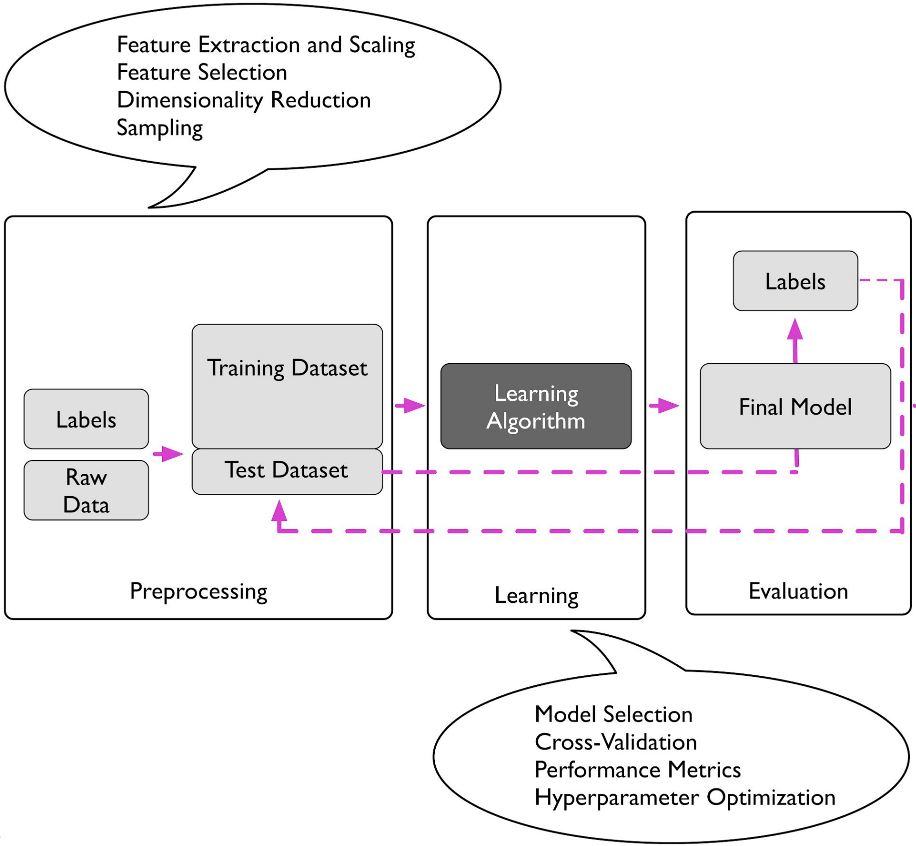
Lecture 14

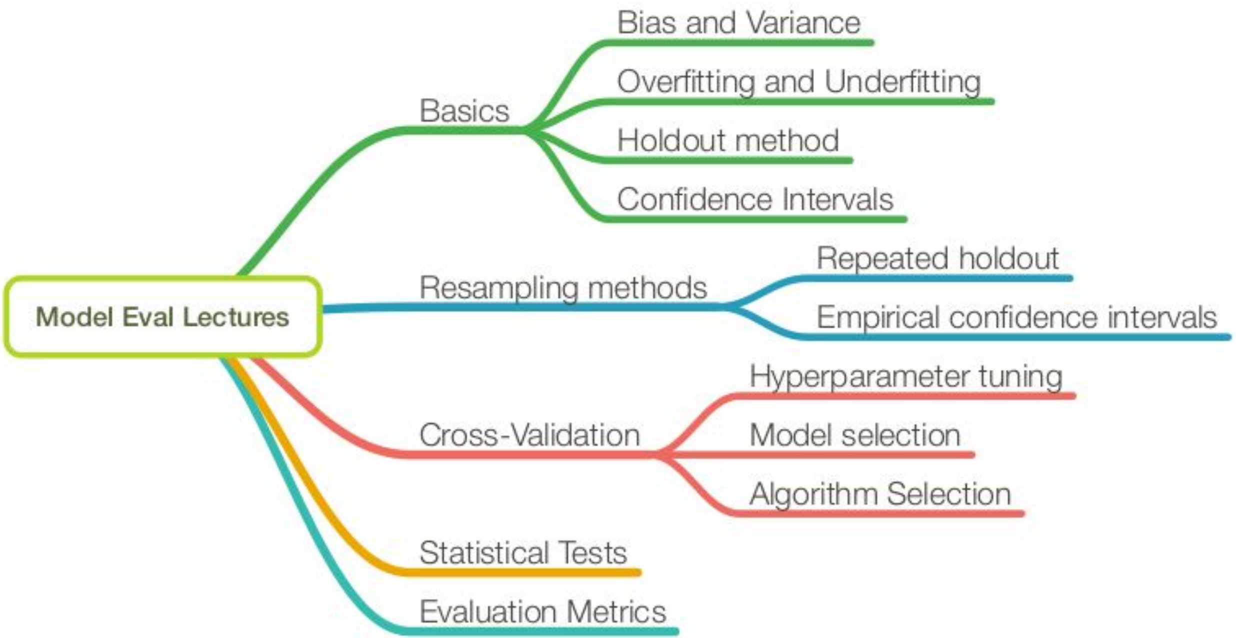
Model evaluation

https://github.com/dalcimar/MA28CP-Intro-to-Machine-Learning
UTFPR - Federal University of Technology - Paraná
https://www.dalcimar.com/

Machine learning pipeline



Lecture overview



Lecturer Overview

- **Overfitting and Underfitting**
- Intro to Bias-Variance Decomposition
- Bias-Variance Decomposition of the Squared Error
- Relationship between Bias-Variance Decomposition and
- Overfitting and Underfitting
- Bias-Variance Decomposition of the 0/1 Loss
- Other Forms of Bias

Generalization Performance

Want a model to "generalize" well to **unseen** data

- "high generalization accuracy" or
- "low generalization error"

Assumptions

i.i.d. assumption: training and test examples are independent and identically distributed (drawn from the same joint probability distribution, P(X, y))

For some random model that **has not been fitted to the training set**, we expect the training error is **approximately similar** the test error

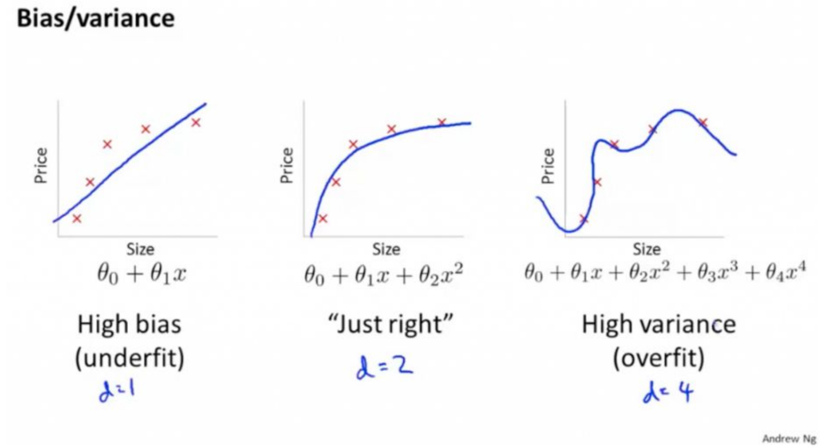
The training error or accuracy provides an **optimistically biased estimate** of the generalization performance

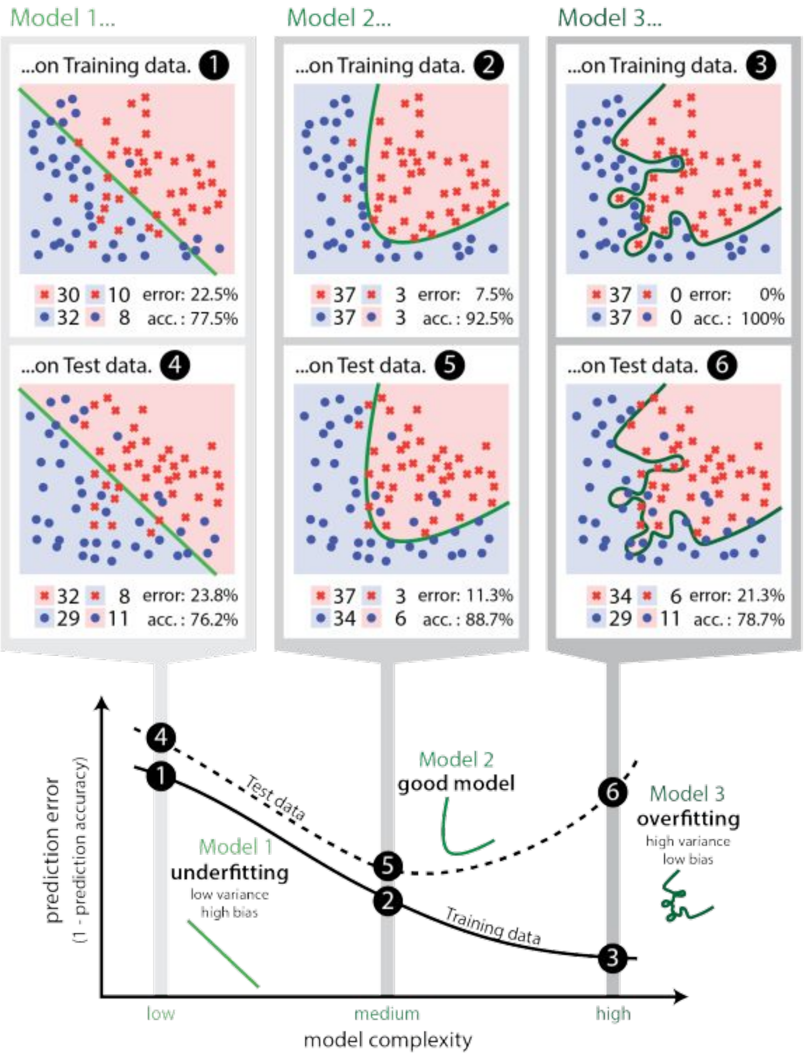
Model Capacity

Underfitting: both the training and test error are high

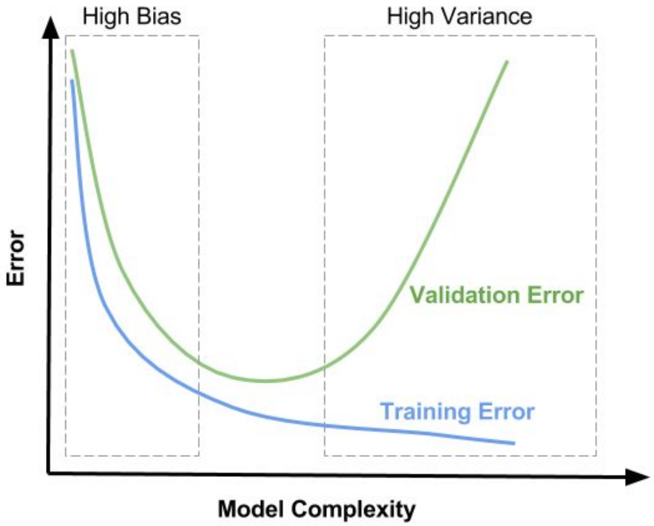
Overfitting: gap between training and test error (where test error is larger)

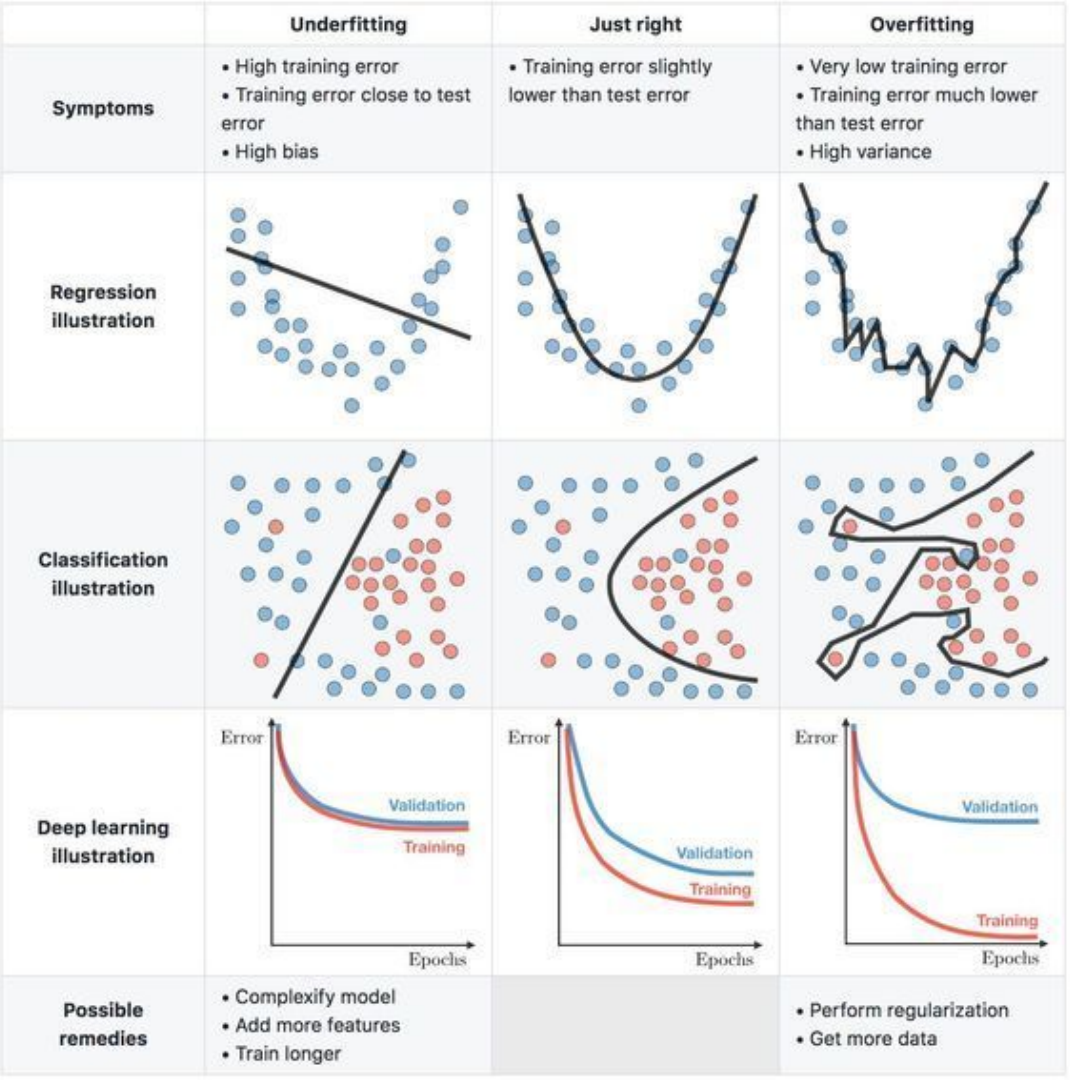
- Large hypothesis space being searched by a learning algorithm -> high tendency to overfit





Overfitting and Underfit





	Underfitting	Just right	Overfitting
Symptoms	• High training error • Training error close to test error • High bias	• Training error slightly lower than test error	• Very low training error • Training error much lower than test error • High variance
Regression illustration			
Classification illustration			
Deep learning illustration	Error Validation Training Epochs	Error Validation Training Epochs	Error Validation Training Epochs
Possible remedies	• Complexify model • Add more features • Train longer		• Perform regularization • Get more data

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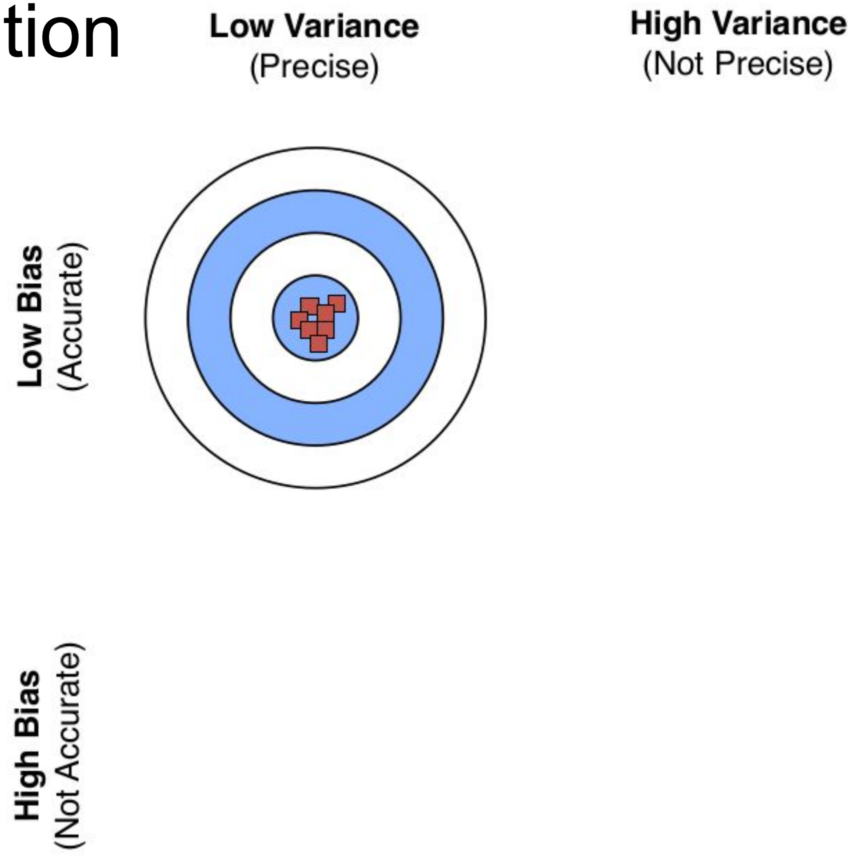
Bias-Variance Decomposition

- Decomposition of the loss into bias and variance help us understand learning algorithms, concepts are related to underfitting and overfitting
- Helps explain why ensemble methods (last lecture) might perform better than single models

Bias-Variance Decomposition

Loss = Bias + Variance + Noise



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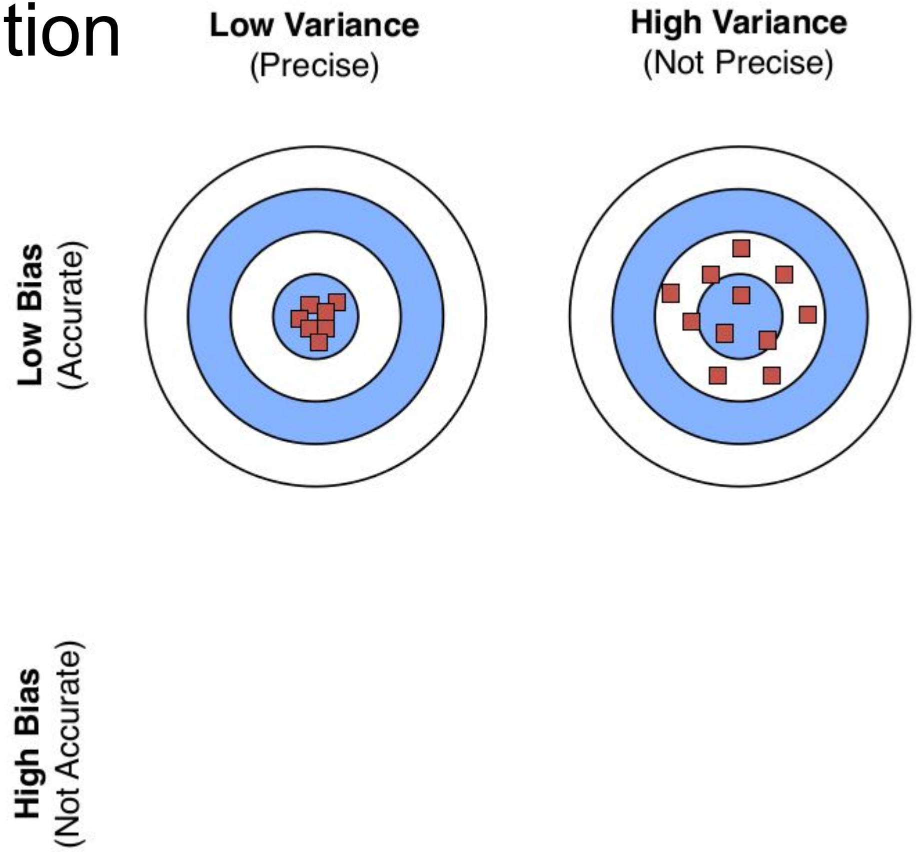

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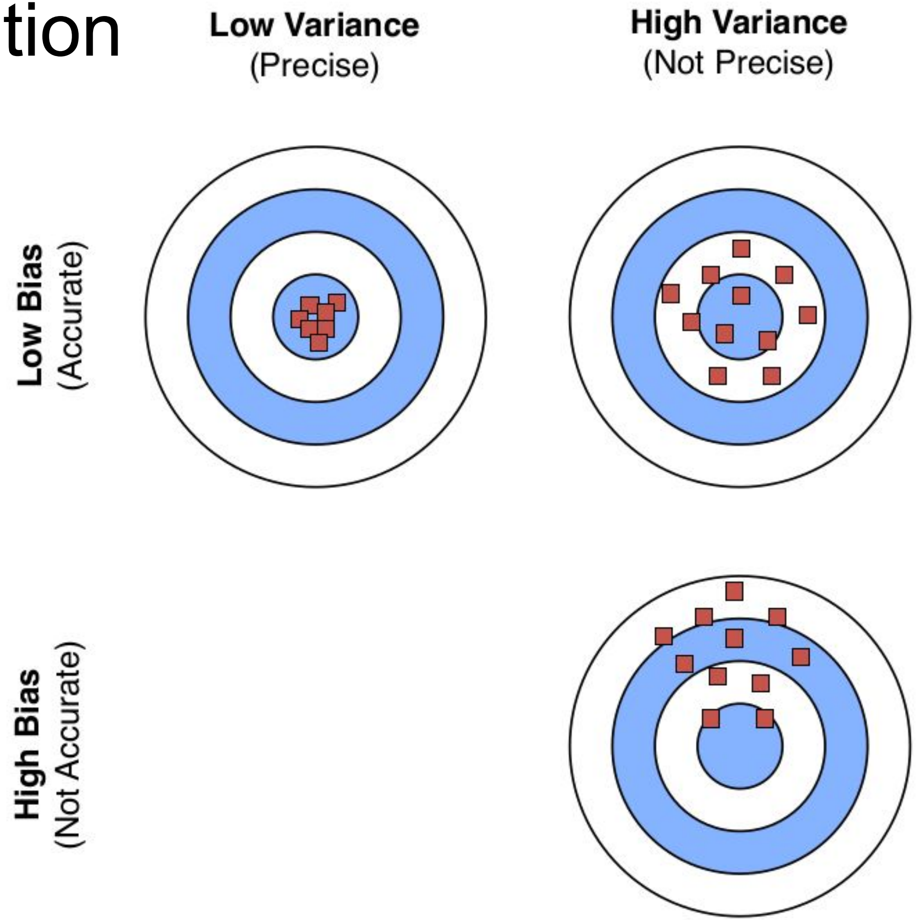

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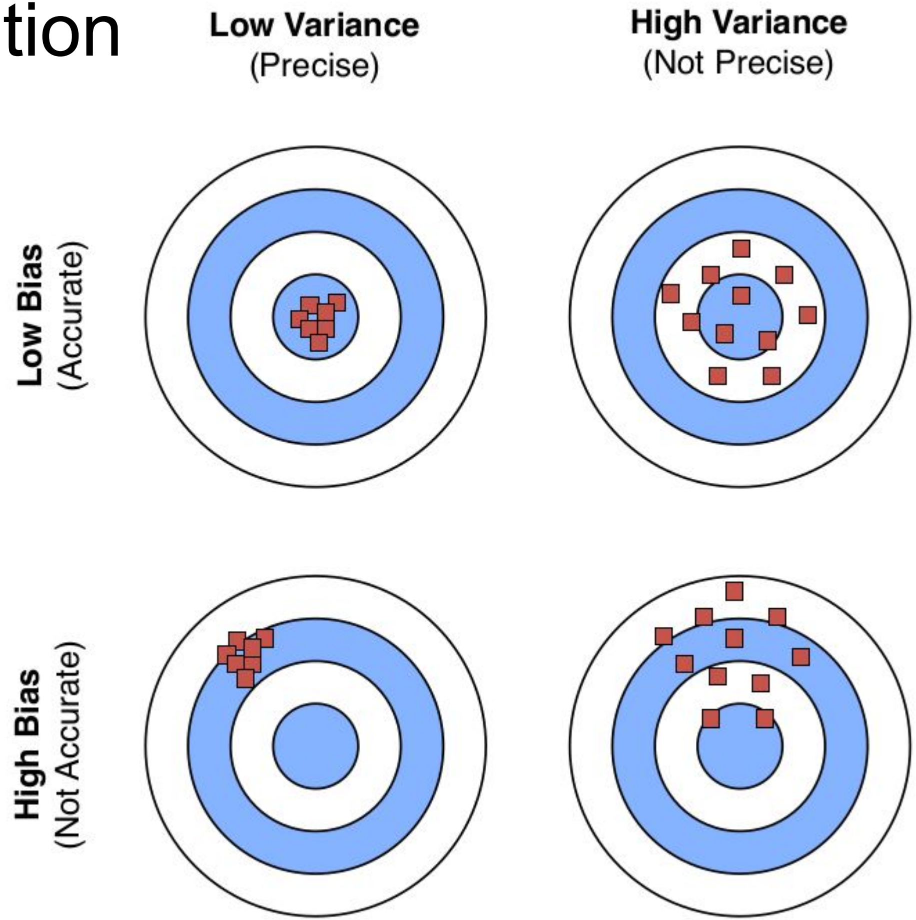
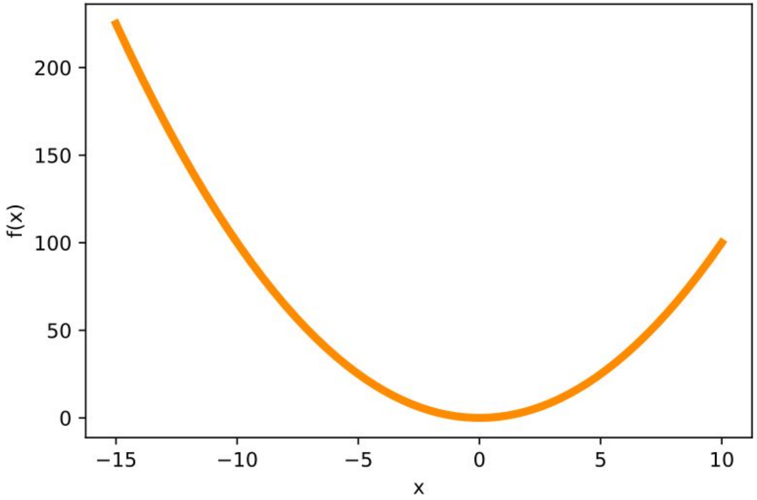
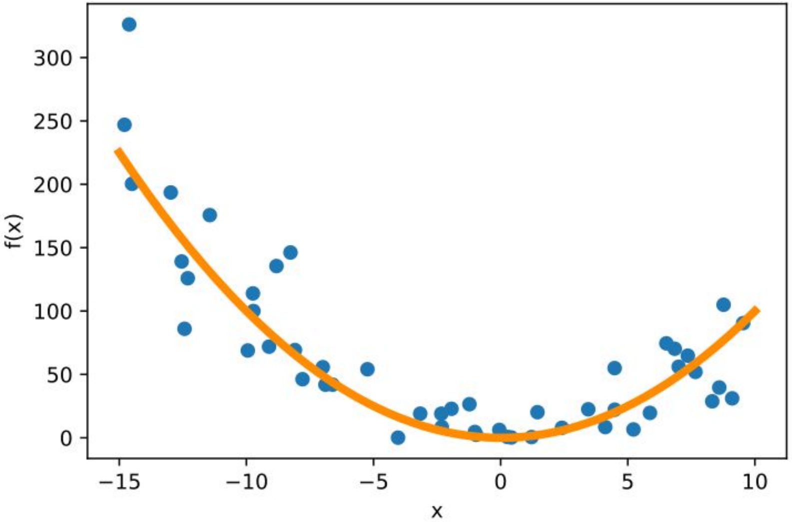


Bias and Variance Intuition



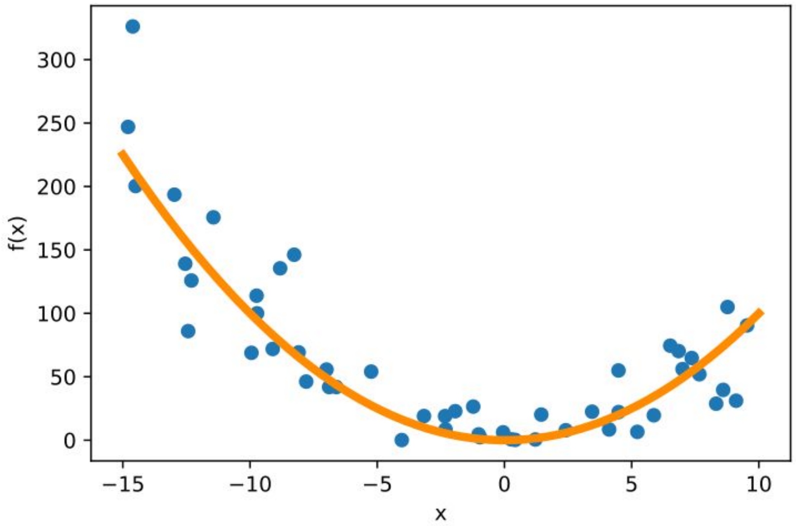
where f(x) is some true (target) function

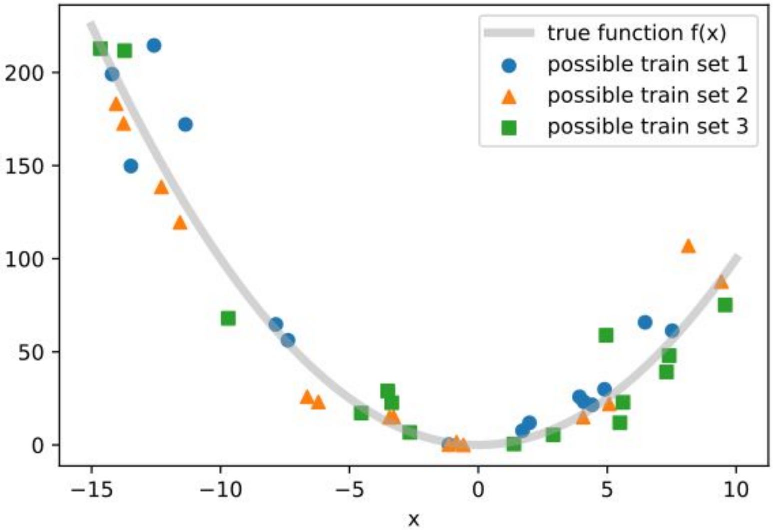


where f(x) is some true (target) function

the blue dots are a training dataset;
here, I added some random Gaussian noise

Bias and Variance Intuition





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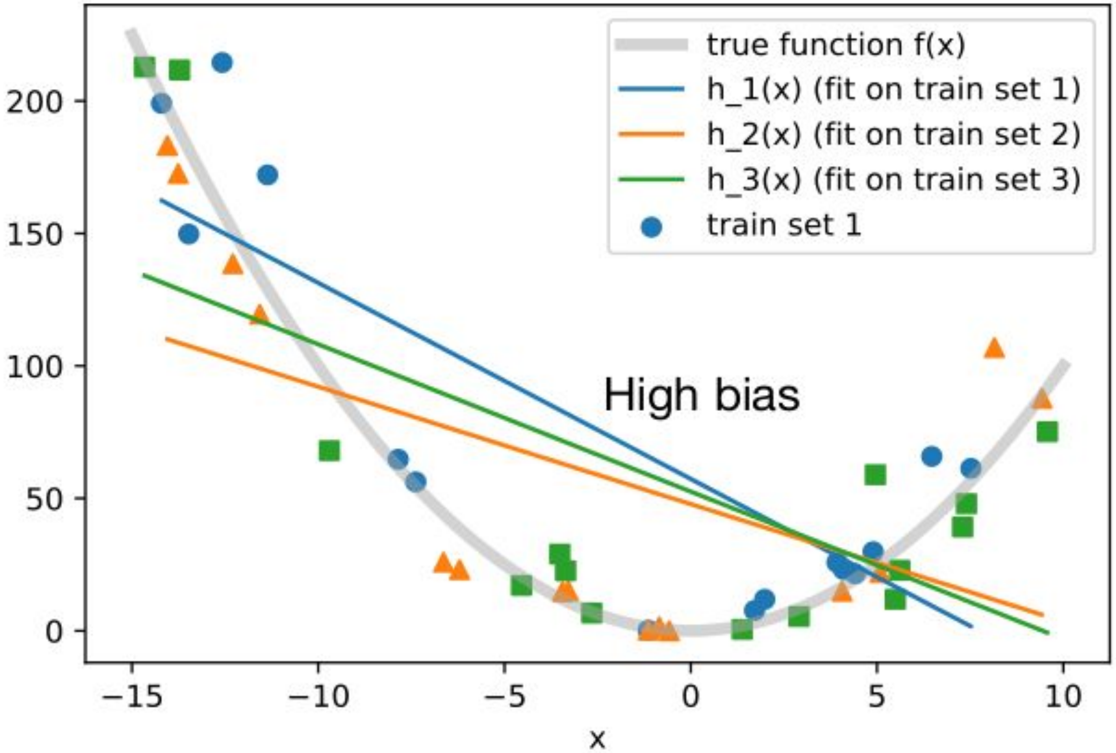
Bias and Variance Intuition

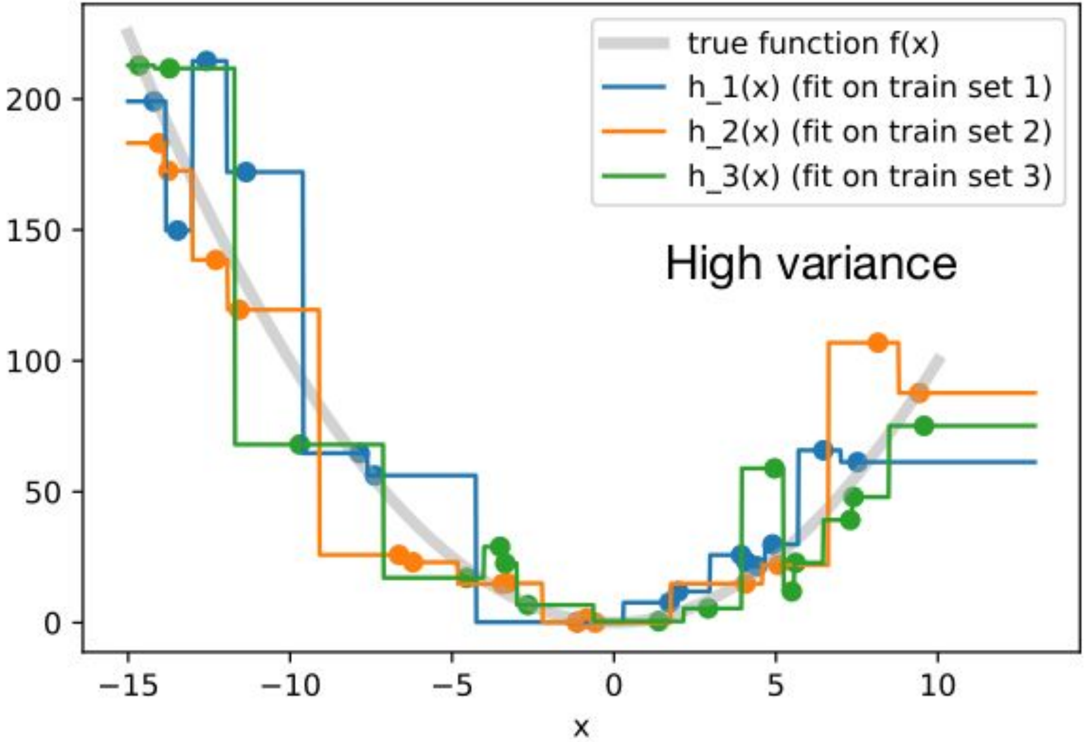
Suppose we have multiple training sets



linear regression models

Bias and Variance Intuition

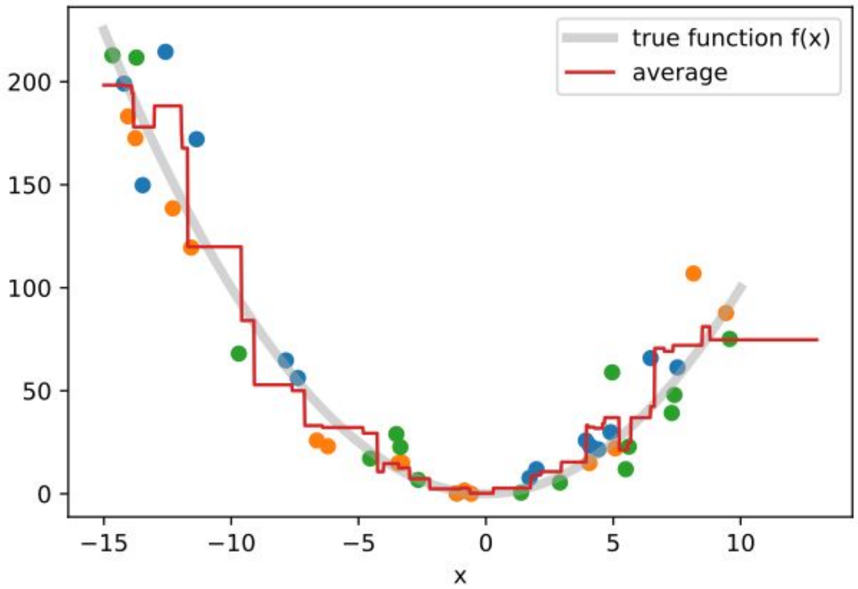
Suppose we have multiple training sets

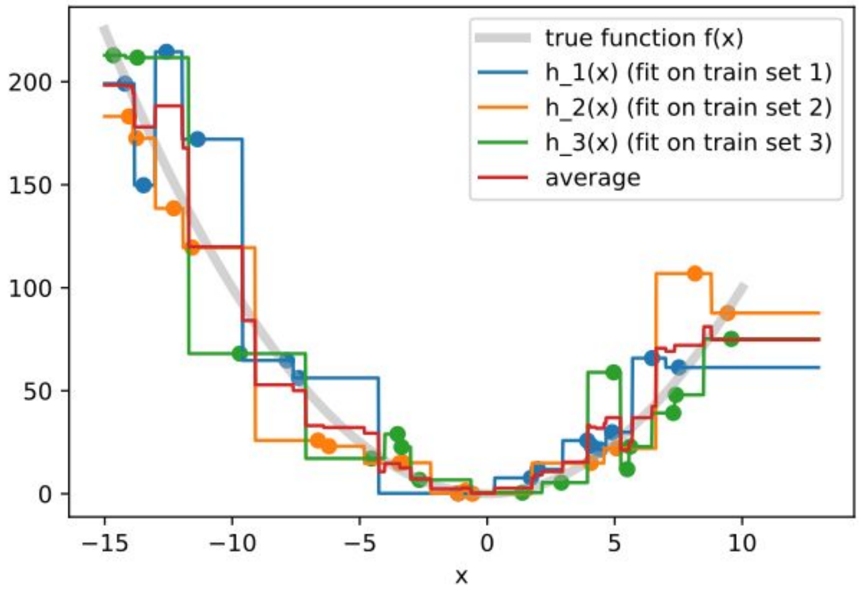


Bias and Variance Intuition

What happens if we take the average?

Does this remind you of something?





Terminology

Point estimator $\hat{\theta}$ of some parameter θ

(could also be a function, e.g., the hypothesis is an estimator of some target function)

$$\text{Bias} = E[\hat{\theta}] - \theta$$

General Definition

$$\text{Bias}[\hat{\theta}] = E[\hat{\theta}] - \theta$$

$$\text{Var}[\hat{\theta}] = E[\hat{\theta}^2] - (E[\hat{\theta}])^2$$

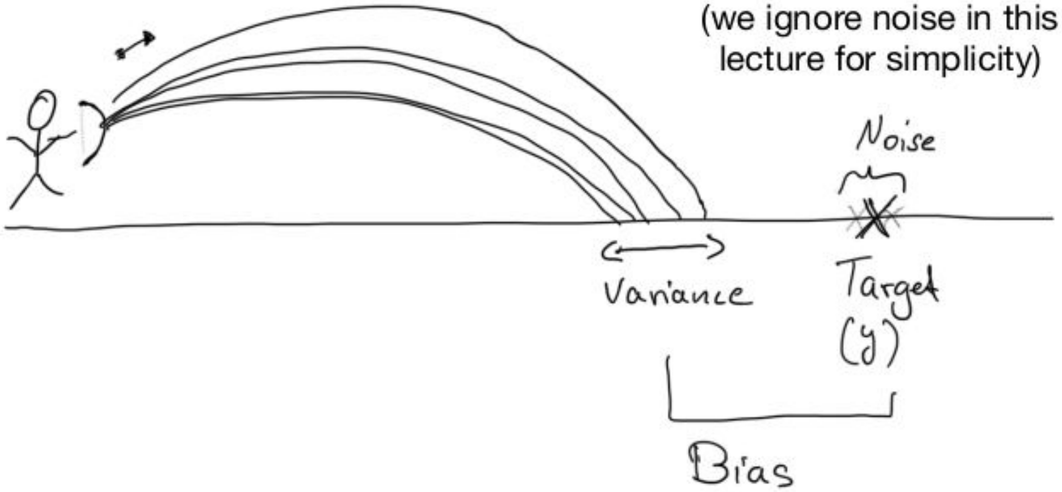
$$\text{Var}[\hat{\theta}] = E\left[(E[\hat{\theta}] - \hat{\theta})^2\right]$$

Terminology

$$\text{Bias}[\hat{\theta}] = E[\hat{\theta}] - \theta \qquad \text{Var}[\hat{\theta}] = E\left[(E[\hat{\theta}] - \hat{\theta})^2\right]$$

Intuition

(we ignore noise in this lecture for simplicity)



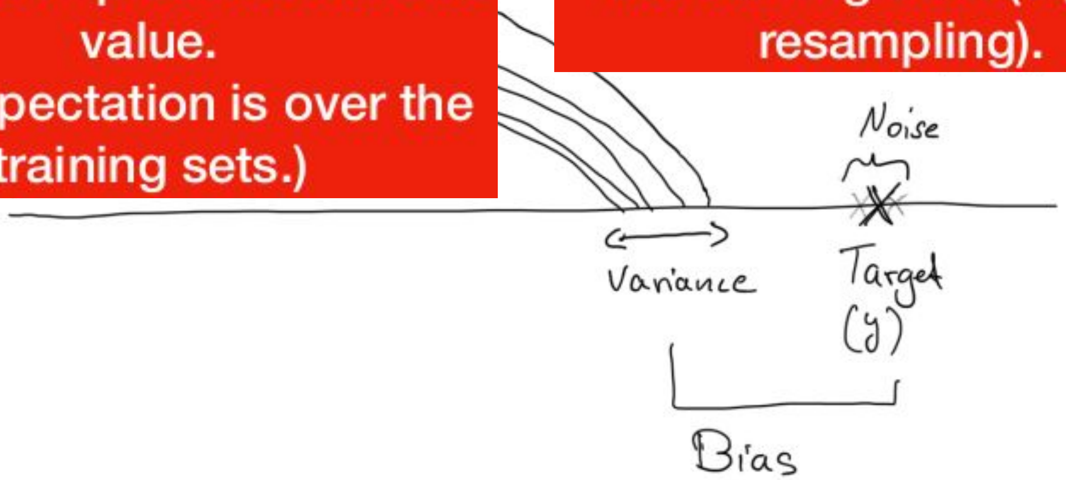
Terminology

$$\text{Bias}[\hat{\theta}] = E[\hat{\theta}] - \theta$$

Bias is the difference between the average estimator from different training samples and the true value.
(The expectation is over the training sets.)

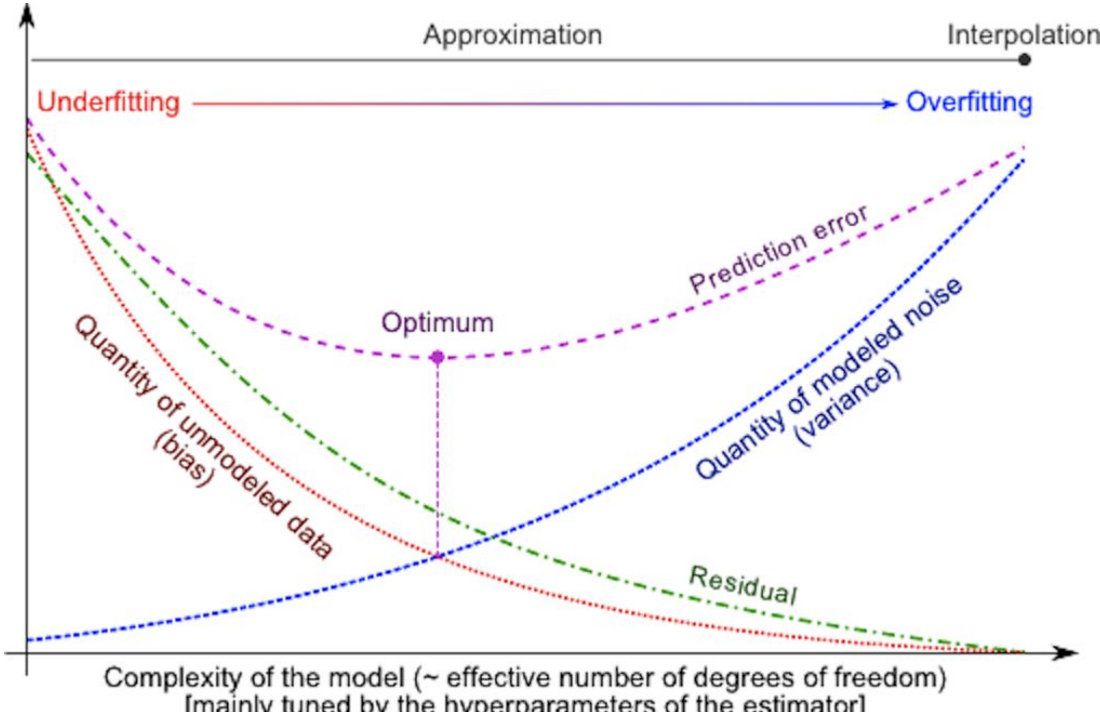
$$\text{Var}[\hat{\theta}] = E\left[(E[\hat{\theta}] - \hat{\theta})^2\right]$$

The variance provides an estimate of how much the estimate varies as we vary the training data (e.g., by resampling).



Bias-Variance Decomposition

Loss = Bias + Variance + Noise



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