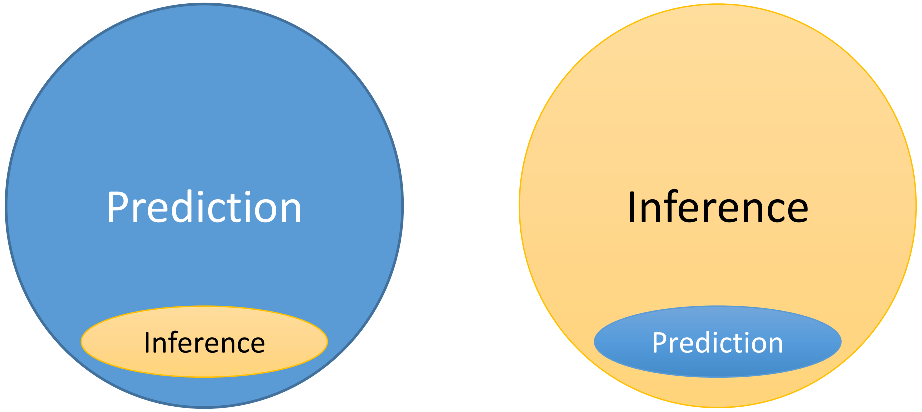
Class 4- Machine Learning concepts
Part I

Motivation

Machine learning fundamental concepts:

- Inference and prediction
- Part I: The Model
  - Parameters and hyperparameters
  - Parametric vs nonparametric ML models
- Part II: Evaluation metrics
- Part III: Bias-Variance tradeoff
- Part IV: Resampling methods and scaling the features
- Part V: How do machines learn?
- Part VI: Solvers/learners (GD, SGD, Adagrad, Adam, …)



Part I
The Model

The Model

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

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:

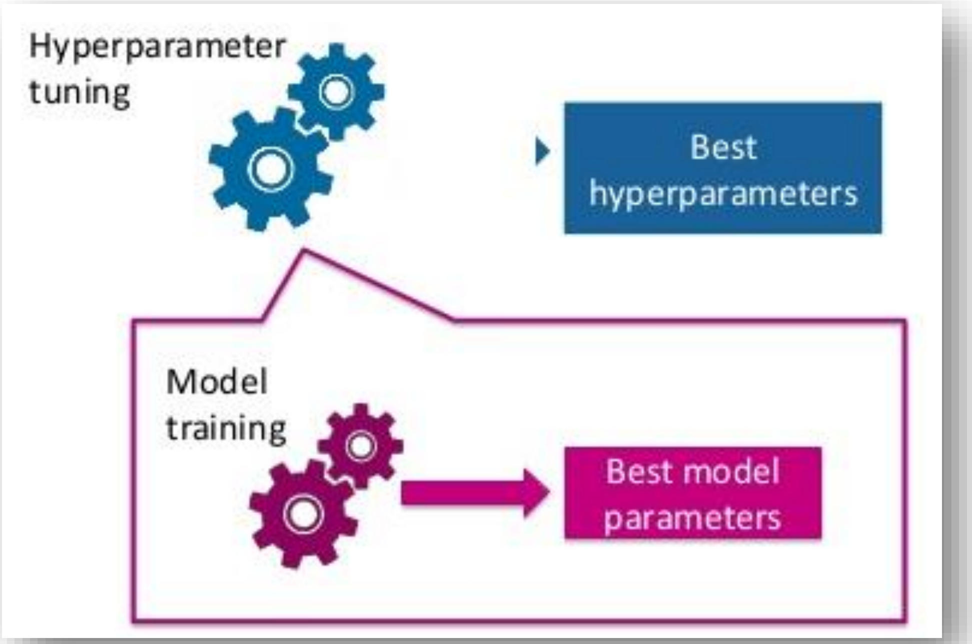
1) Inference (interpretable ML)

2) Prediction

Parameters and Hyperparameters

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

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

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

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, ….

	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

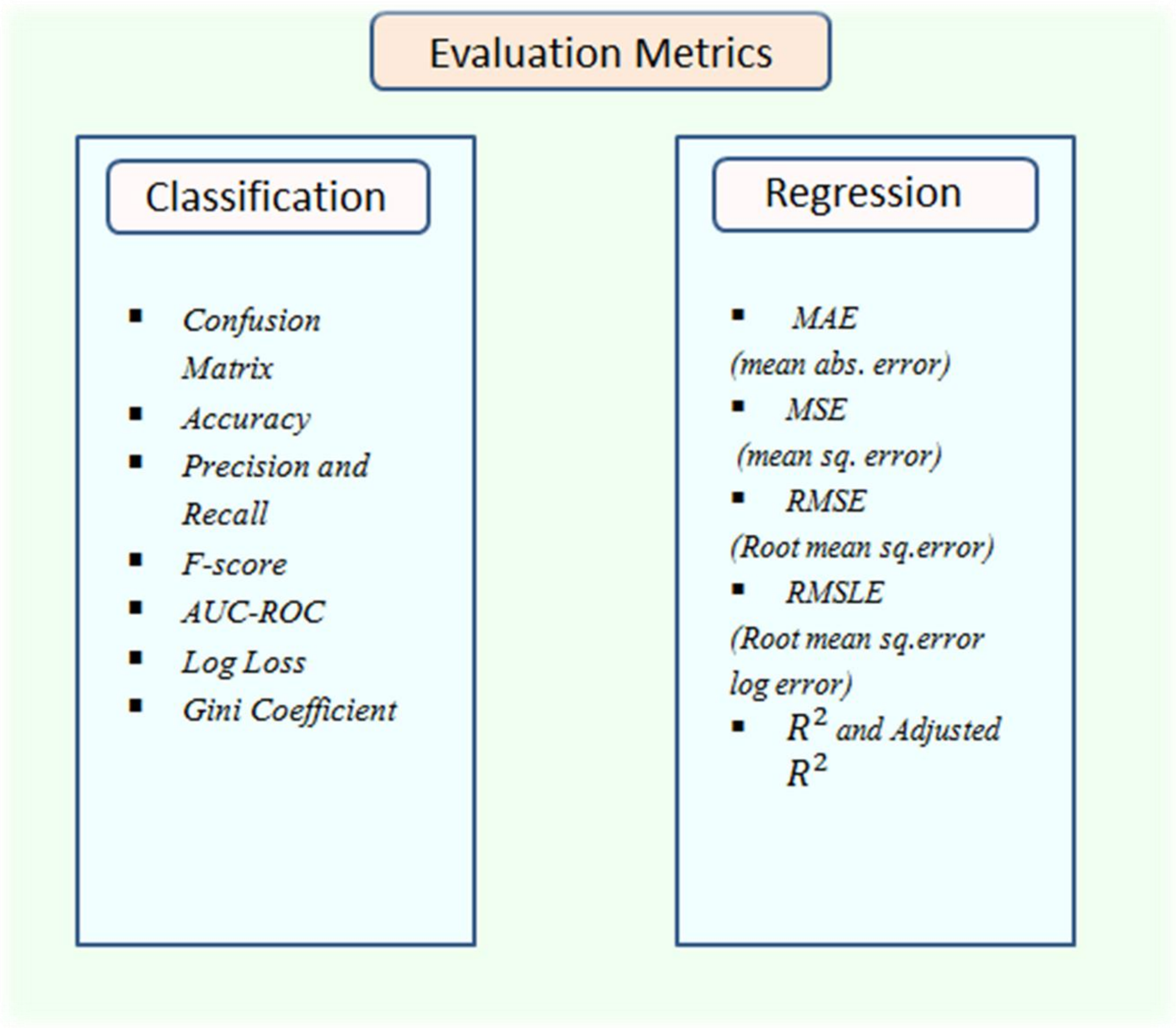
Part II
Evaluation Metrics

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

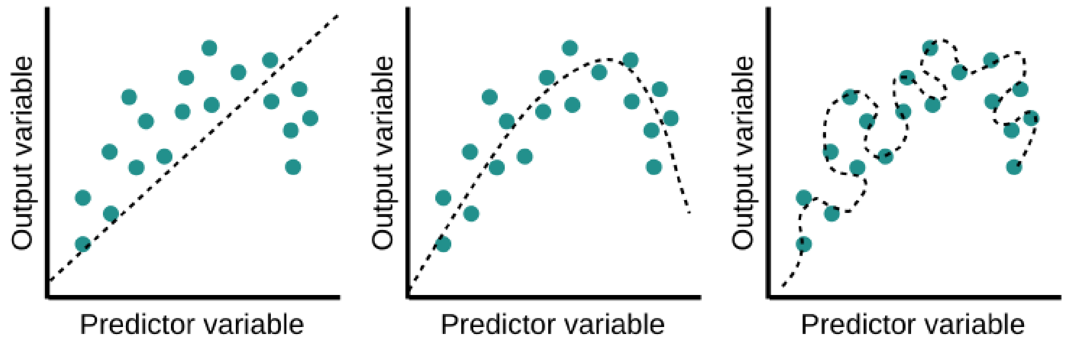
- Disadvantages
  - Can produce overly complex models
  - Difficult to interpret
  - Sensitive to noise
  - Can overfit!

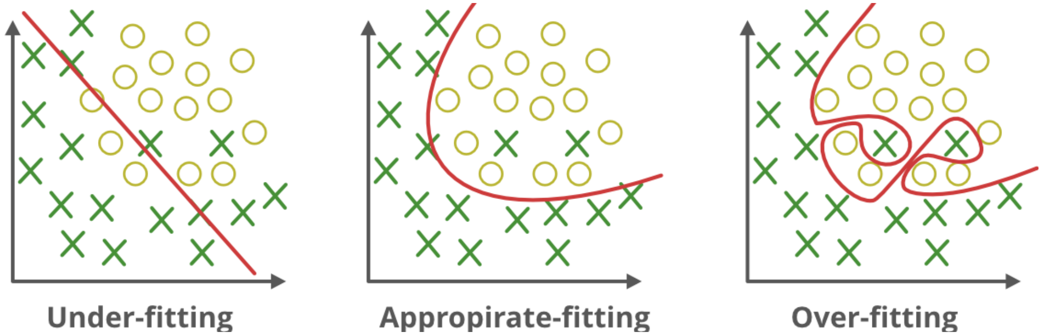
	Statistical Learning	**Machine Learning**
Focus	Hypothesis testing & interpretability	Predictive accuracy
Driver	Math, theory, hypothesis	Fitting data
Data size	Any reasonable set	Big data
Data type	Structured	Structured, unstructured, semi-structured
Dimensions / scalability	Mostly low dimensional data	High dimensional data
Model choice	Parameter significance & in-sample goodness of fit	Cross-validation of predictive accuracy on partitions of data
Interpretability	High	Low
Strength	Understand **causal** relationship & behavior	Prediction (forecasting and nowcasting)

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!





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):

$$\mathbb{E}[\hat{\epsilon}^2] = \mathbb{E}[(y - \hat{f}(\mathbf{x}))^2] = \mathbb{E}[(f(\mathbf{x}) + \epsilon - \hat{f}(\mathbf{x}))^2]$$
$$= \underbrace{\mathbb{E}[(f(\mathbf{x}) - \hat{f}(\mathbf{x}))^2]}_{\text{total quadratic error}} + \underbrace{\mathbb{E}[\epsilon^2]}_{\text{irreducible error}}$$

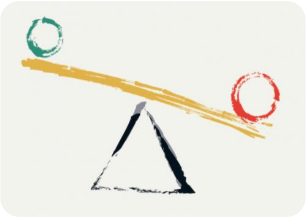
$$\ldots\ldots = \underbrace{\mathbb{V}[\hat{f}(\mathbf{x})]}_{\text{variance of model}} + \underbrace{\mathbb{E}[(f(\mathbf{x}) - \hat{f}(\mathbf{x}))]^2}_{\text{squared bias}} + \sigma^2$$

MSE decomposition

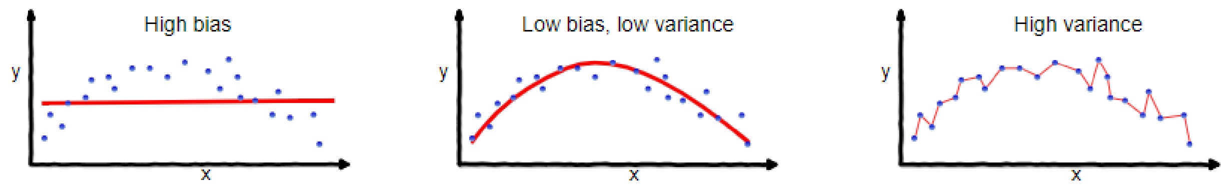
$$MSE = \text{model variance} + \text{model bias} + \text{irreducible error}$$

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.



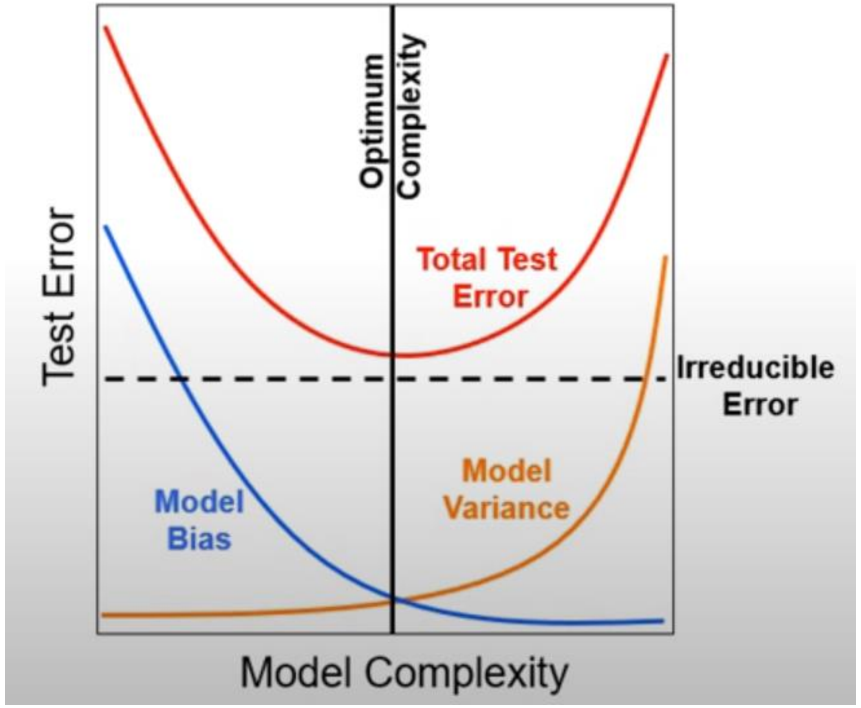
Representations of the bias-variance tradeoff



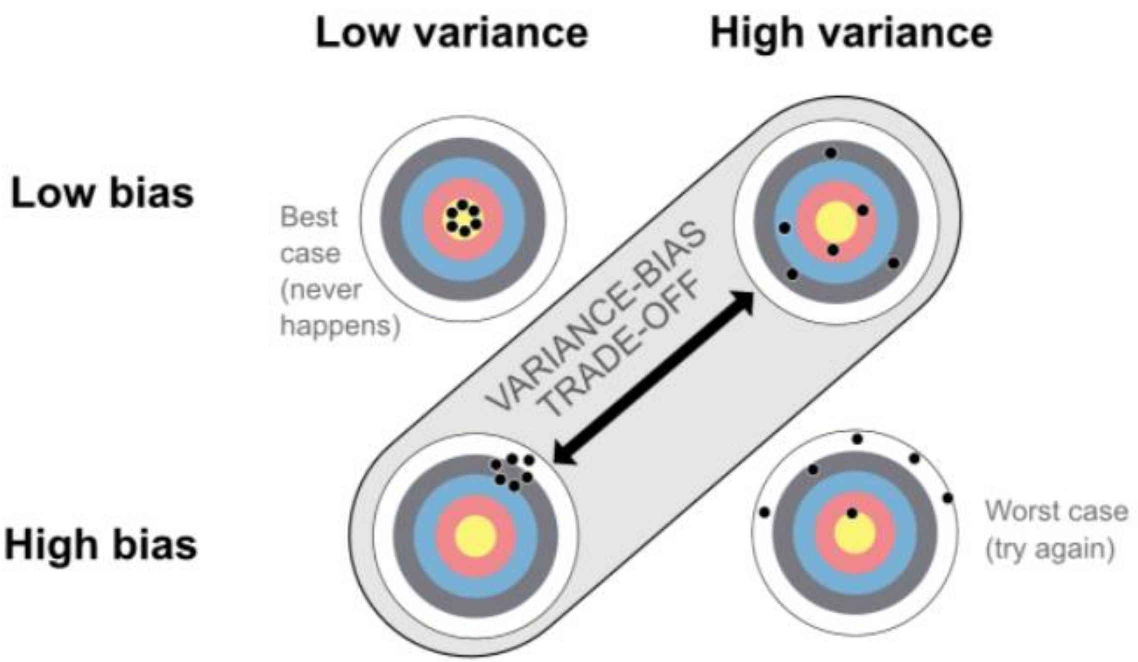
underfitting

Good balance

overfitting



Other representations of the bias-variance tradeoff

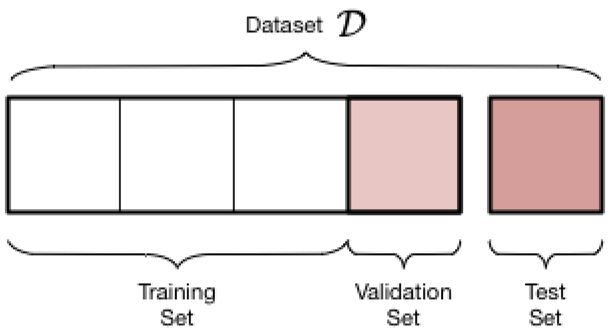


Part IV
Resampling methods
Scaling the features

Partitioning of the dataset

The data set is typically divided into three <u>non-overlapping</u> 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.

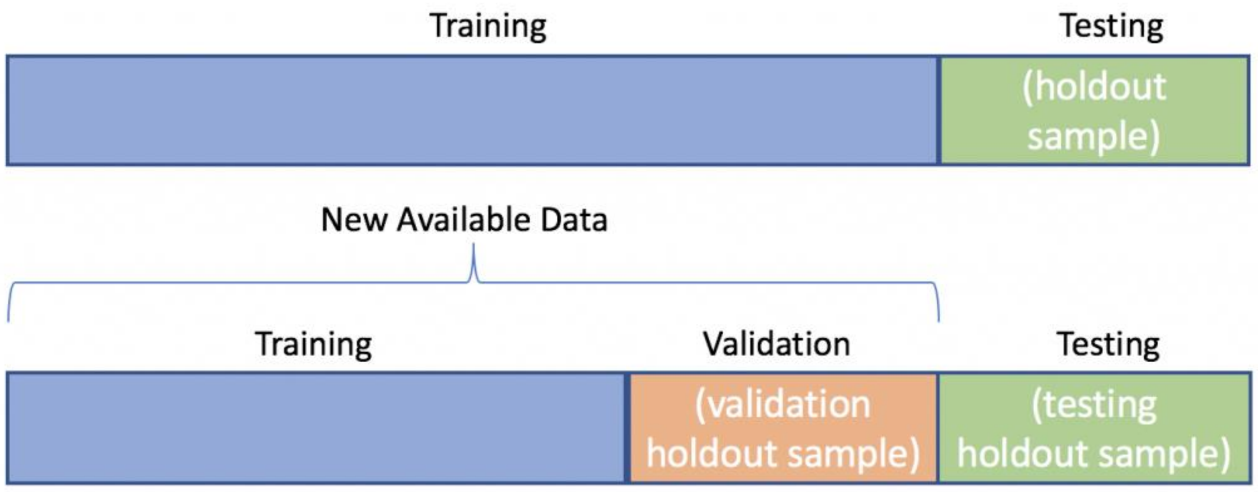
Large dataset is needed! But what if we don't have it?

Resampling methods

Cross validation

- Sometimes we cannot afford to split the data in three because the algorithm may not learn anything from a small training dataset!
- Small validation set is also problematic because we cannot tune the hyperparameters properly!

- 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.



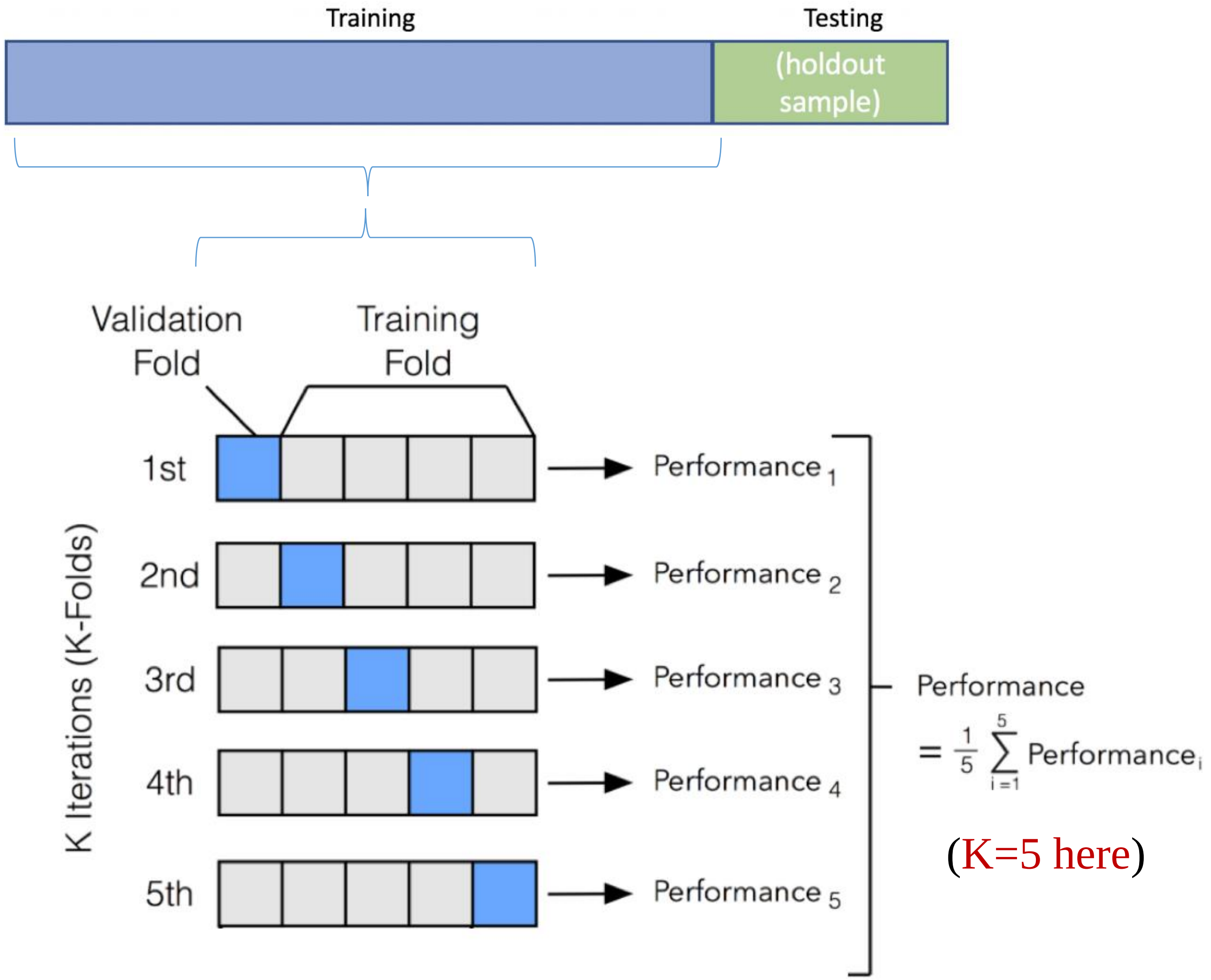
K-fold Cross Validation

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) Performance can be any of the evaluation metrics for regression or classification models. For example, MSE, accuracy, …

3) 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.

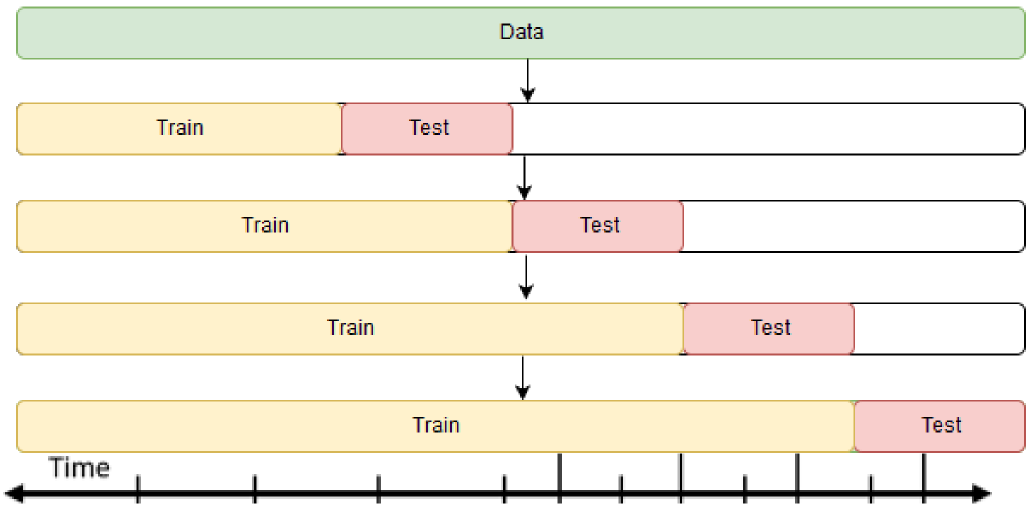


(K=5 here)

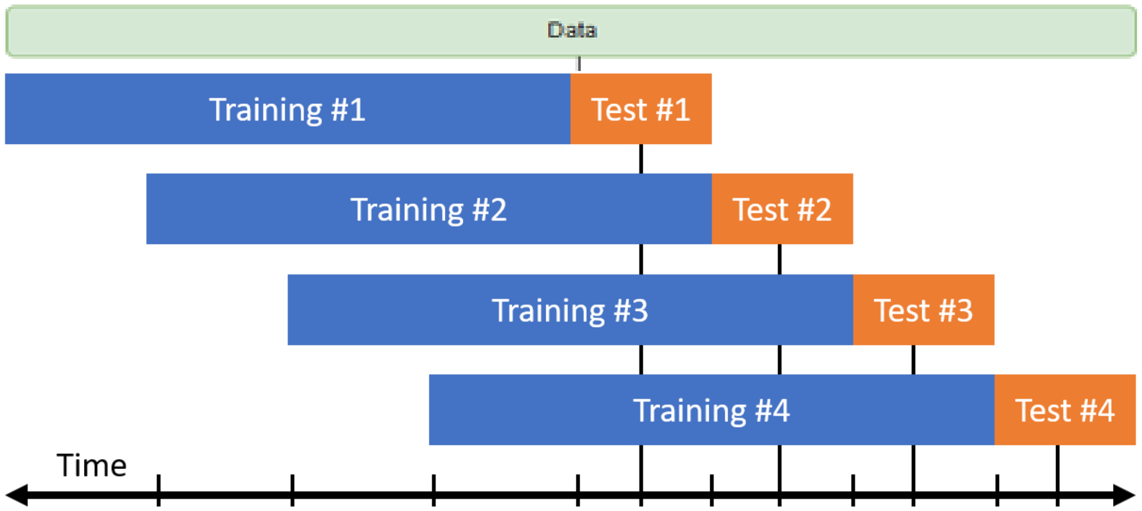
Time Series Cross Validation

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

Walk forward cross validation
Expanding windows



Walk forward cross validation
Rolling windows

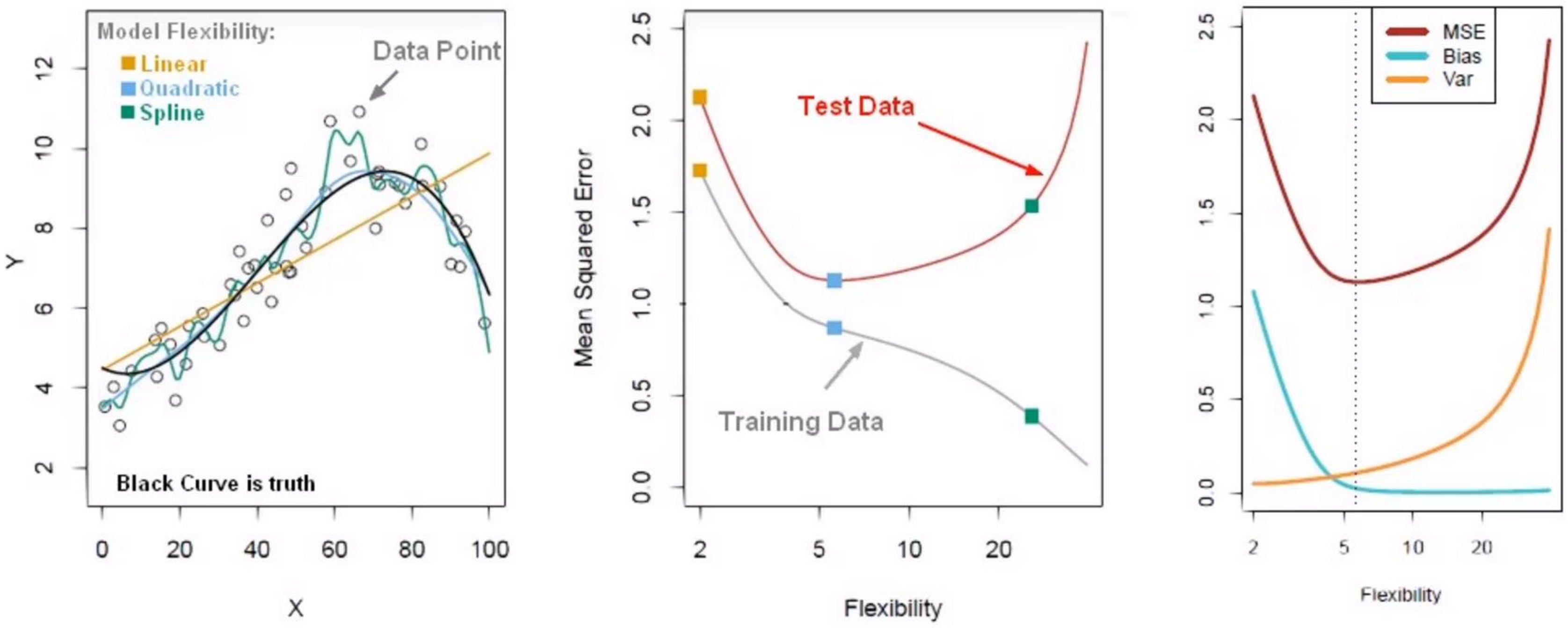


Mitigate overfitting

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

1) Complexity reduction (regularization)

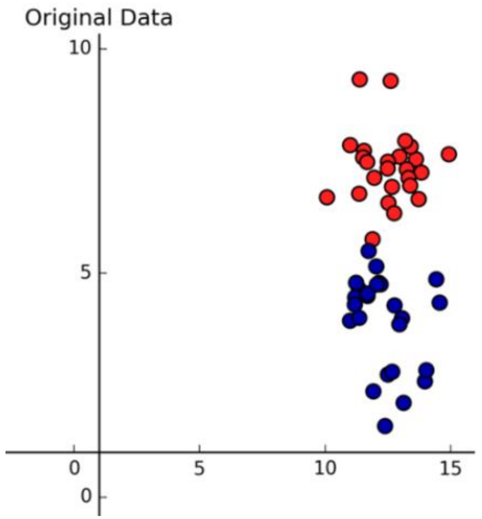
2) Cross validation (estimate the test error)

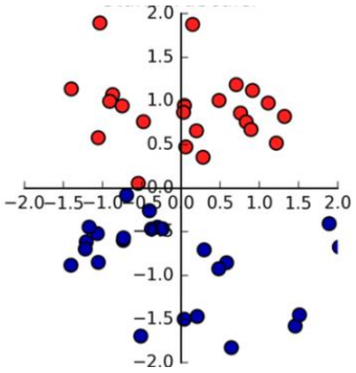


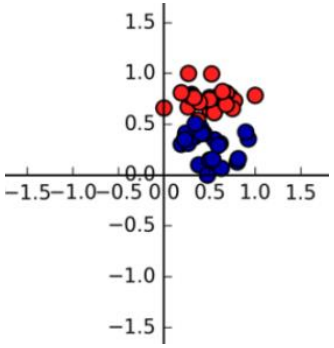
Scaling the features

Let us use x_i for raw input and $\widetilde{x_i}$ for the transformed data. Common scaling practices include:

- Standardization (Z-score normalization): $\widetilde{x_i} = \left(\frac{x_i - \mu_x}{\sigma_x}\right)$
- Normalization:
    - Min-Max scaler over [0,1]: $\widetilde{x_i} = \left(\frac{x_i - \mathrm{Min}(X)}{Max(X) - Min(X)}\right)$
    - Min-Max scaler over [-1,1]: $\widetilde{x_i} = 2 * \left(\frac{x_i - \mathrm{Min}(X)}{Max(X) - Min(X)}\right) - 1$







Scaling the features

- Normalization is good to use when the distribution of the data does not follow a Normal distribution. (ideal for non-parametric algorithms like KNN)
- Standardization, can be helpful in cases where the data follows a Normal distribution. However, this does not have to be necessarily true.
- Unlike normalization, standardization does not have a bounding range. So, even if you have outliers in your data, they will not be affected by standardization.
- Be careful when scaling the time series data! Why?
- To avoid data leakage, It is a good practice to fit the scaler on the training data and then use it to transform the testing data.
- The choice of using normalization or standardization will depend on your problem and the machine learning algorithm you are using

Question of the day!

Students' questions

1) I am having a hard time grasping the difference between bias and variance.
2) I'm loving these principles! Machine learning seemed to be a nebulous field before these few classes, but now that I'm taking this class it seems to be simpler than I thought.
3) I'm having some difficulty understanding why we might use both cross-validation AND a confusion matrix to evaluate the best machine learning method. Can you please elaborate a bit on this in class?
4) Do we use hyperparameters in every ML model?
5) The only thing I did not understand was how to know what data is the testing set and what data is the training set.
6) How do you know what models to include/exclude when doing cross validation? What is the next deciding factor if cross validation results are similar?
7) Is there a way you'd recommend taking notes in class?
8) The graph in the CFA reading?

thank you all
CLASS DISMISSED