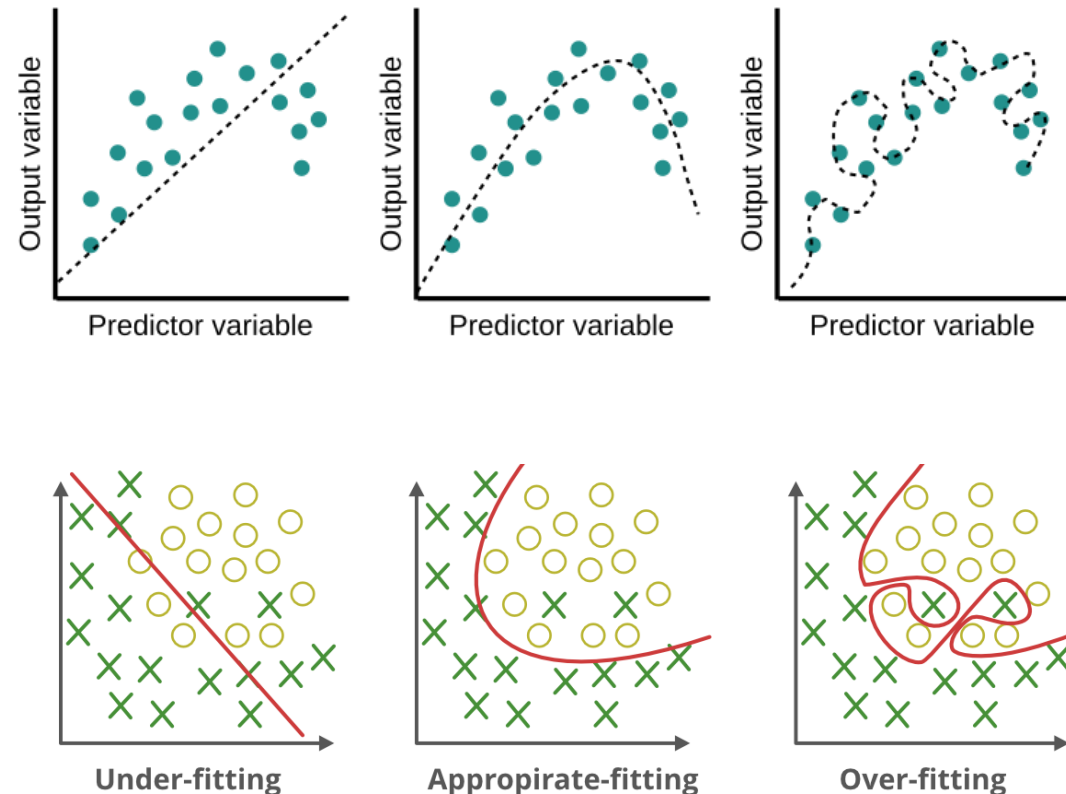
Optimization
Vs
Generalization

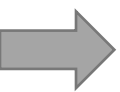


Overfitting

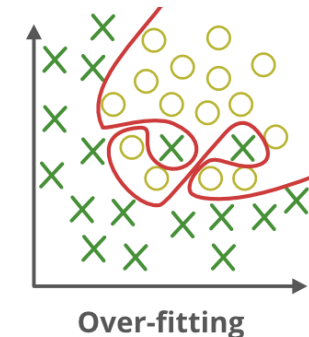
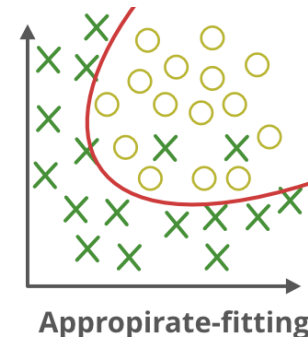
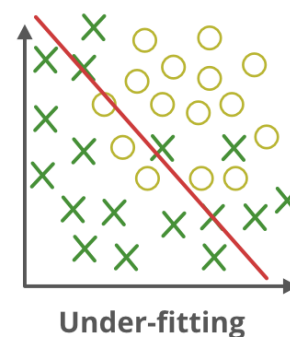
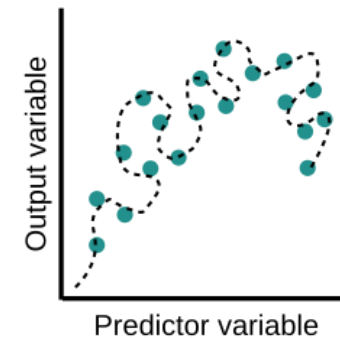
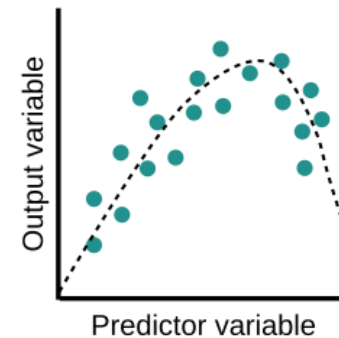
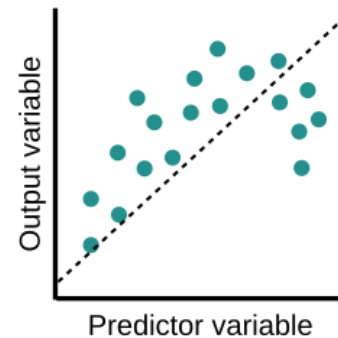
Overfitting happens when the fitted algorithm does **not generalize** well to new data:

- 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**!





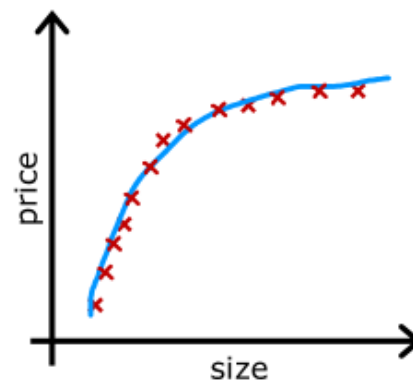
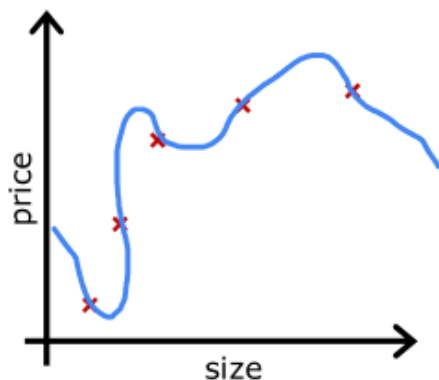
Overfitting



➔ 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)

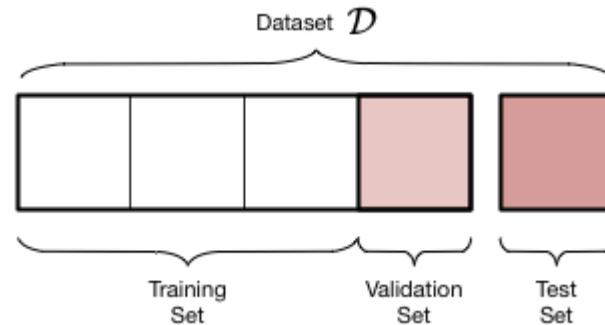


With more training example

→ Partitioning of the dataset

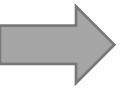
The data set is typically divided into three non-overlapping samples:

- 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**)



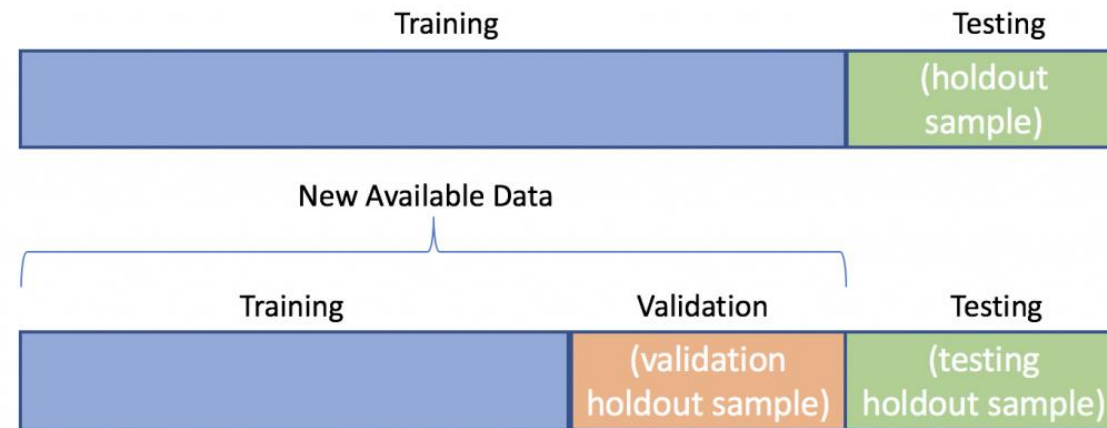
To be valid and useful, any supervised machine learning model **must** generalize well beyond the training data.

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



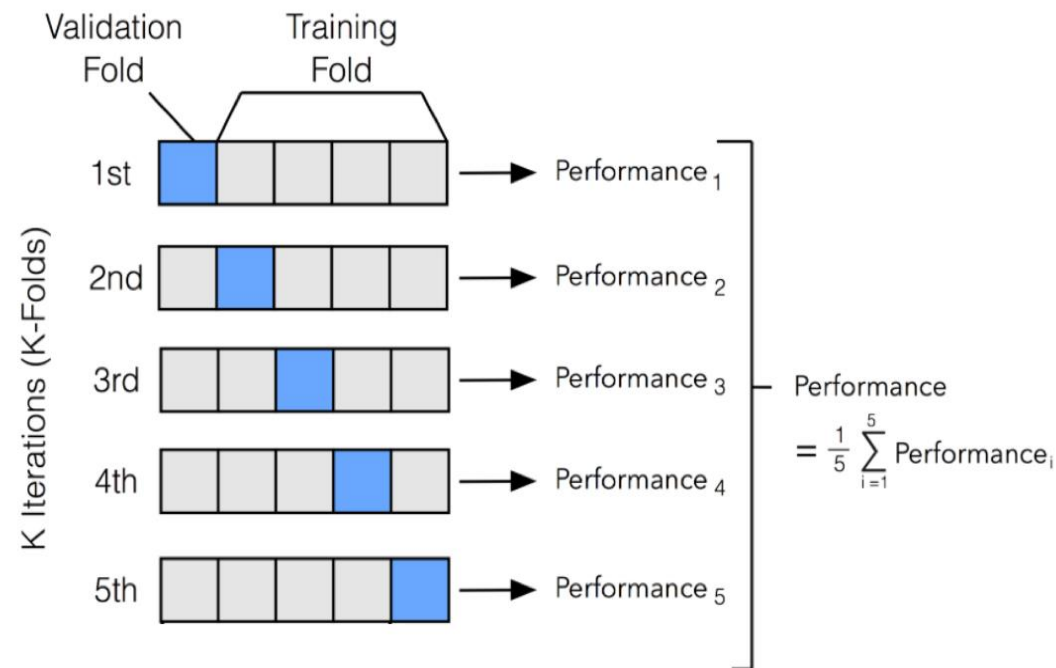
Resampling methods

- 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.



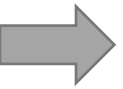
➔ Why do we use Cross Validation?

Cross validation is mainly used for two purposes:

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



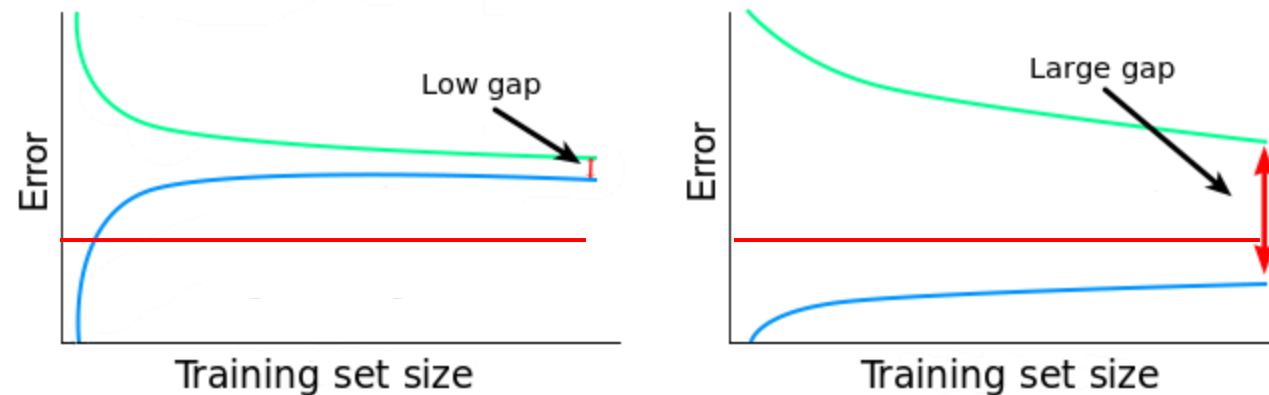
- After selecting the **best model architecture**, we estimate the generalization error using the test set.
- **Different model comparison** is based on **test set** performance!



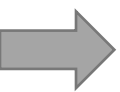
The Learning Curve: Do we need to collect more data?

- 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)

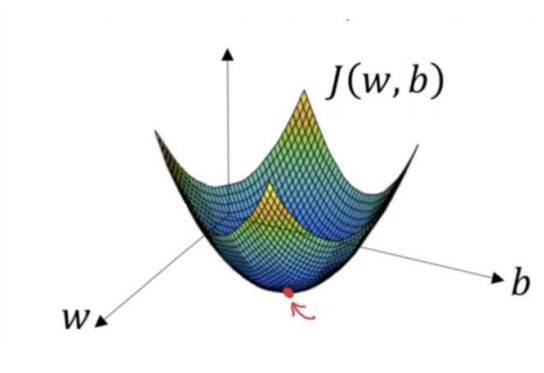


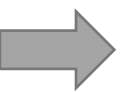
How do Machines Learn?



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)!

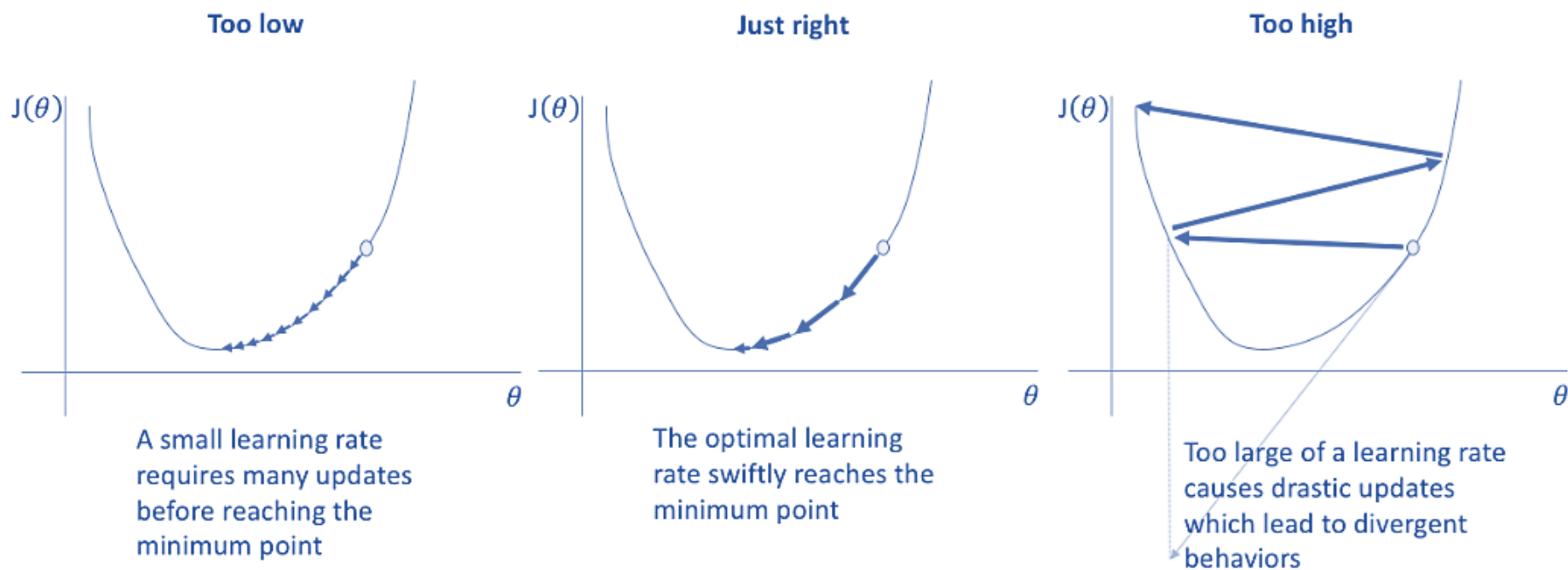
- **Gradient Descent**: is an **iterative** optimization algorithm for finding the minimum of a function.
- We start at some random point and take steps proportional to the **negative** of the gradient of the function at the current point.

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

- 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.

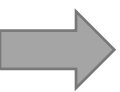


➔ Beyond Gradient Descent?

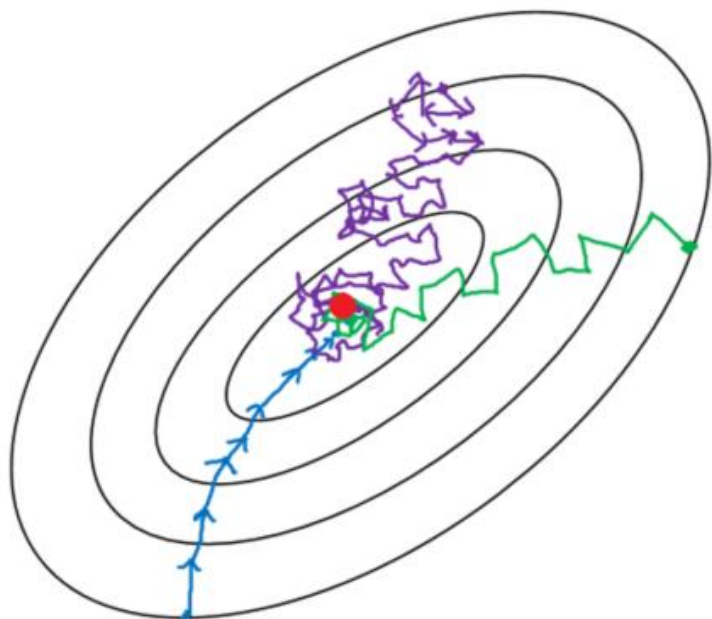
Disadvantages of gradient descent:

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

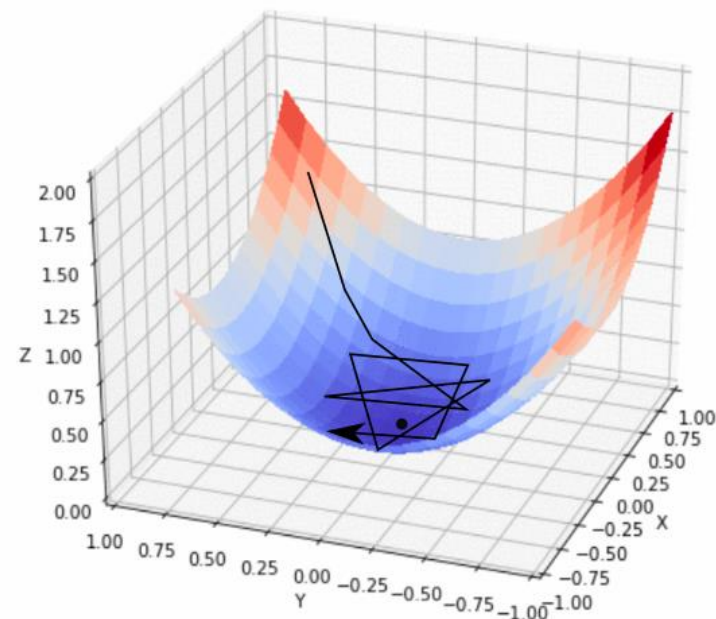
(Minibatch) Stochastic Gradient Descent: is a version of the algorithm that speeds up the computation by approximating the gradient using **smaller batches** (subsets) of the training data. SGD itself has various “upgrades”.

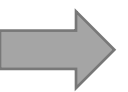


SGD vs GD



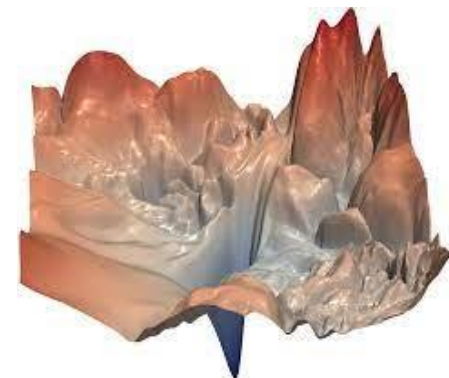
- Batch gradient descent
- Mini-batch gradient Descent
- Stochastic gradient descent





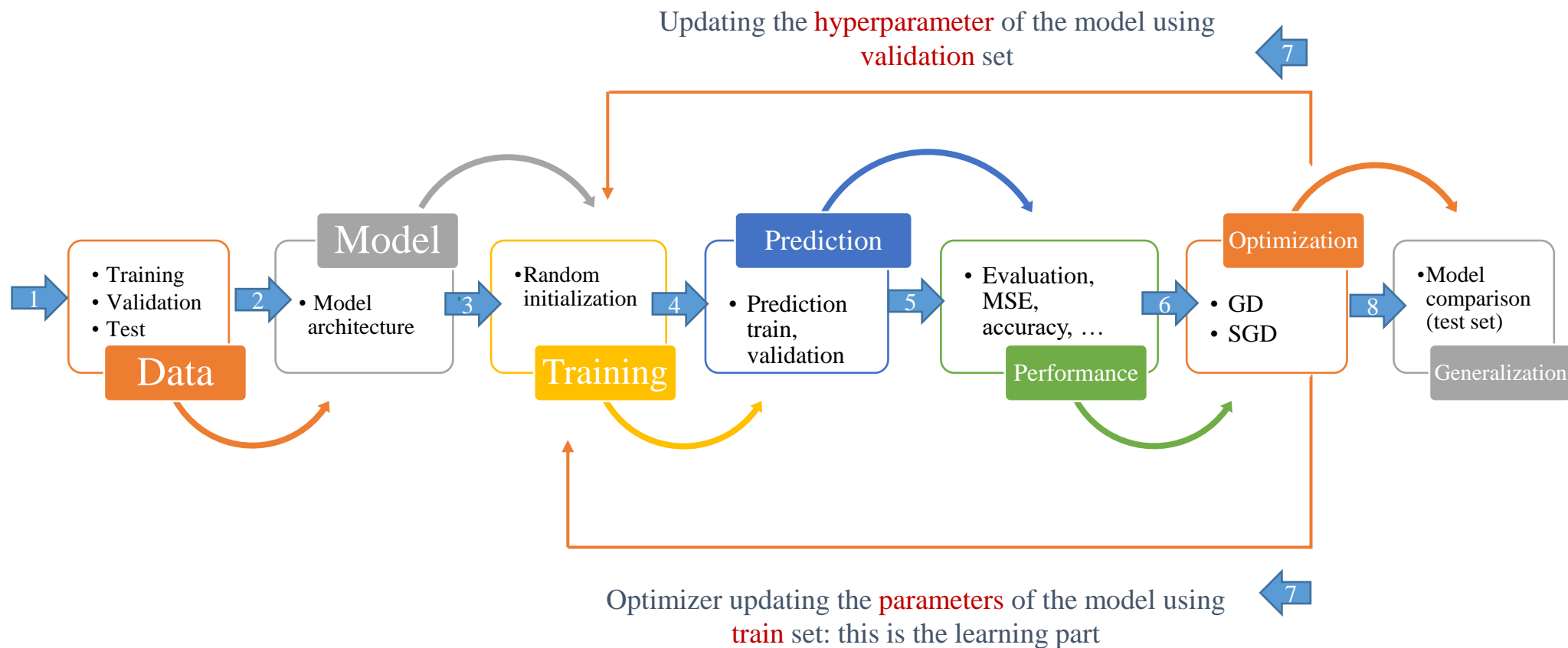
Beyond SGD?

- Loss functions can be difficult to optimize!
- *Visualizing the loss landscape of neural nets*, Li et al, 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, Adadelata, Adagrad, RMSProp!

How do machines actually learn?



Module 3 – Part II

Machine Learning Boosting models

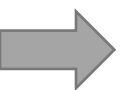
dmlc
XGBoost



CatBoost

 **LightGBM**

The LightGBM logo icon consists of four colored triangles (red, green, blue, and yellow) arranged in a square pattern, with a white stylized 'L' shape in the center.



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**

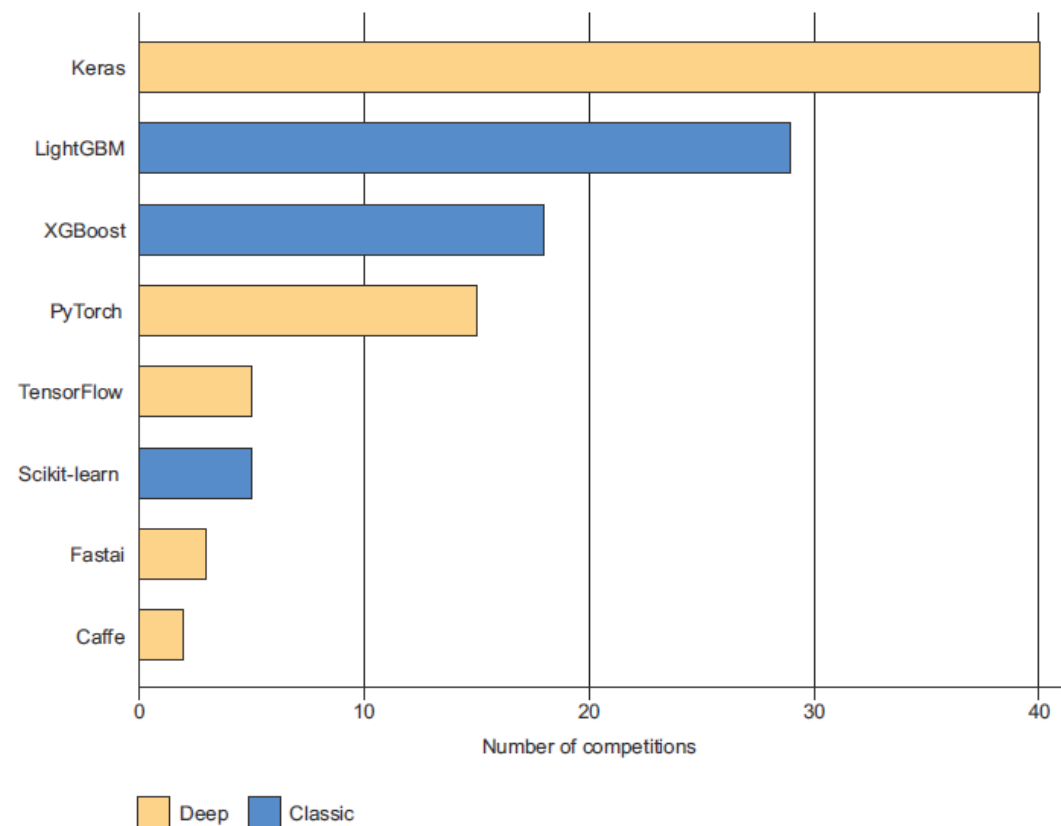
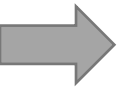
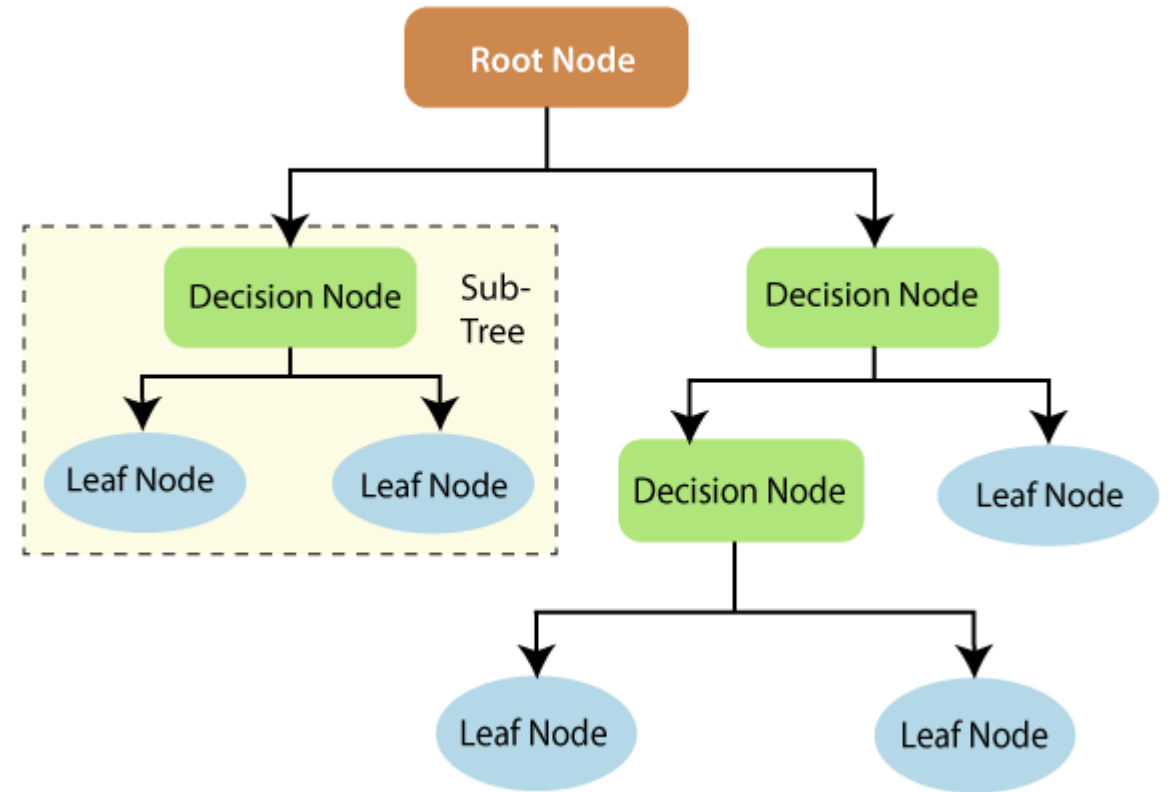


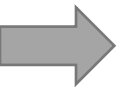
Figure 1.12 Machine learning tools used by top teams on Kaggle



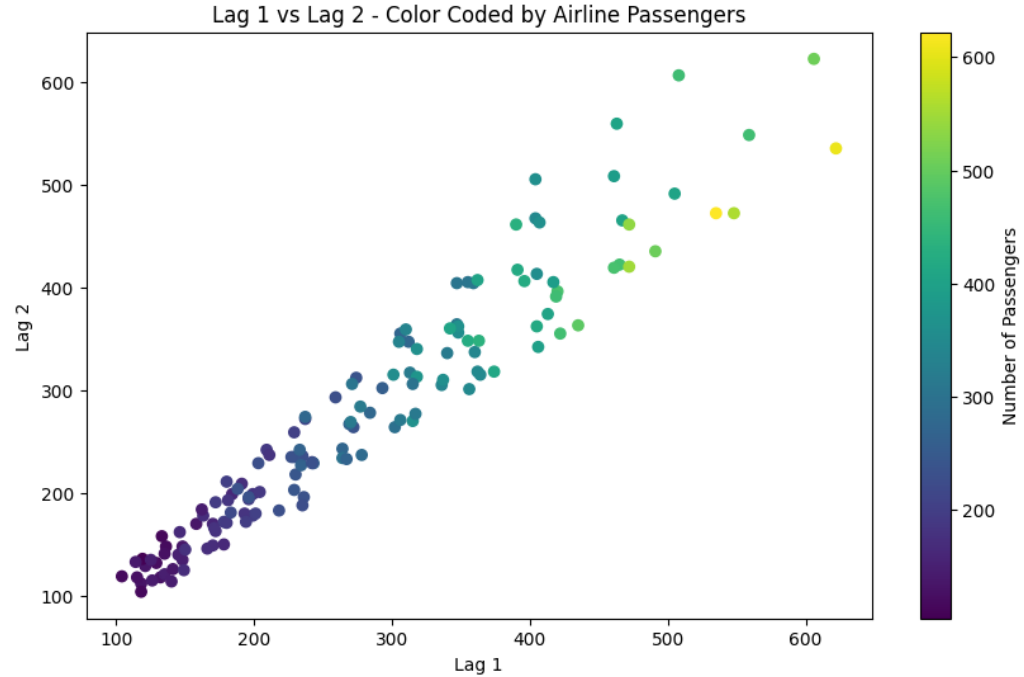
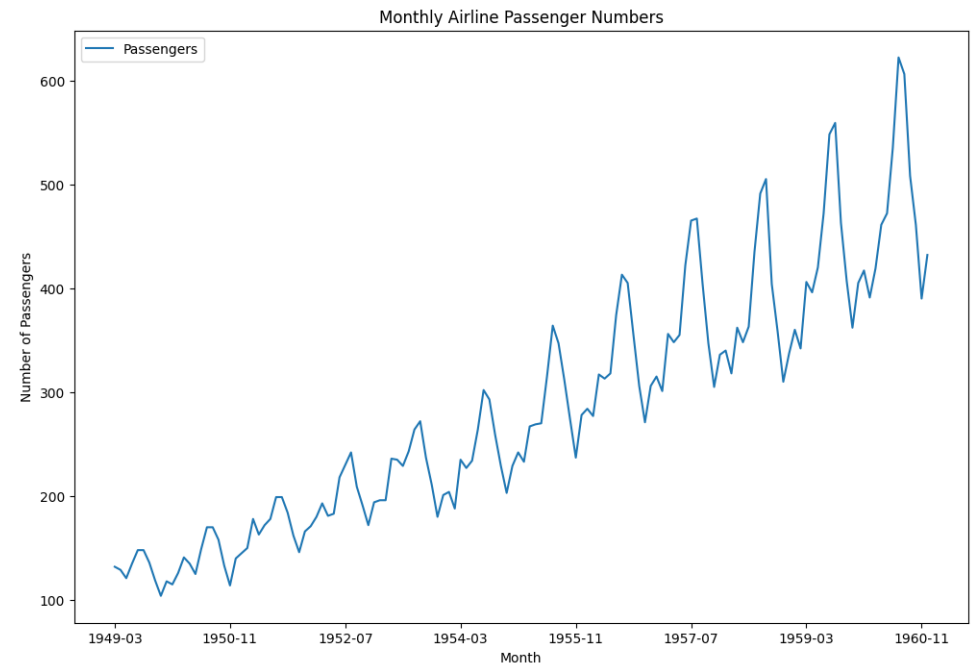
Decision Trees Fundamental questions

- Four fundamental questions to be answered:
 - 1) What **feature** and **cut off** to start with?
 - 2) How to **split** the samples?
 - 3) How to **grow** a tree?
 - 4) How to combine trees?

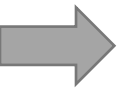




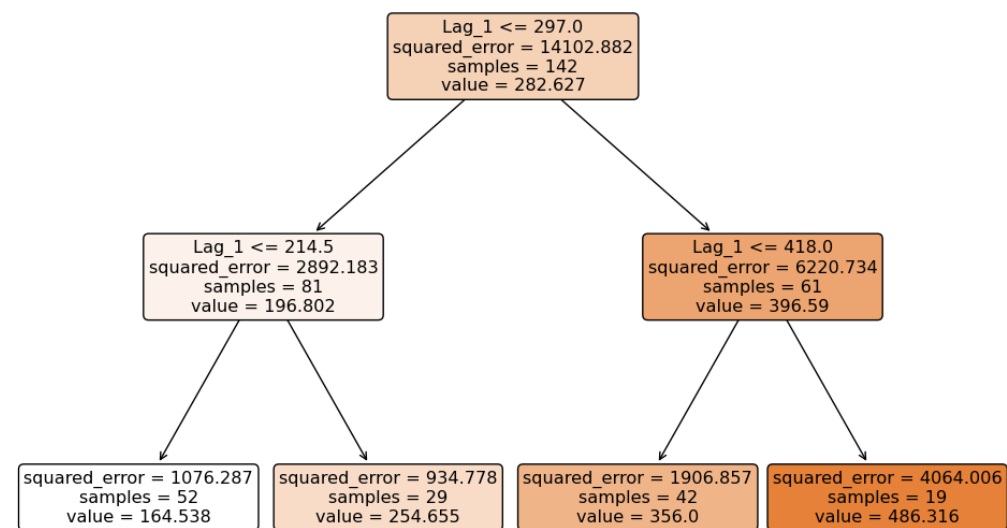
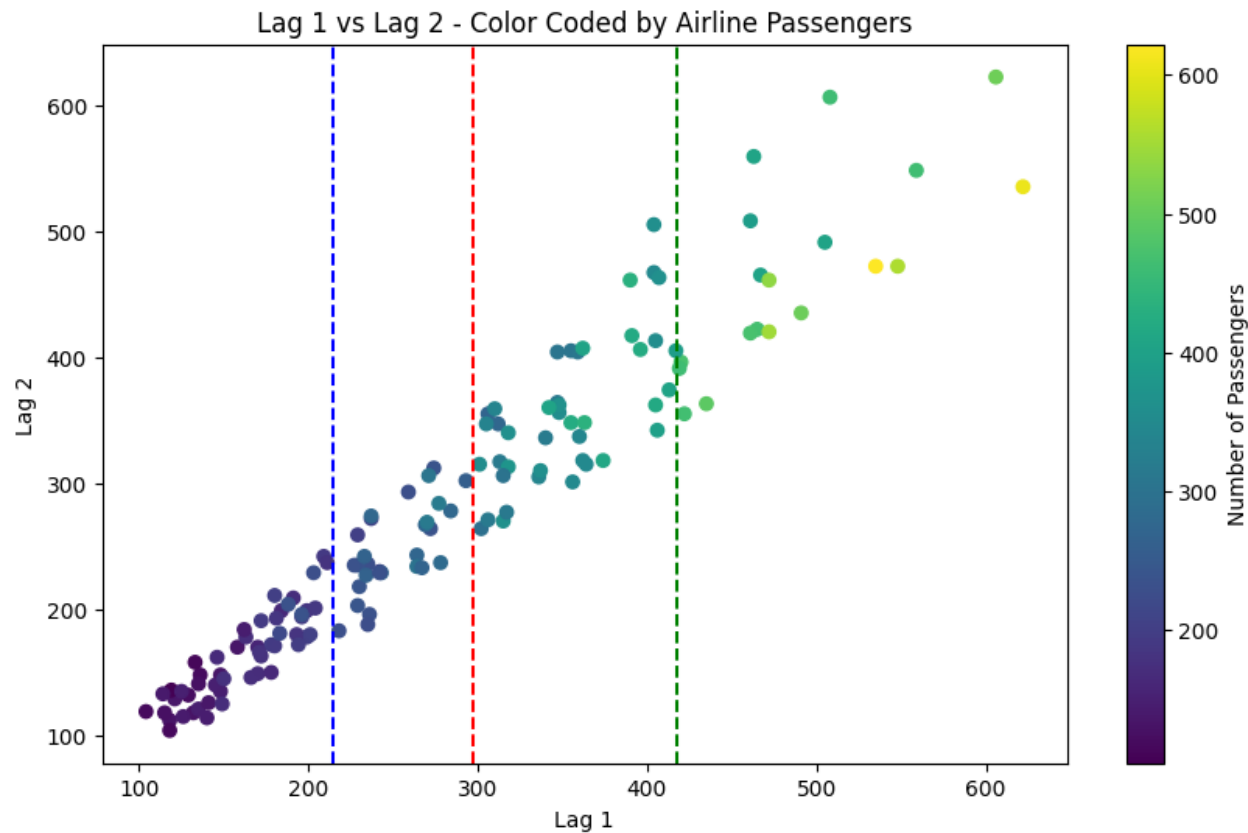
Decision Tree TS regression (Intuition)

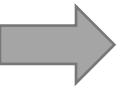


	Passengers	Lag_1	Lag_2
Month			
1949-01	112	NaN	NaN
1949-02	118	112.0	NaN
1949-03	132	118.0	112.0
1949-04	129	132.0	118.0
1949-05	121	129.0	132.0

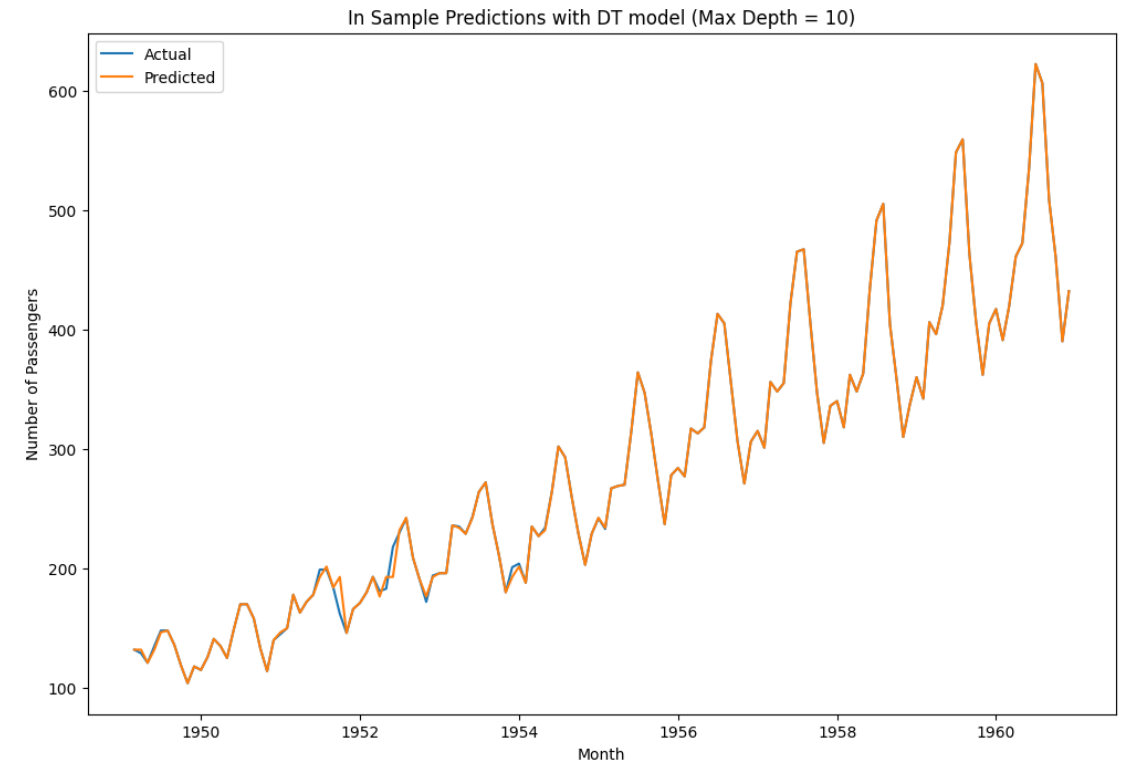
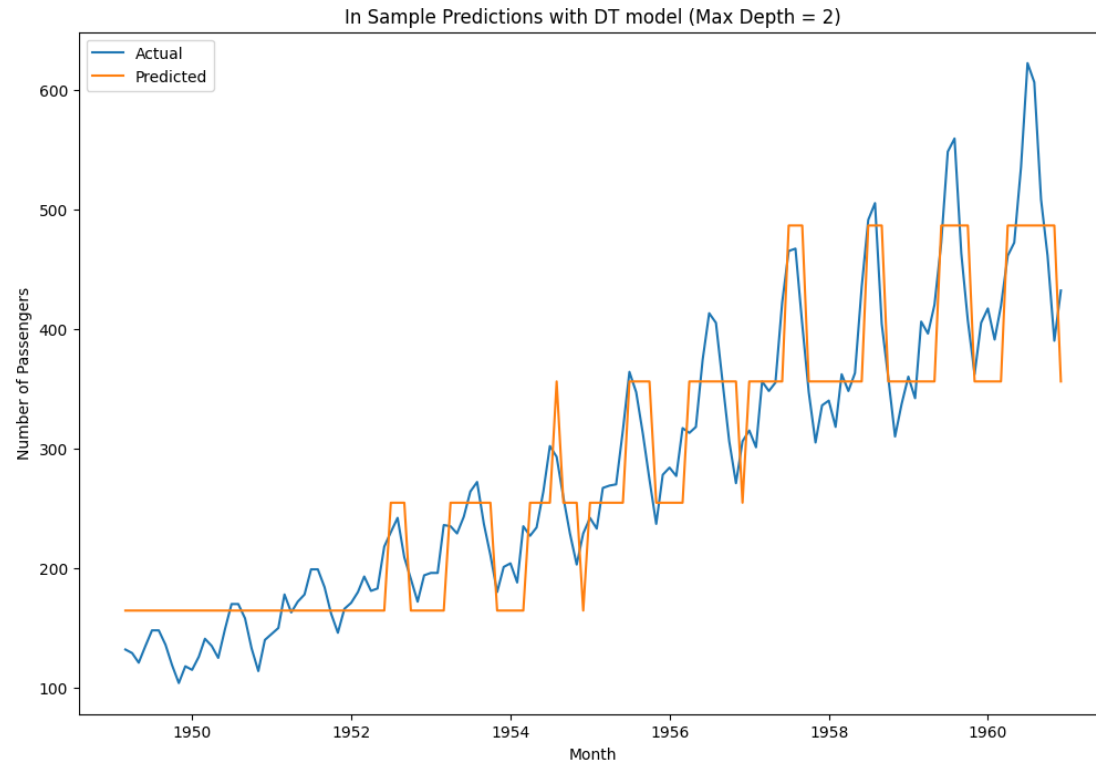


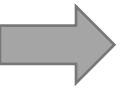
Decision Tree TS regression (Intuition)





Decision Tree TS regression (Intuition)

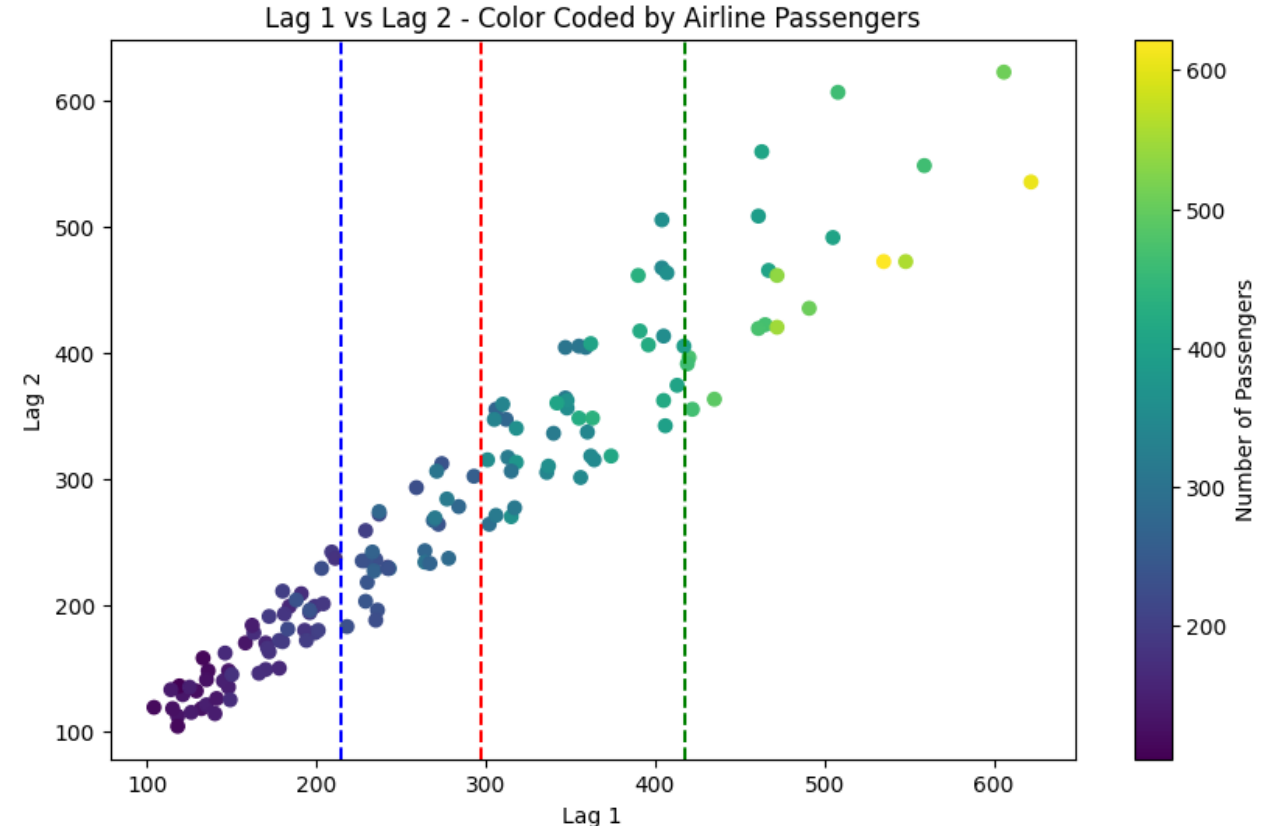




What feature and cut off to start with?

- 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

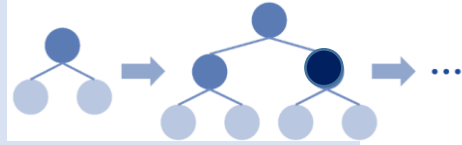
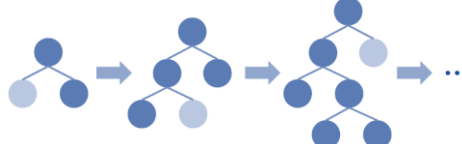

$$\sum_{j=1}^J \sum_{i \in R_j} (y_i - \hat{y}_{R_j})^2$$



→ How to split the samples?

Method	Description
Pre-sorted and histogram based	This method sorts the data and creates histograms of the values before splitting the tree. This allows for faster splits but can result in less accurate trees.
GOSS (Gradient-based One-Side Sampling)	This method uses gradient information as a measure of the weight of a sample for splitting. Keeps instances with large gradients while performing random sampling on instances with small gradients.
Greedy method	This method selects the best split at each step without considering the impact on future splits. This method May result in suboptimal trees

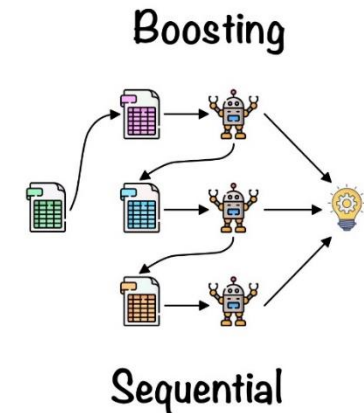
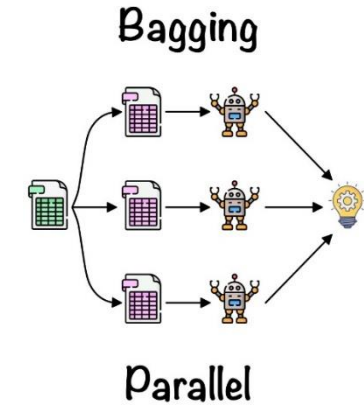
→ How to grow a tree?

Algorithm	Description	
Depth-Wise Level-Wise	This strategy grows the tree one level at a time , ensuring all nodes at the current level are fully expanded before moving on to the next. 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.	

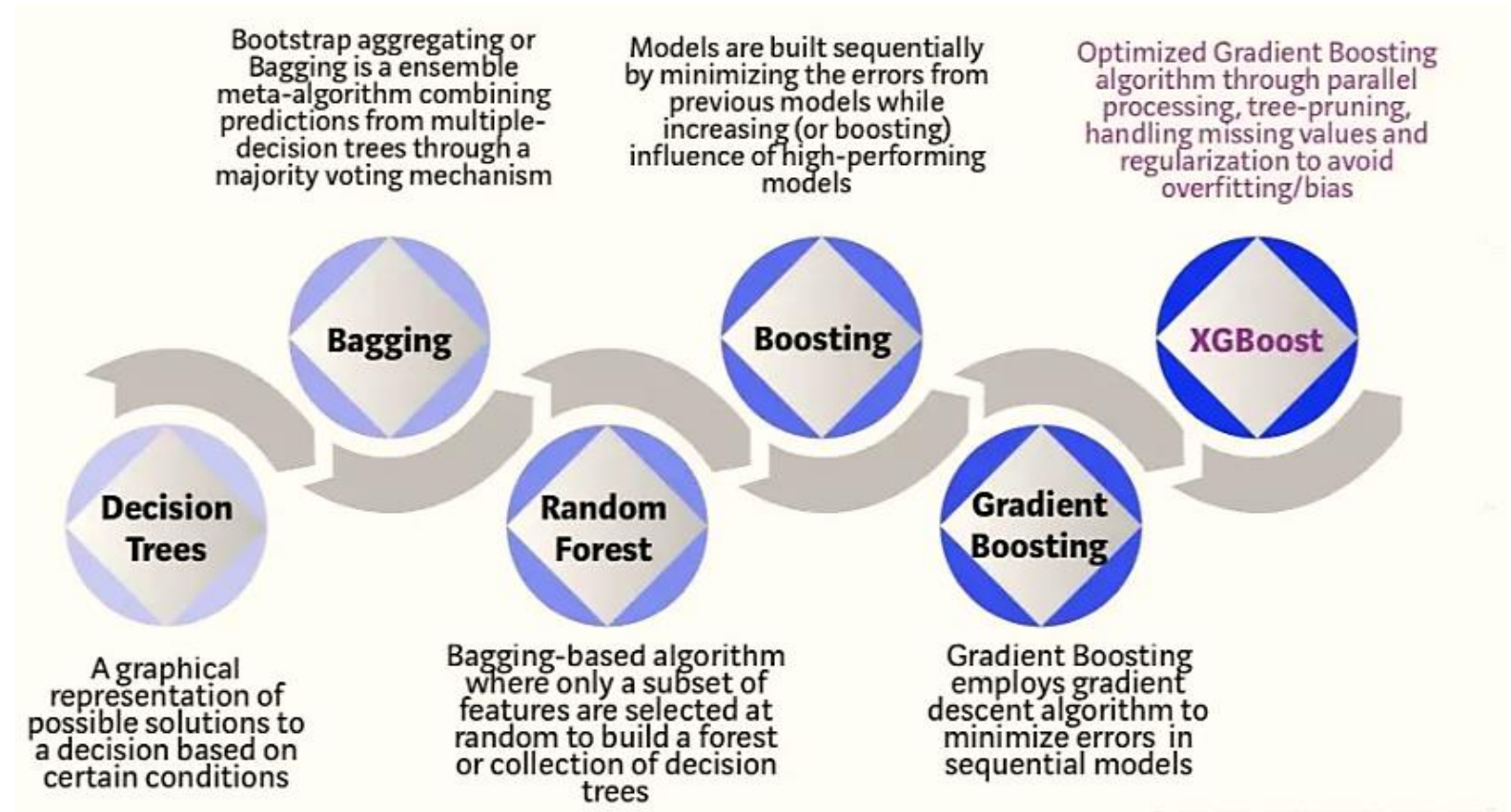
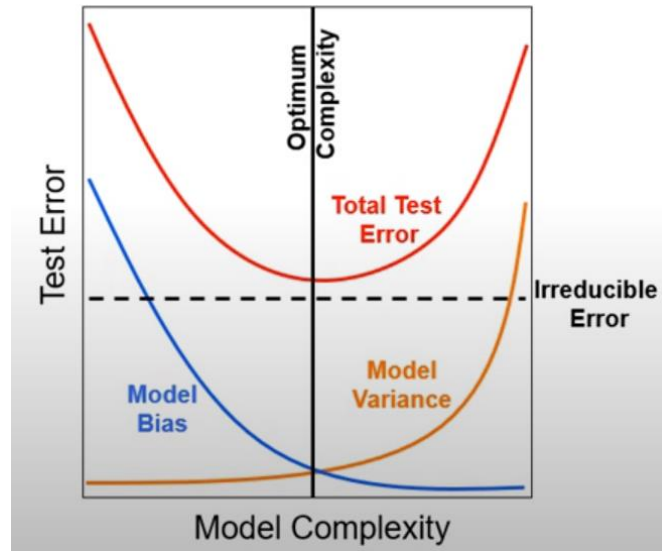
All the methods, repeatedly split the data along the feature with the highest information gain

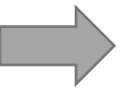
➔ How to combine trees?

- **Bagging** consists of creating many “copies” of the training data (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** 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.



➔ Evolution of XGBoost

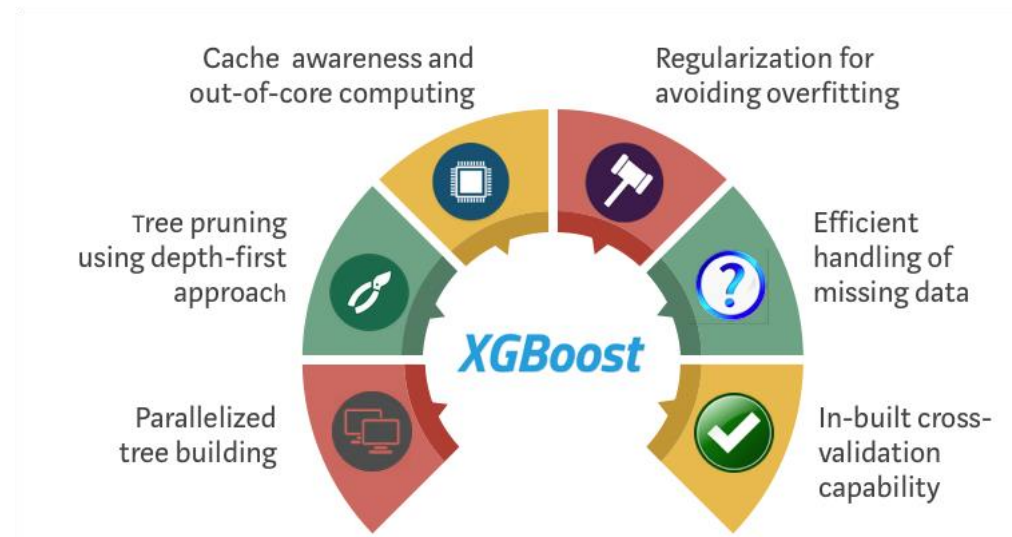


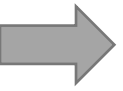


XGBoost: eXtreme Gradient Boosting

- XGBoost is an open-source gradient boosting library developed by **Tianqi Chen** (2014) focused on developing **efficient** and **scalable** machine learning algorithms.
- **Extreme** refers to the fact that the algorithms and methods have been customized to push the limit of what is possible for gradient boosting algorithms.
- XGBoost includes several other features that can improve **model performance**, such as handling missing values, automatic feature selection, and model ensembling.

dmlc
XGBoost





LightGBM (Light Gradient Boosted Machine)

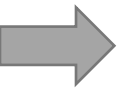
- LightGBM is an open-source gradient boosting library developed by **Microsoft** (2016) that is fast and efficient, making it suitable for **large-scale learning tasks**.
- LightGBM can handle **categorical features**, but requires one-hot encoding, ordinal encoding or other preprocessing
- LightGBM includes several other features that can improve **model performance**, such as handling missing values, automatic feature selection, and model ensembling.



➔ CatBoost (Category Boosting)

- CatBoost is an open-source gradient boosting library developed by **Yandex** (2017) that is specifically designed **to handle categorical data**.
- CatBoost can handle **categorical features directly**, without the need for one-hot encoding or other preprocessing.
- CatBoost includes several other features that can improve **model performance**, such as handling missing values, automatic feature selection, and model ensembling.

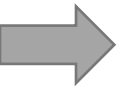




XGBoost vs LightGBM vs CatBoost

	XGBoost	LightGBM	CatBoost
Developer	Tianqi Chen (2014)	Microsoft (2016)	Yandex (2017)
Base Model	Decision Trees	Decision Trees	Decision Trees
Tree growing algorithm	Depth-wise tree growth Leaf-wise is also available	Leaf-wise tree growth	Symmetric tree growth
Parallel training	Single GPU	Multiple GPUs	Multiple GPUs
Handling categorical features	Encoding required (one-hot, ordinal, target, label, ...)	Automated encoding using categorical feature binning	No encoding required
Splitting method	Pre-sorted and histogram based	GOSS and histogram based	Greedy method



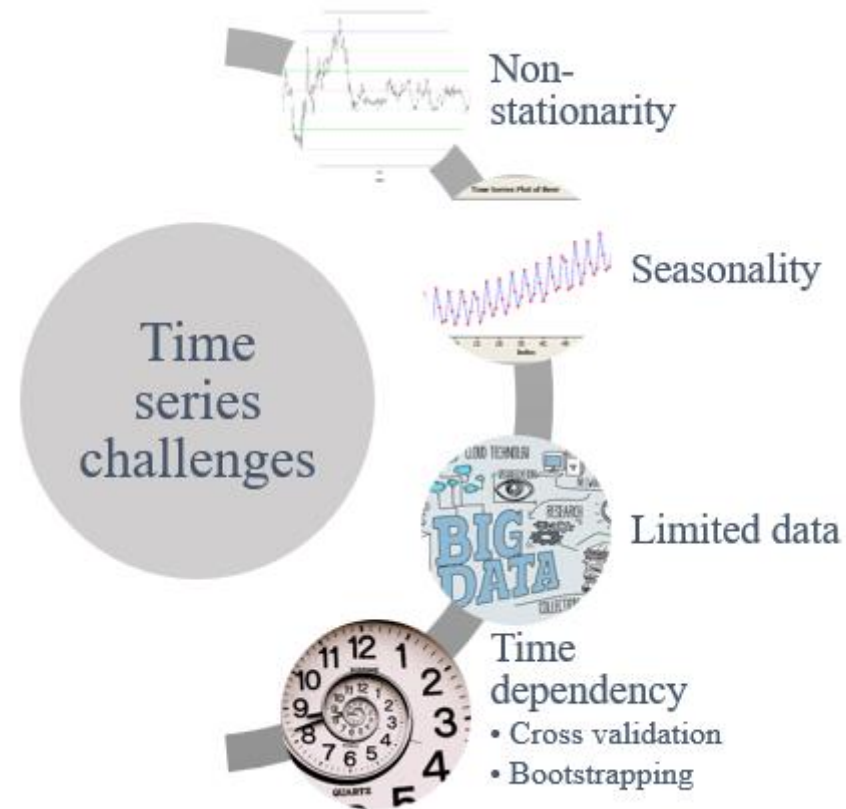


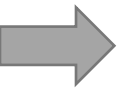
Cost functions and minimization methods

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)

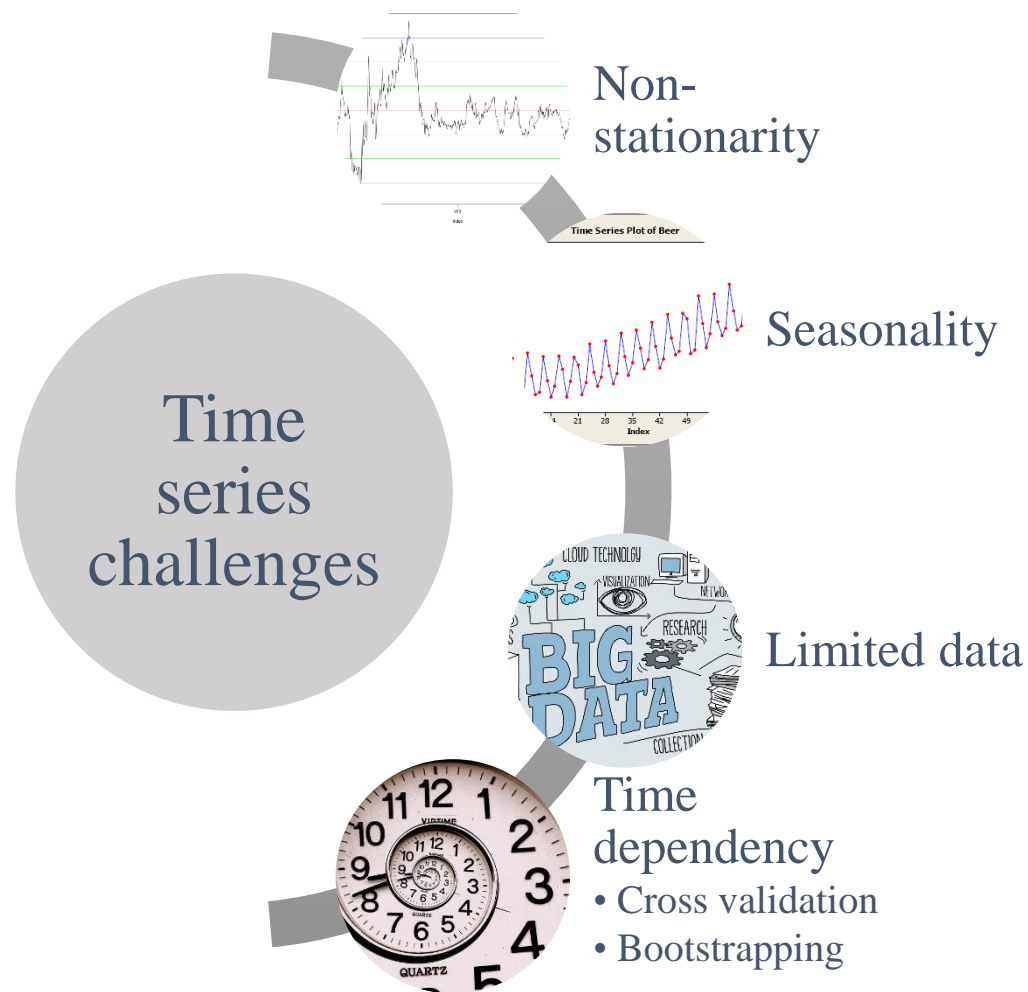
Module 3 – Part III

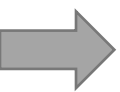
Challenges in Time Series Machine Learning





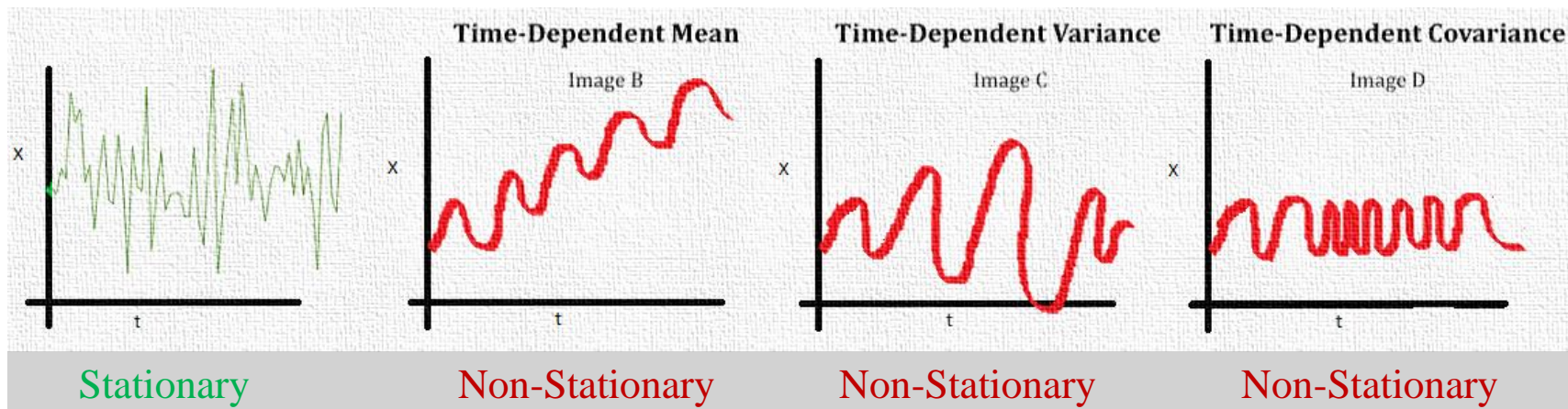
Challenges in Time Series Machine Learning





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**



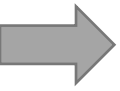
- Data with **trend** and **seasonality** are **NOT** stationary!

→ 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

Iteration 1	Test	Train	Train	Train	Train
Iteration 2	Train	Test	Train	Train	Train
Iteration 3	Train	Train	Test	Train	Train
Iteration 4	Train	Train	Train	Test	Train
Iteration 5	Train	Train	Train	Train	Test



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.

Iteration 1	Test	Train	Train	Train	Train
Iteration 2	Train	Test	Train	Train	Train
Iteration 3	Train	Train	Test	Train	Train
Iteration 4	Train	Train	Train	Test	Train
Iteration 5	Train	Train	Train	Train	Test

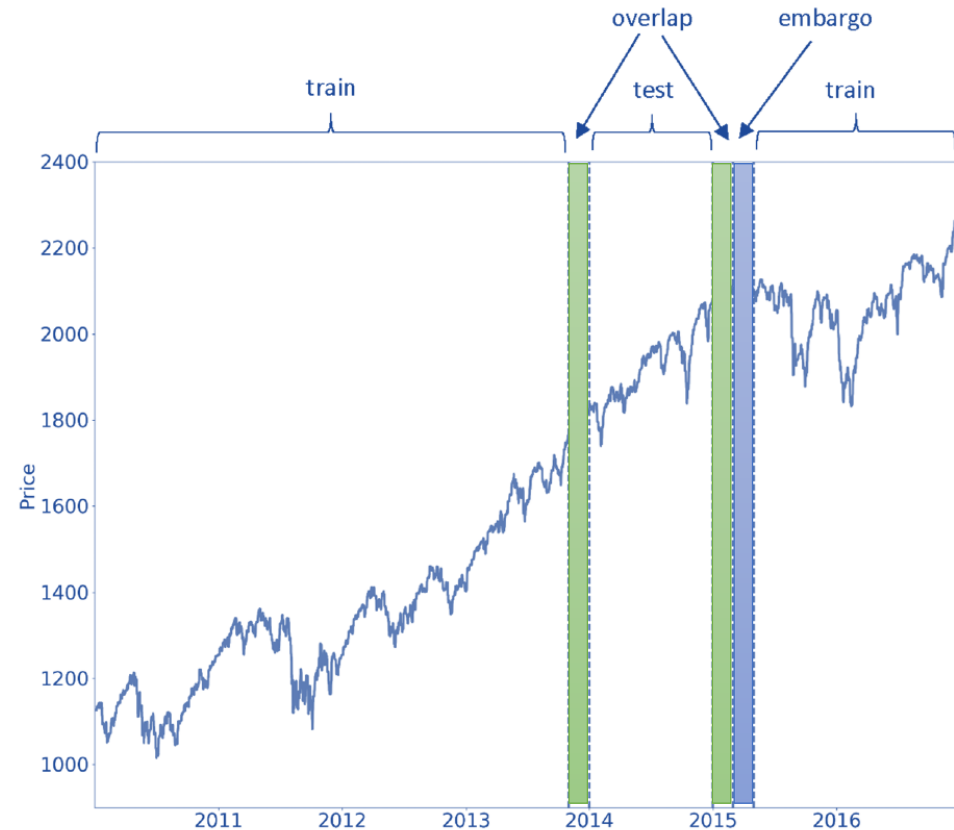
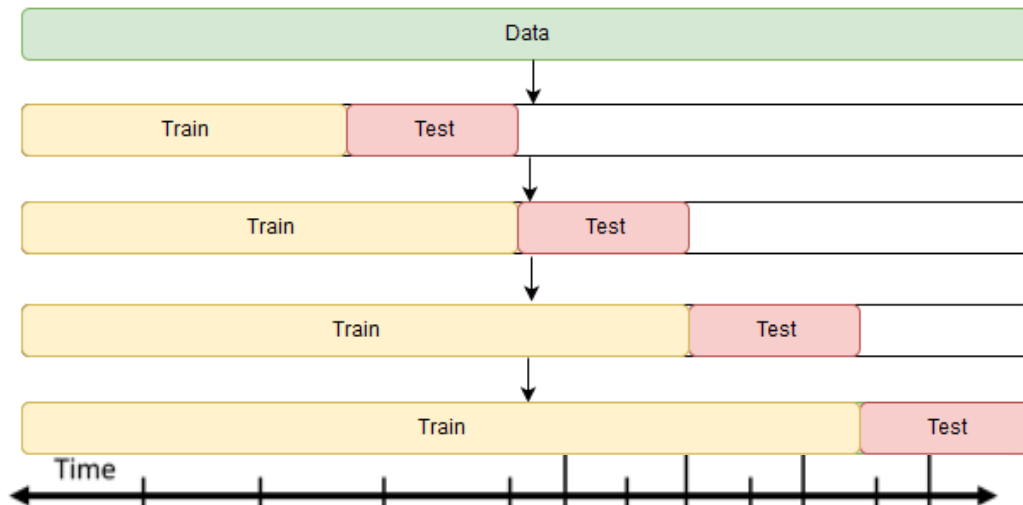


FIGURE 7.3 Embargo of post-test train observations

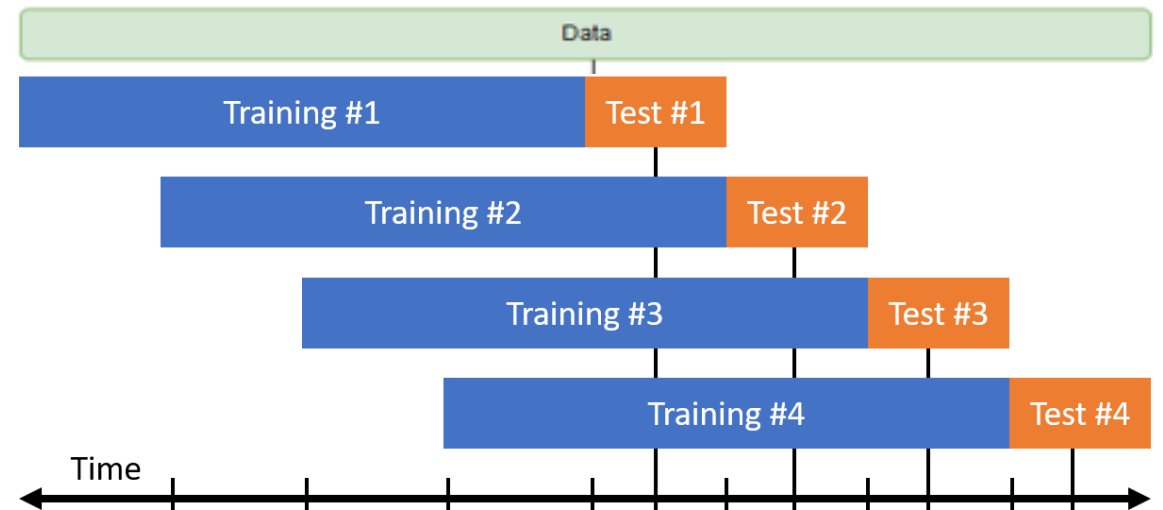


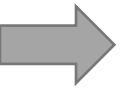
→ Walk Forward Cross Validation

Walk forward cross validation
Expanding windows



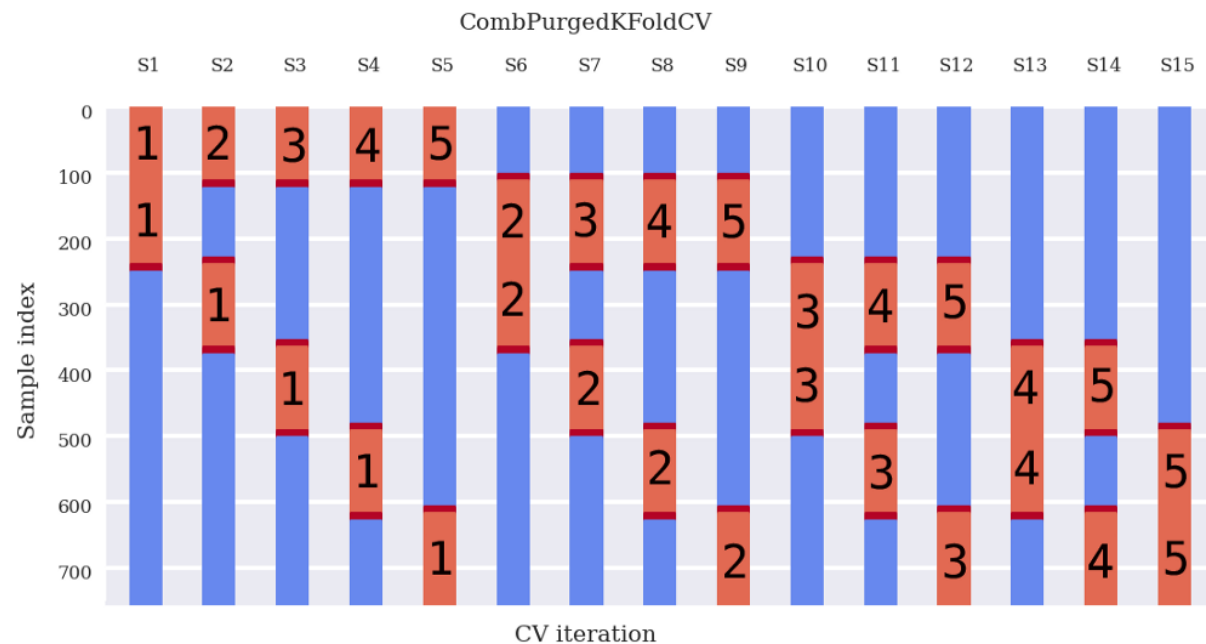
Walk forward cross validation
Rolling windows





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.

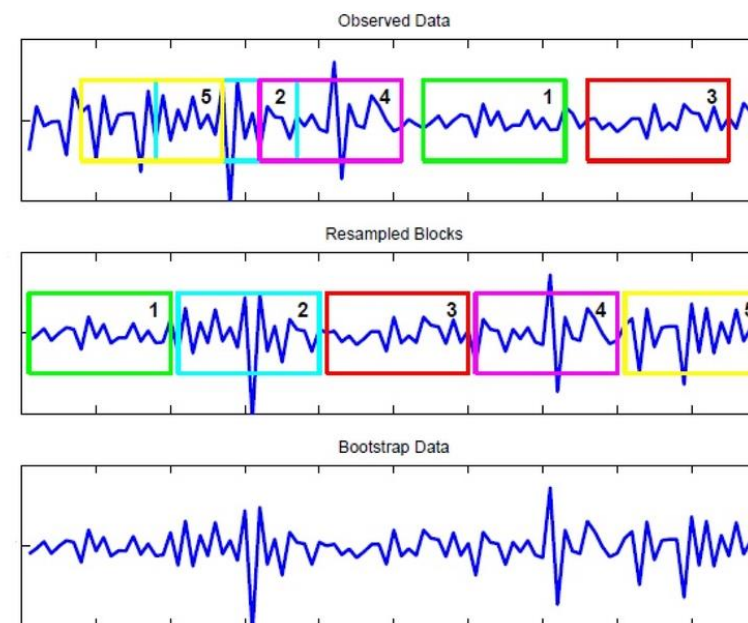
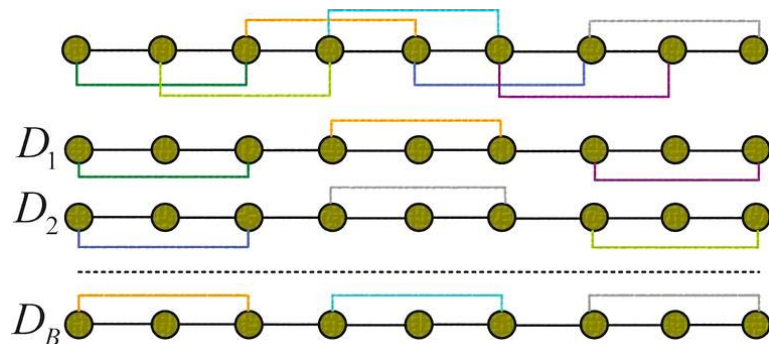


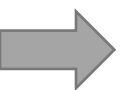
→ Time Series Bootstrapping

- 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)

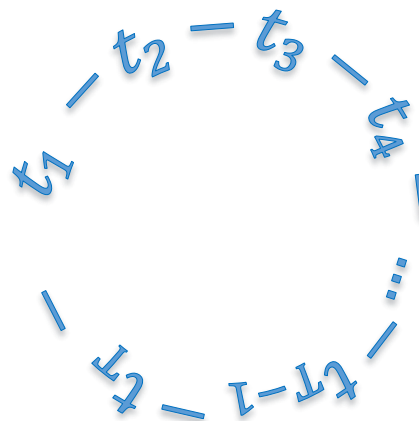
- Moving Block Bootstrap, samples **overlapping fixed size** blocks of m consecutive observations.
- Blocks starts at indices $1, \dots, T-m+1$





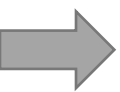
Circular Block Bootstrap (CBB)

- 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)

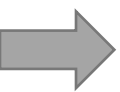
- In SB, the **block size is no longer fixed**.
- Chooses an **average block size of m** rather than an exact block size.
- Popularity of SB stems from difficulty in determining optimal m
- Once applied to stationary data, the resampled **pseudo time series** by SB are **stationary**. This is not the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



Preparing data for machine learning

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

Features (X)				Target (y)
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}

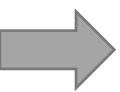


Single-Output (one-step ahead)

Input Features				Single-Output
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}

➔ Single-Output (multiple-step ahead)

Input Features				Single-Output
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}



Multi-Output

Input Features				Multi-Output		
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}



➔ 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

