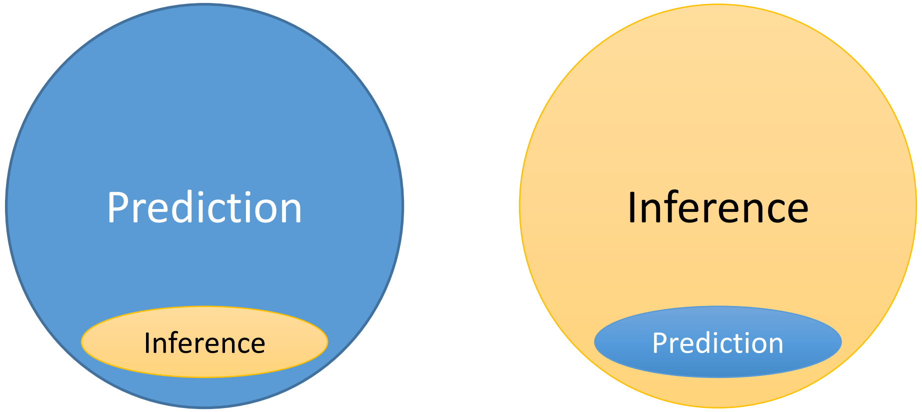
Class 4- Machine Learning concepts
Part I

Motivation

Machine learning fundamental concepts:

- Inference and prediction
- Part I: The Model
- Part II: Evaluation metrics
- Part III: Bias-Variance tradeoff
- Part IV: Resampling methods
- Part V: Solvers/learners (GD, SGD)
- Part VI: How do machines learn?
- Part VII: Scaling the features



Part I
The Model

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:

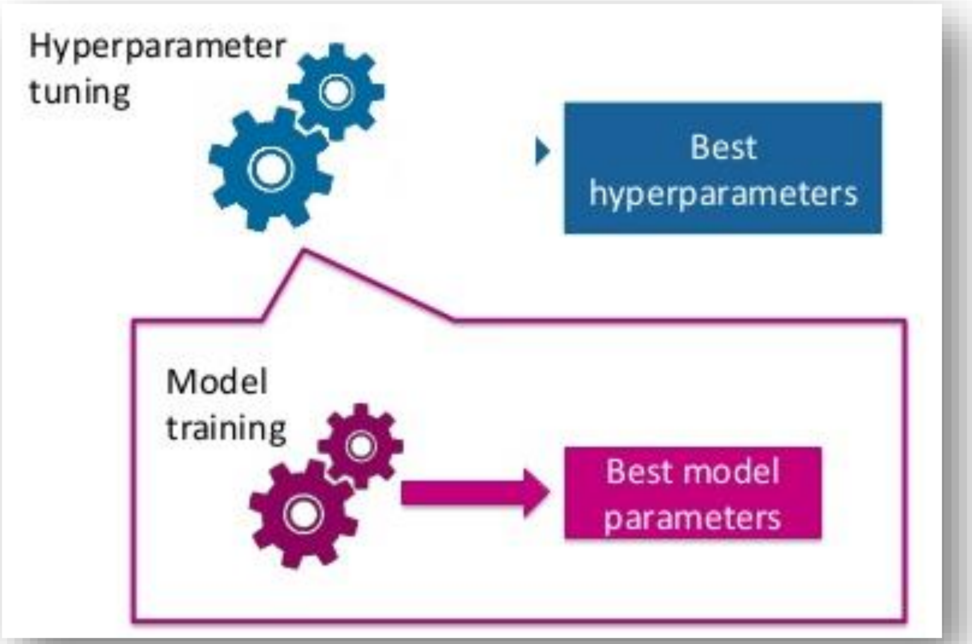
1) Inference (interpretable ML)

2) Prediction

Parameters and Hyperparameters

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

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, ….

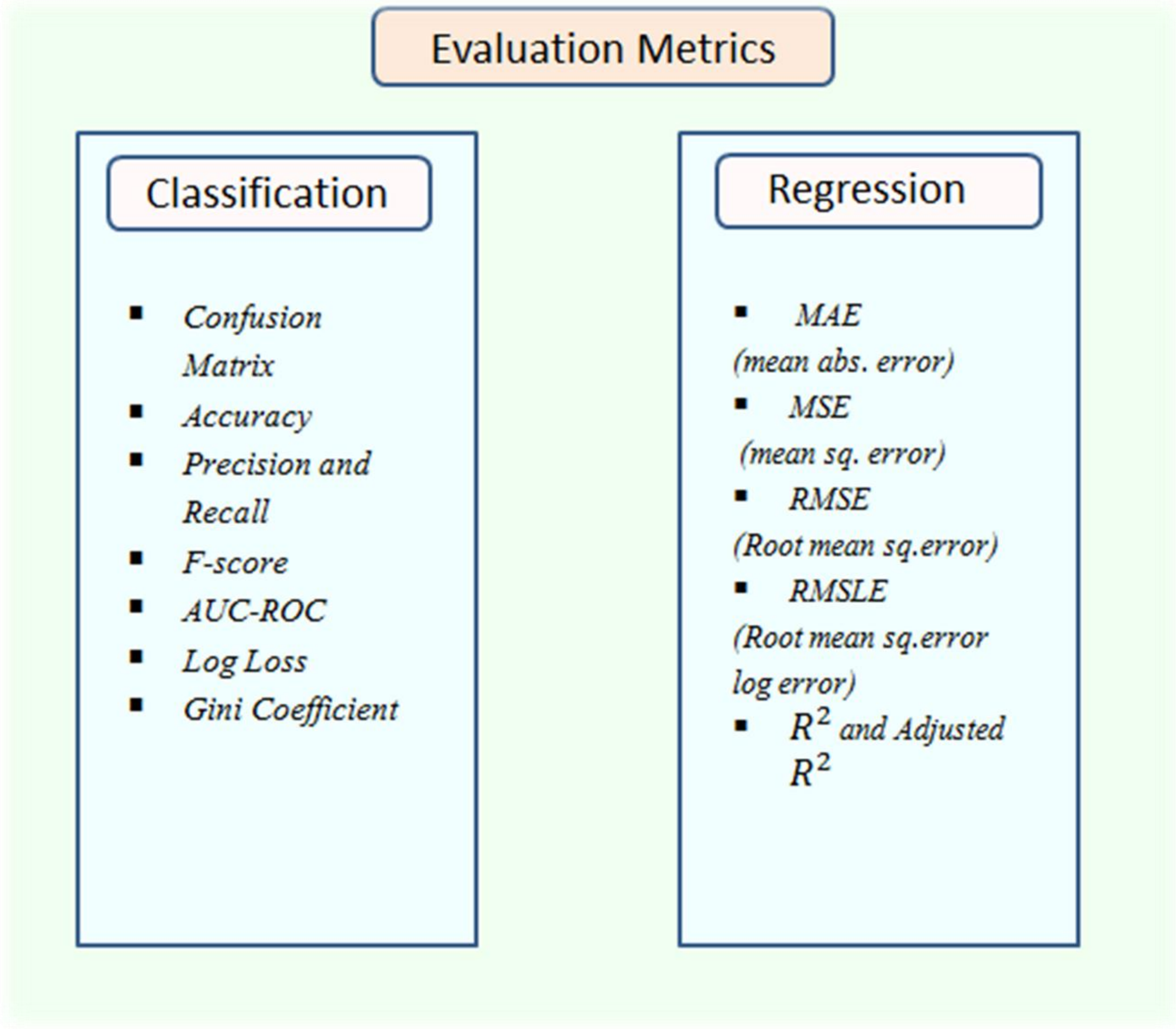
	Pros	Cons
Parametric algorithms	**Simpler** Easier to understand and to interpret **Faster** Very fast to fit your data **Less data** Require "few" data to yield good perf.	**Limited complexity** Because of the specified form, parametric algorithms are more suited for "simple" problems where you can guess the structure in the data

Part II
Evaluation Metrics

Evaluation metrics

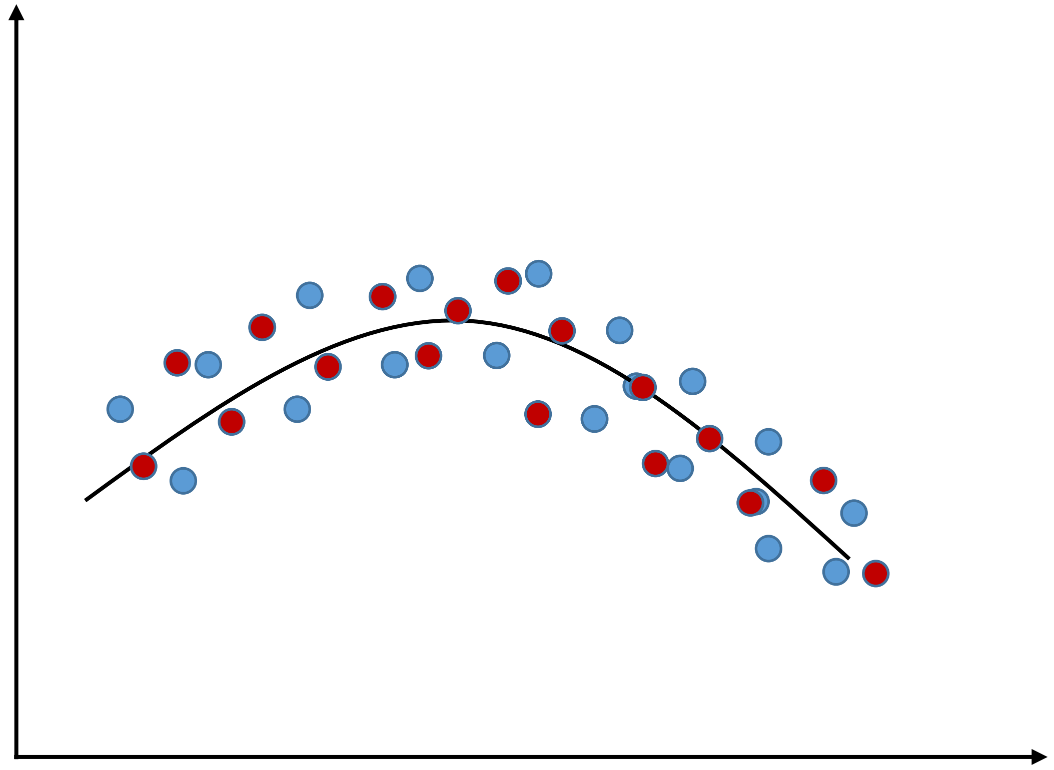
In general, we want to compare how close are the predictions to the actual numbers in the test set.

This is typically assessed using
- MSE for quantitative response
- Misclassification rate for qualitative response



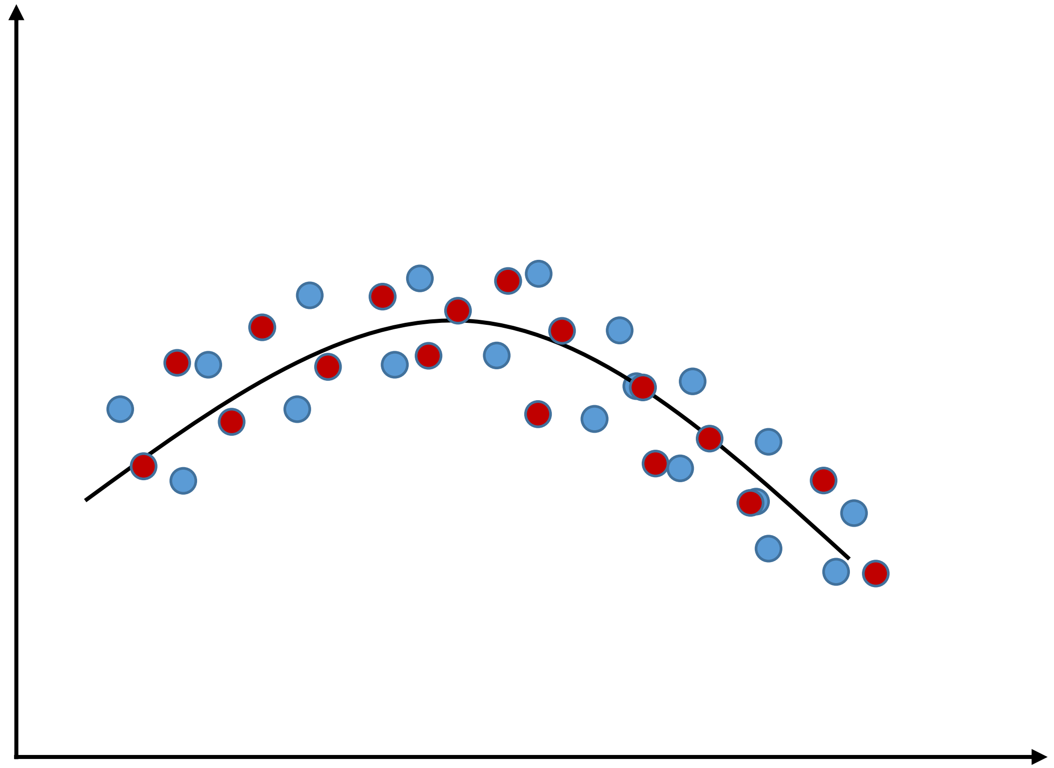
Part III
Bias-Variance Tradeoff

Model Bias & Model Variance in machine learning



JON M. HUNTSMAN SCHOOL OF BUSINESS UtahStateUniversity

Model Bias & Model Variance in machine learning



MSE decomposition

$$MSE = \color{blue}{model\ variance} + \color{green}{model\ bias} + \color{red}{irreducible\ error}$$

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.

MSE decomposition

The bias-variance tradeoff is one of the core concepts in <u>supervised</u> learning.

Assume that the data is generated by a simple model!

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

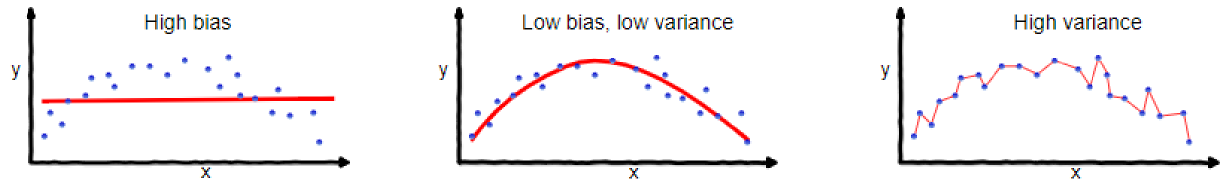
The estimated model yields

$$\hat{y_i} = \hat{f}(X_i)$$

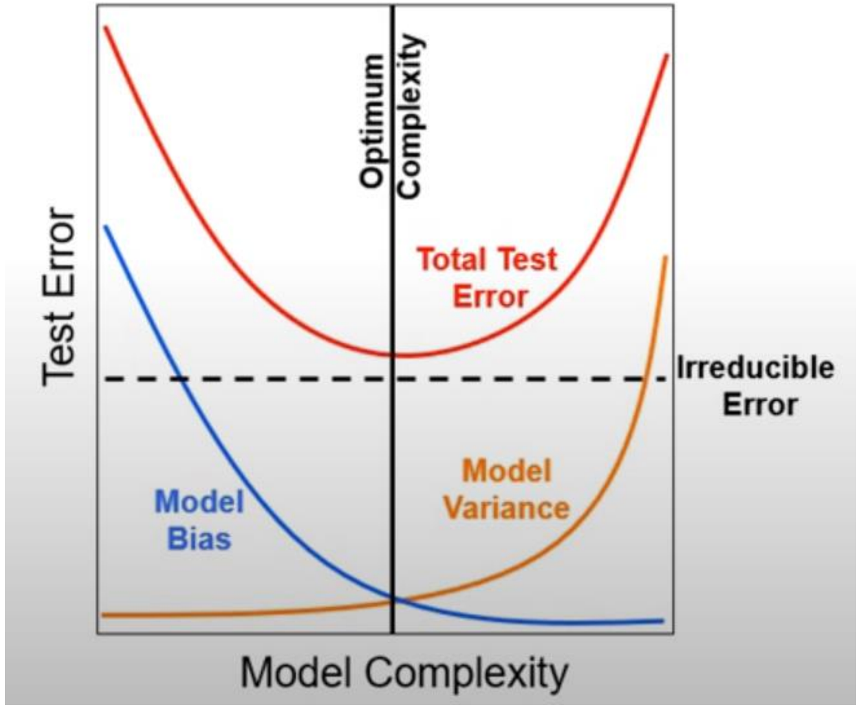
Let us decompose the mean squared error (MSE):

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

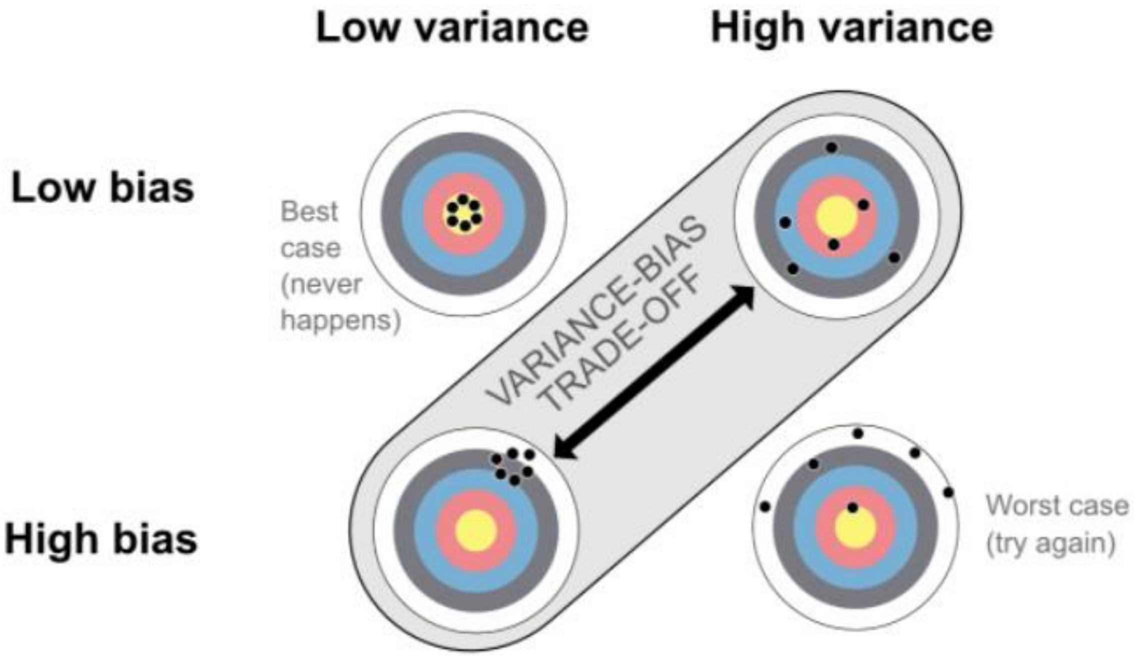
Representations of the bias-variance tradeoff



underfitting | **Good balance** | **overfitting**



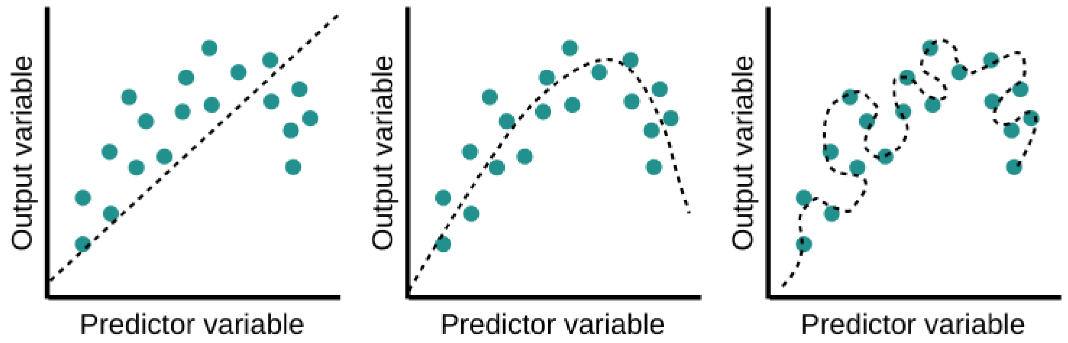
Other representations of the bias-variance tradeoff

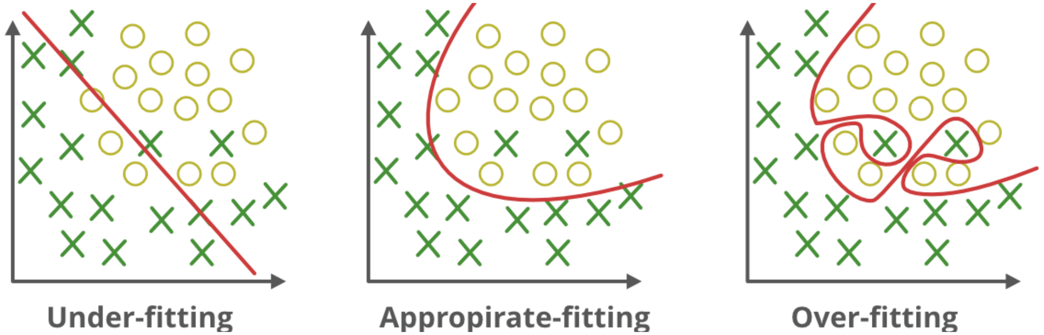


Overfitting

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!



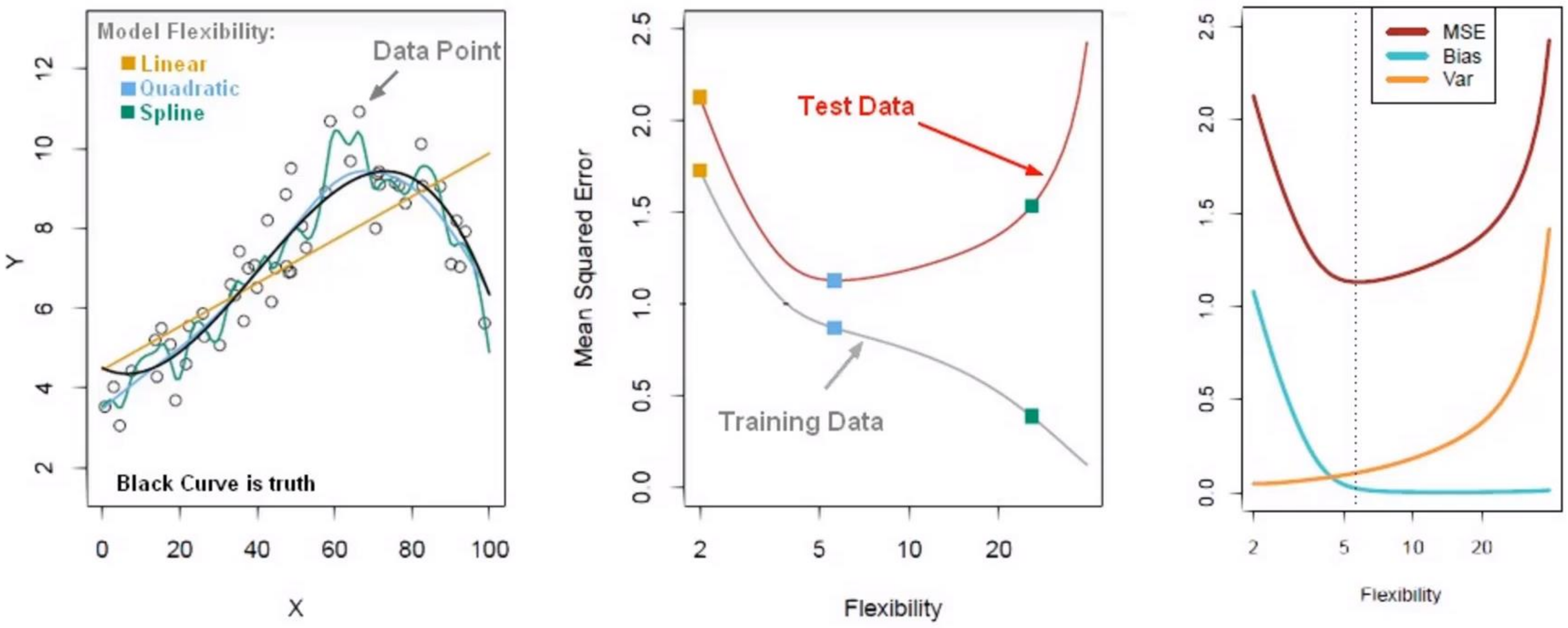


Mitigate overfitting

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!


class
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