Class 4- Machine Learning concepts
Part I

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Motivation

Machine learning fundamental concepts:

- Inference and prediction
- Parameters and hyperparameters
- Parametric vs nonparametric ML models
- Evaluation metrics
- Bias-Variance tradeoff
- Resampling methods

Part I
The Model

The Model

$$y = f(X) + \epsilon = f(X_1, X_2 \; \dots, X_m) + \epsilon$$

y : response, dependent variables, output, Target

X: predictors, independent variables, input, Features

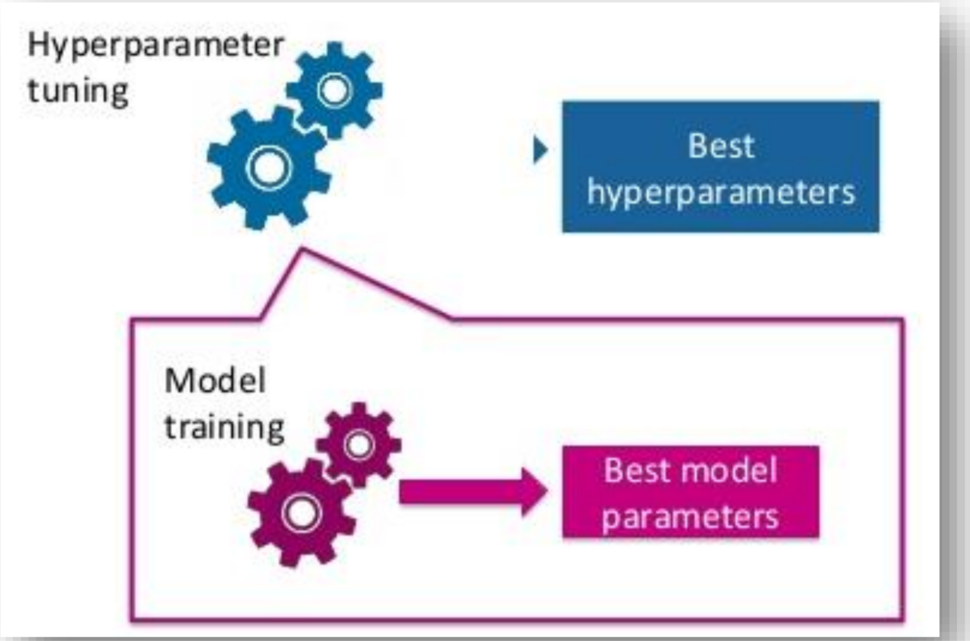
✓ It is all about estimating f by $\hat{f}$ for two purposes:

1) Inference (interpretable ML)
2) Prediction

Parameters and Hyperparameters

$$y = f(X) + \epsilon = f(X_1, X_2\ \ldots, X_m) + \epsilon$$

Model parameters are estimated from data automatically and model hyperparameters are set manually (prior to training the model) and are used in processes to help estimate model parameters.



Example?

Parametric Vs. Nonparametric models

$$y = f(X) + \epsilon$$

The true relationship, $f(X)$ is unknown and the goal is to see which ML algorithm is better at approximating it. An algorithm learns/estimates $f(X)$ from training data.

$f(X)$ is assumed. Examples: Linear regression, GLM, logistic regression, simple Neural networks, ….

$f(X)$ is NOT assumed. Free to learn any functional form. Examples:

KNN, CART, Random forest, SVM, ANN, …

	Pros	Cons
Parametric algorithms	**Simpler** Easier to understand and to interpret **Faster** Very fast to fit your data **Less data** Require "few" data to yield good perf.	**Limited complexity** Because of the specified form, parametric algorithms are more suited for "simple" problems where you can guess the structure in the data
Nonparametric algorithms	**Flexibility** Can fit a large number of functional forms, which doesn't need to be assumed **Performance** Performance will likely be higher than parametric algorithms as soon as data structures get complex	**Slower** Computations will be significantly longer **More data** Require large amount of data to learn **Overfitting** We'll see in a bit what this is, but it affects model performance

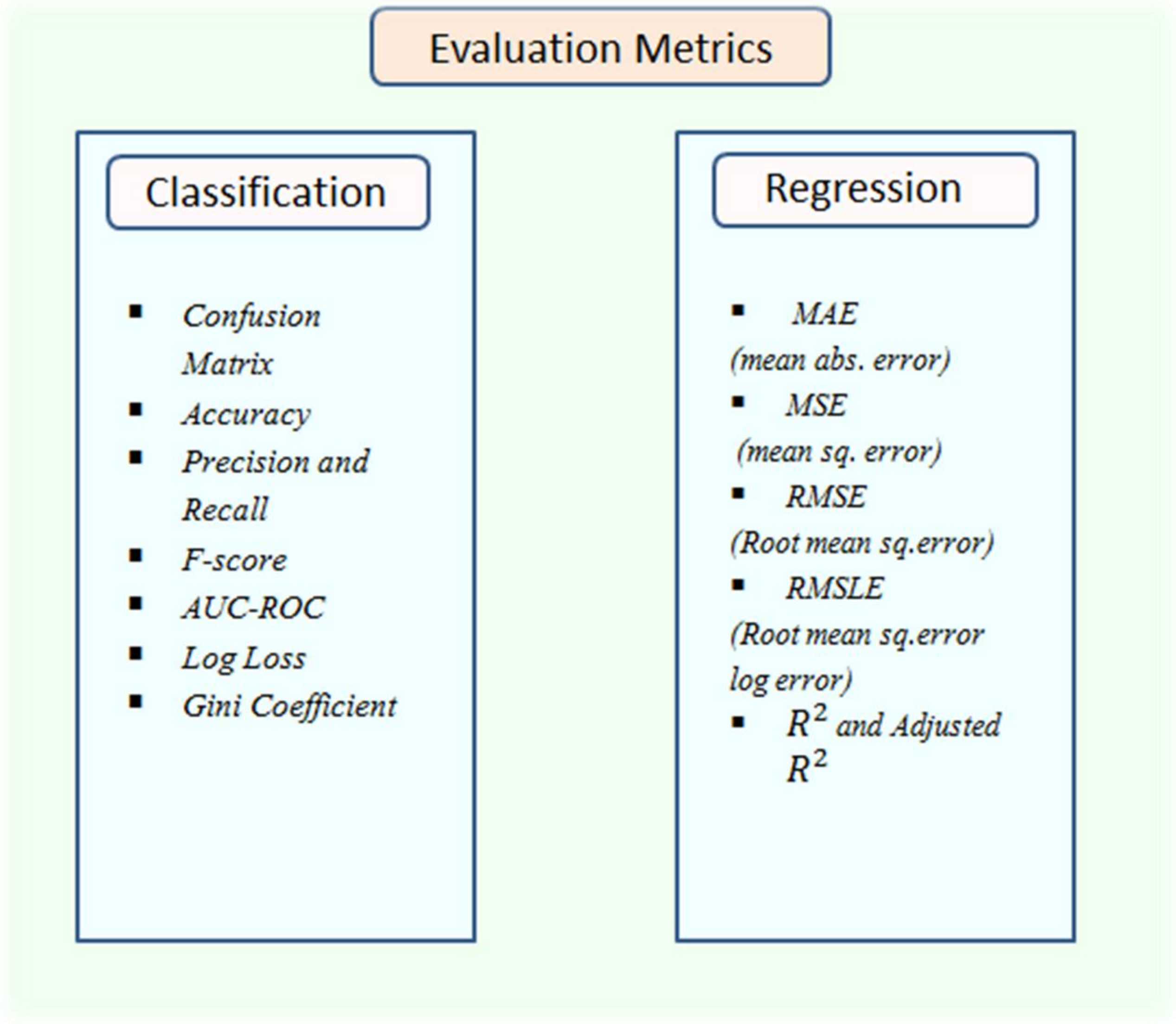
Part II
Evaluation Metrics

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



Part III

Bias-Variance Tradeoff

ML relative to statistical learning algorithms

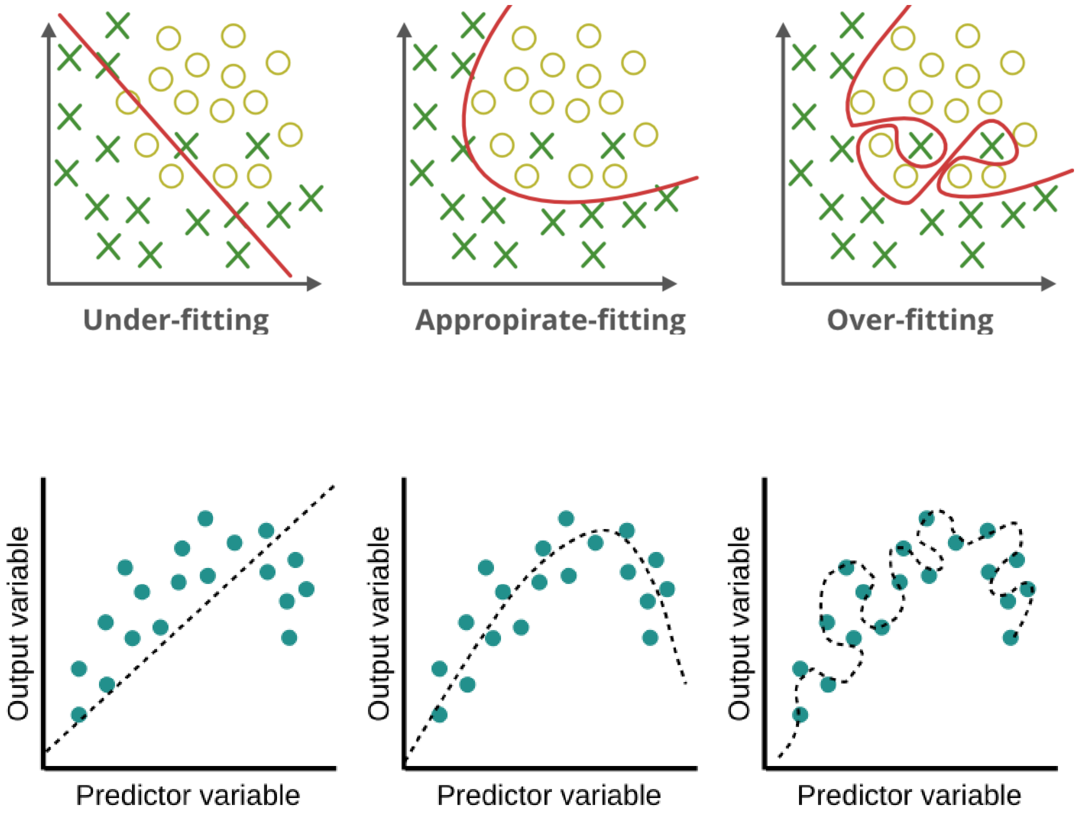
- Advantages
  - Ability to uncover complex interactions
  - Process massive amount of data quickly
  - Capture non-linear relationships
  - Predict structural changes between features and target

- Disadvantages
  - Can produce overly complex models
  - Difficult to interpret
  - Sensitive to noise
  - Can overfit!

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 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!



MSE decomposition

The bias-variance tradeoff is one of the core concepts in supervised learning.

Assume that the data is generated by a simple model!

$$y_i = f(\mathbf{x}_i) + \epsilon_i, \quad \mathbb{E}[\boldsymbol{\epsilon}] = 0, \quad \mathbb{V}[\boldsymbol{\epsilon}] = \sigma^2$$

The estimated model yields

$$\hat{y}_i = \hat{f}(X_i)$$

Let us decompose the mean squared error (MSE):

$$\begin{aligned}\mathbb{E}[\hat{\epsilon}^2] &= \mathbb{E}[(y - \hat{f}(\mathbf{x}))^2] = \mathbb{E}[(f(\mathbf{x}) + \epsilon - \hat{f}(\mathbf{x}))^2] \\ &= \underbrace{\mathbb{E}[(f(\mathbf{x}) - \hat{f}(\mathbf{x}))^2]}_{\text{total quadratic error}} + \underbrace{\mathbb{E}[\epsilon^2]}_{\text{irreducible error}}\end{aligned} \quad \ldots\ldots \quad = \underbrace{\mathbb{V}[\hat{f}(\mathbf{x})]}_{\text{variance of model}} + \underbrace{\mathbb{E}[(f(\mathbf{x}) - \hat{f}(\mathbf{x}))]^2}_{\text{squared bias}} + \sigma^2$$

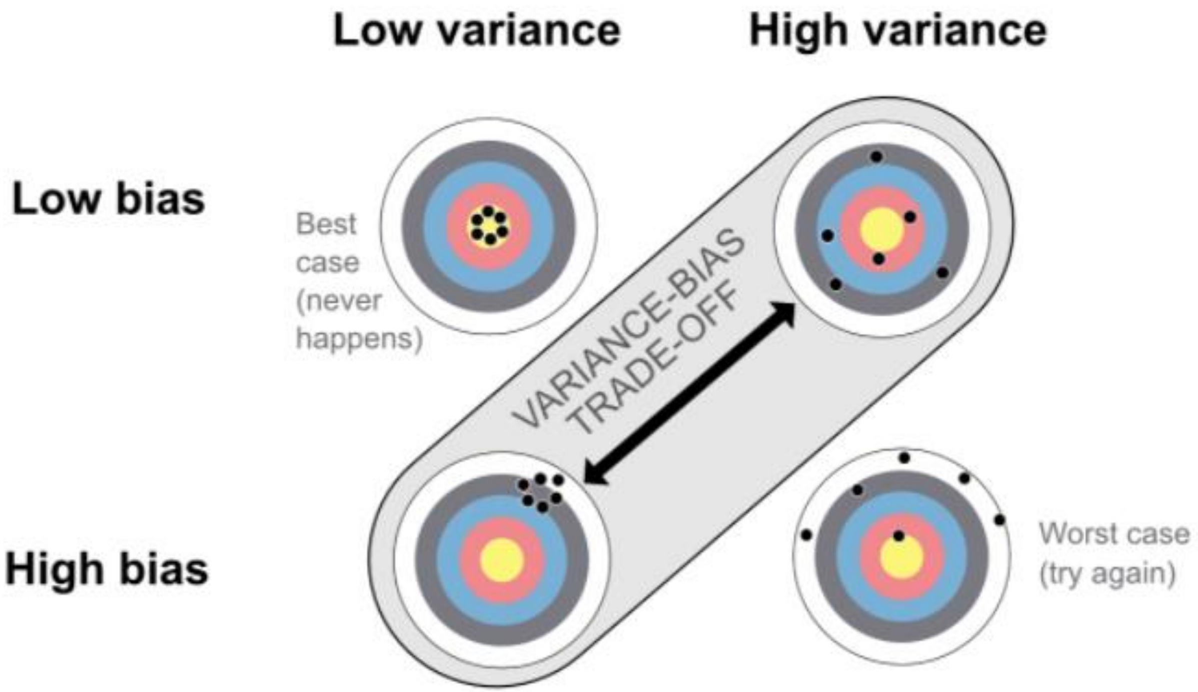
MSE decomposition

$$MSE = model\ variance + model\ bias + irreducible\ error$$

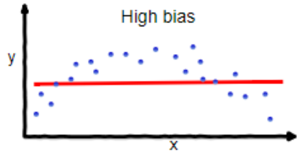
1) Model variance is the variance if we had estimated the model with a different **training set**
2) Model bias is the error due to using an approximate model (model is too simple)
3) Irreducible error is due to missing variables and limited samples. Can't be fixed with modeling

- The goal is to minimize the sum of model variance and model bias.
- This is known as the bias-variance tradeoff because reducing one often leads to increasing the other.
- Choosing the flexibility (complexity) of $\hat{f}(X)$, will amount to bias-variance tradeoff.

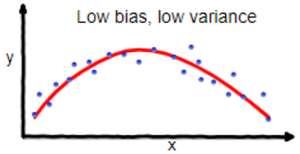
Representations of the bias-variance tradeoff



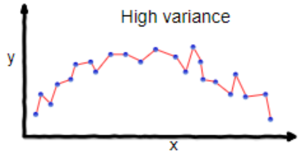
Other representations of the bias-variance tradeoff



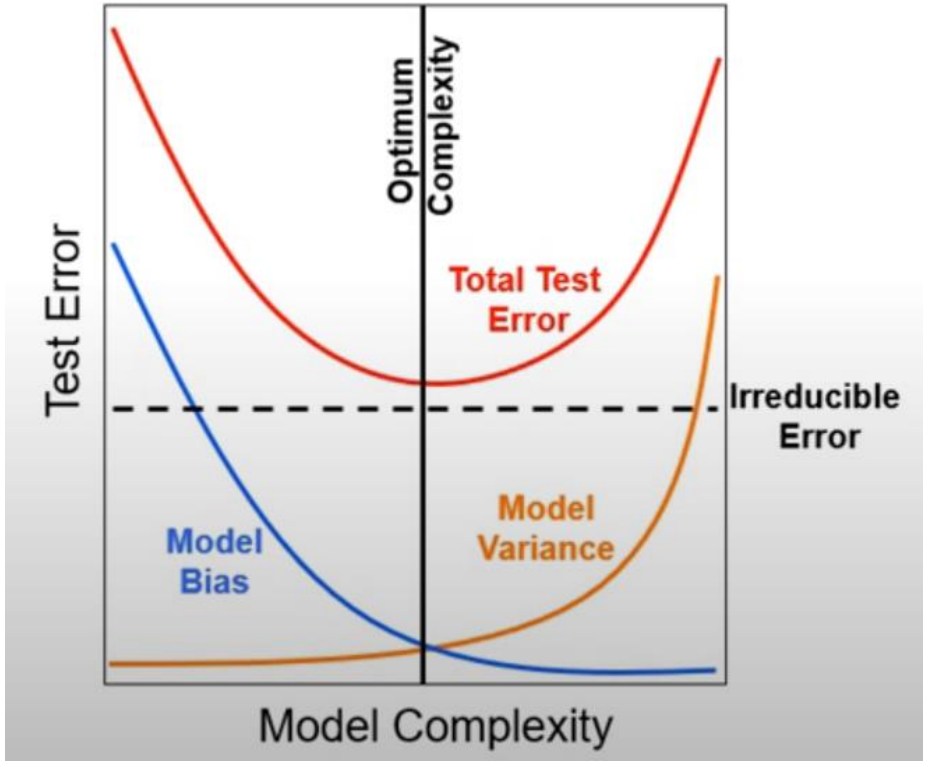
underfitting



Good balance



overfitting

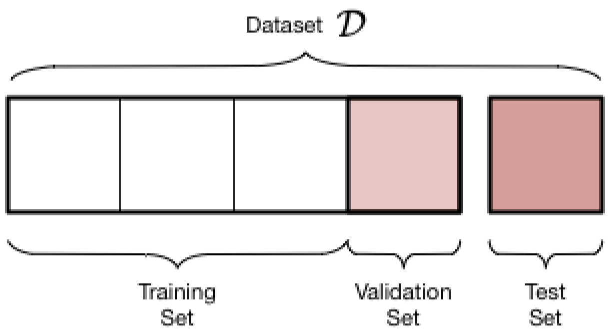


Part IV
Resampling methods

Partitioning of the dataset

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

1) Training set used to train the model
2) Validation set for validating and tuning the model
3) Test set (holdout set) for testing the model's ability to predict well on new data



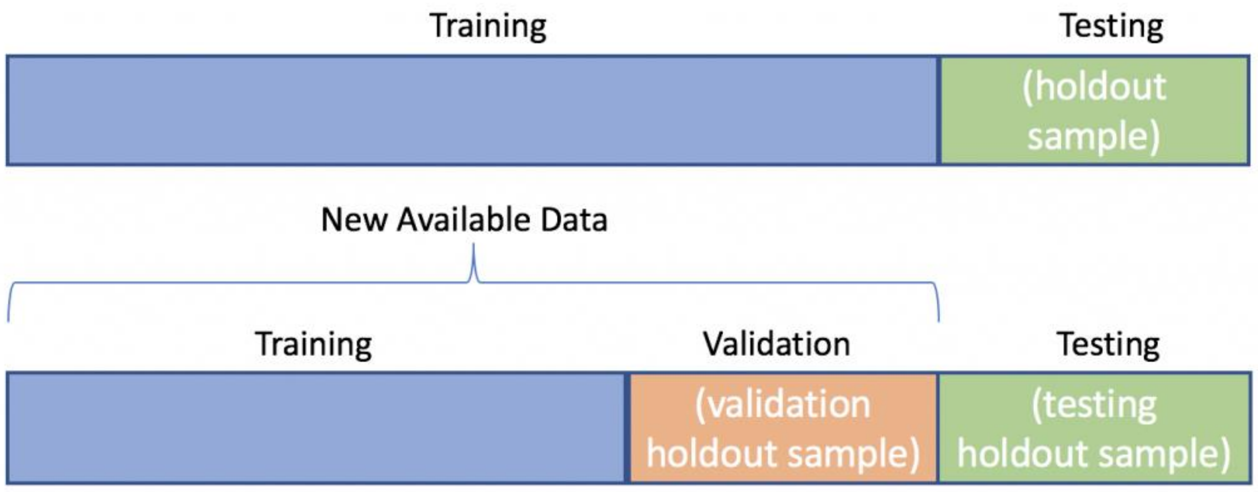
To be <u>valid</u> and <u>useful</u>, any supervised machine learning model must generalize well beyond the training data.

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

Resampling methods

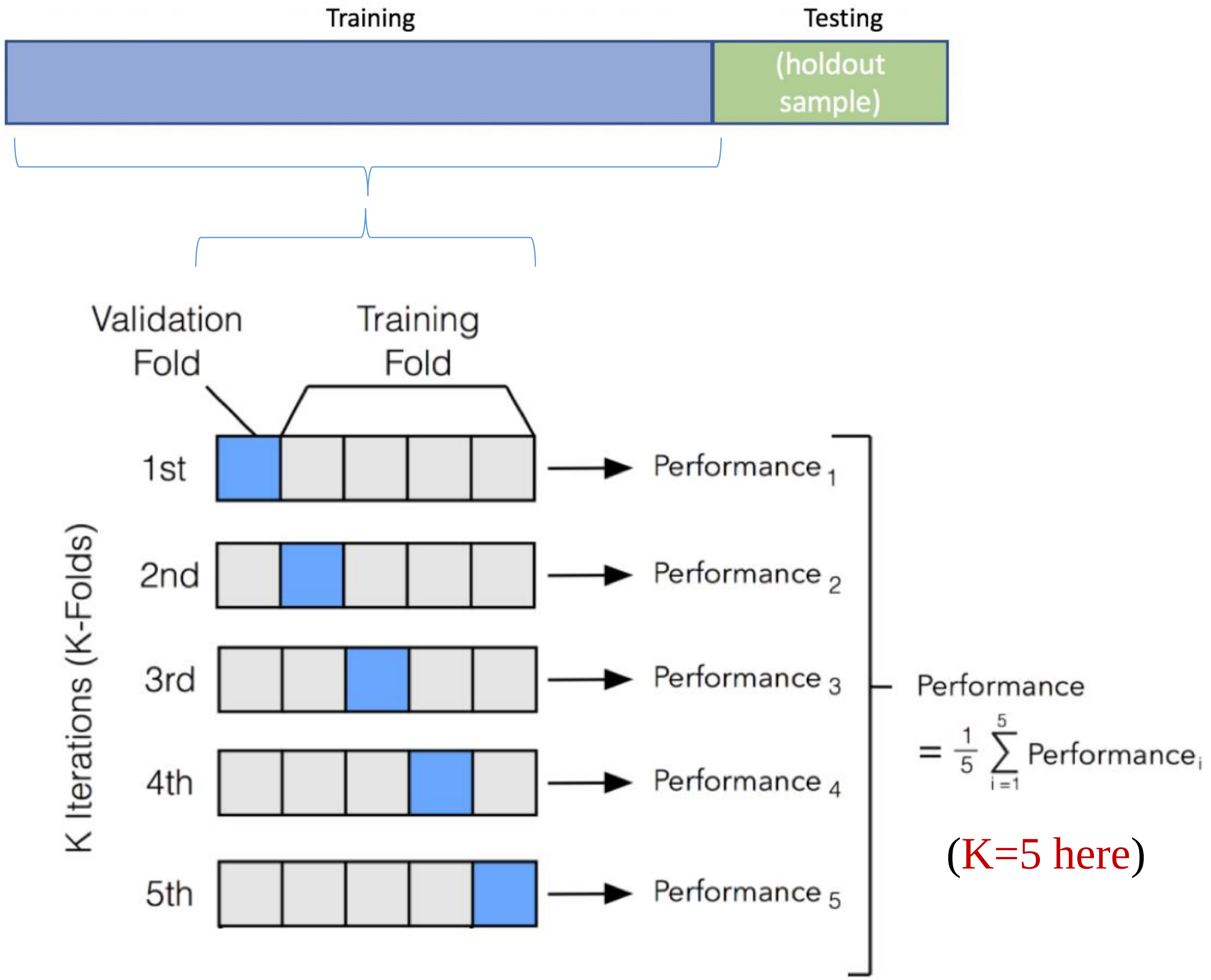
Cross validation

- Sometimes we cannot afford to split the data in three because the algo may not learn anything from a small training dataset!
- When we don't have a decent validation set to tune the hyperparameters on, we can use cross validation technique.
- Solution: combining the training and validation sets!
- The goal is to obtain additional information about the fitted model! For example, to provide estimates of test set prediction errors.



K-fold Cross Validation

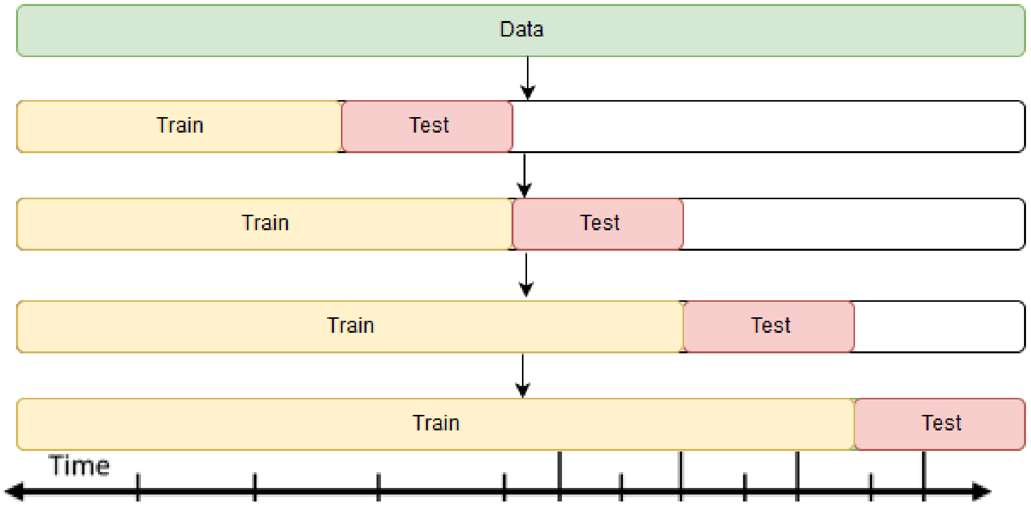
- Divide the training data into K roughly equal-sized non-overlapping groups. Leave out k^{th} part and fit the model to the other $k - 1$ parts. Finally, obtain predictions for the left-out k^{th} part.
- Performance can be any of the evaluation metrics for regression or classification models. For example, MSE, accuracy, …
- This is done in turn for each part $k = 1,2, \dots . K$, and then the results are combined.
- Leave one out CV (LOOCV): if there is only 1 observation in each fold.



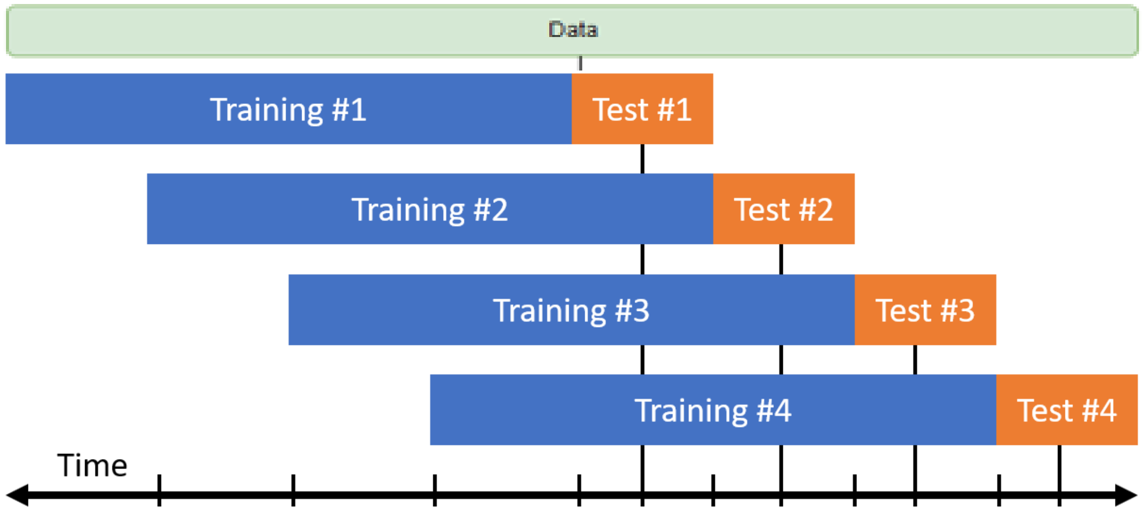
(K=5 here)

Time Series Cross Validation

Walk forward cross validation
Expanding windows



Walk forward cross validation
Rolling windows



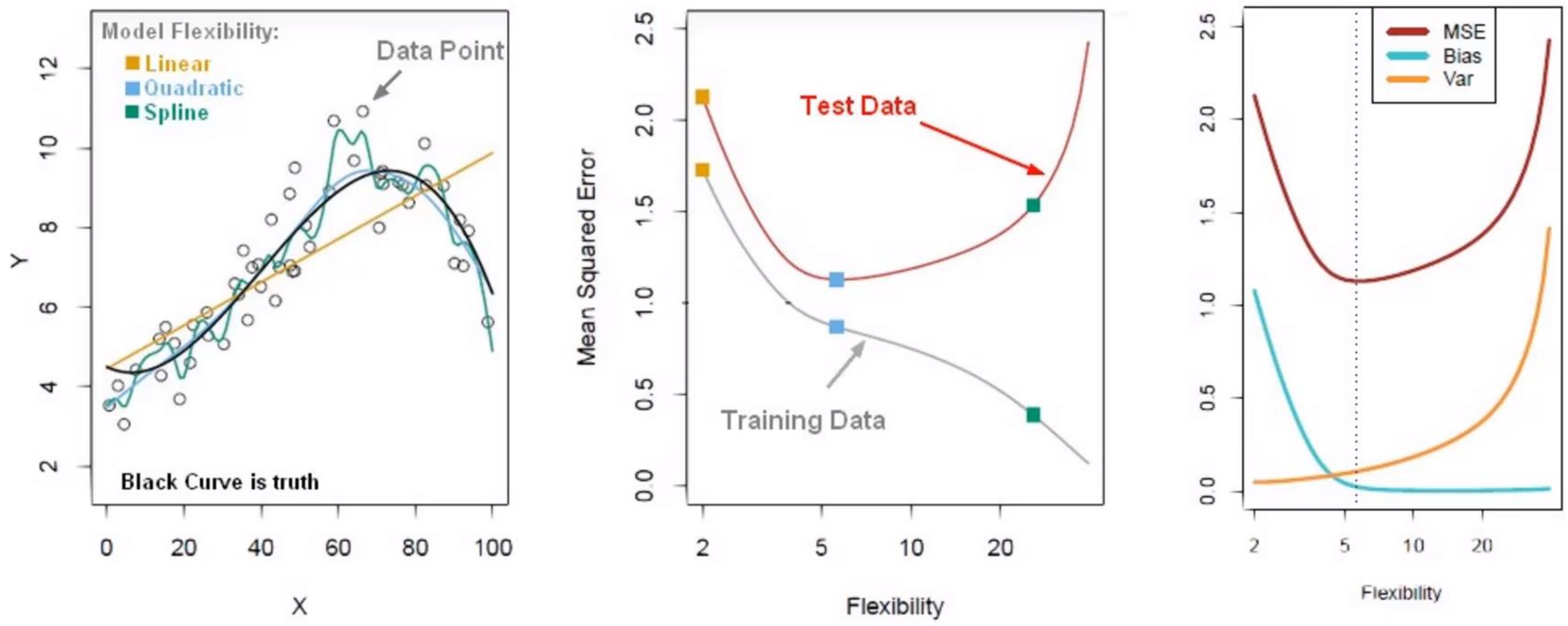
In time series data, we cannot shuffle the data! We also need to avoid look ahead bias!

Mitigate overfitting

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

1) Complexity reduction (regularization)

2) Cross validation (estimate the test error)



Question of the day!