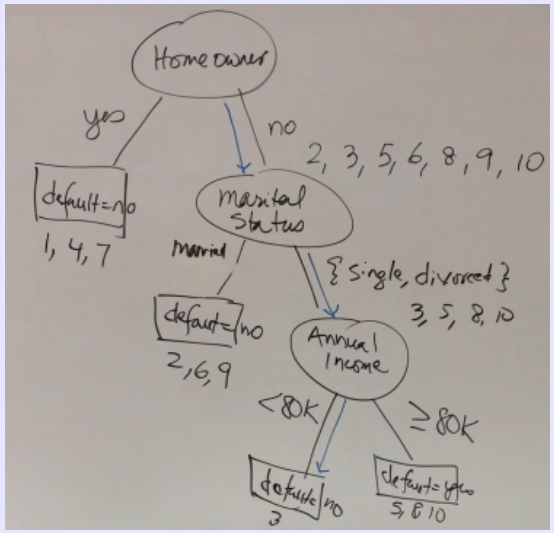
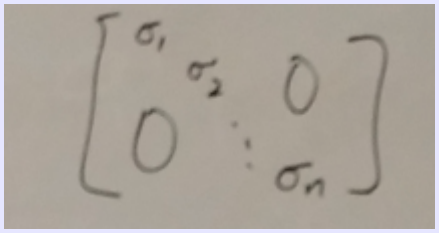
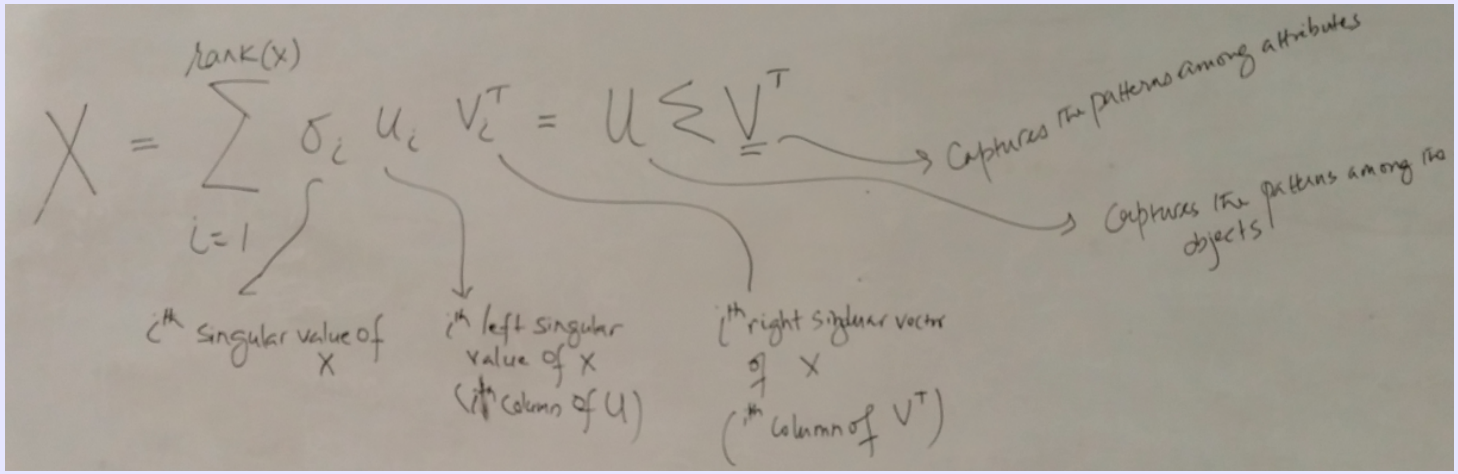
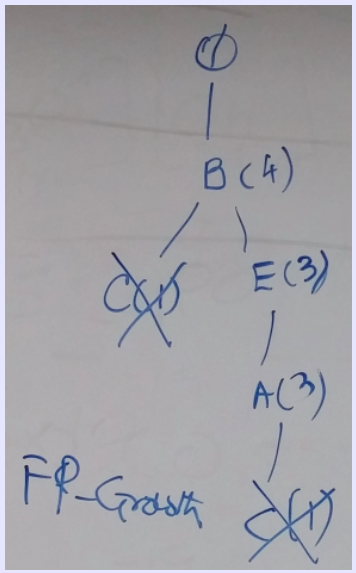






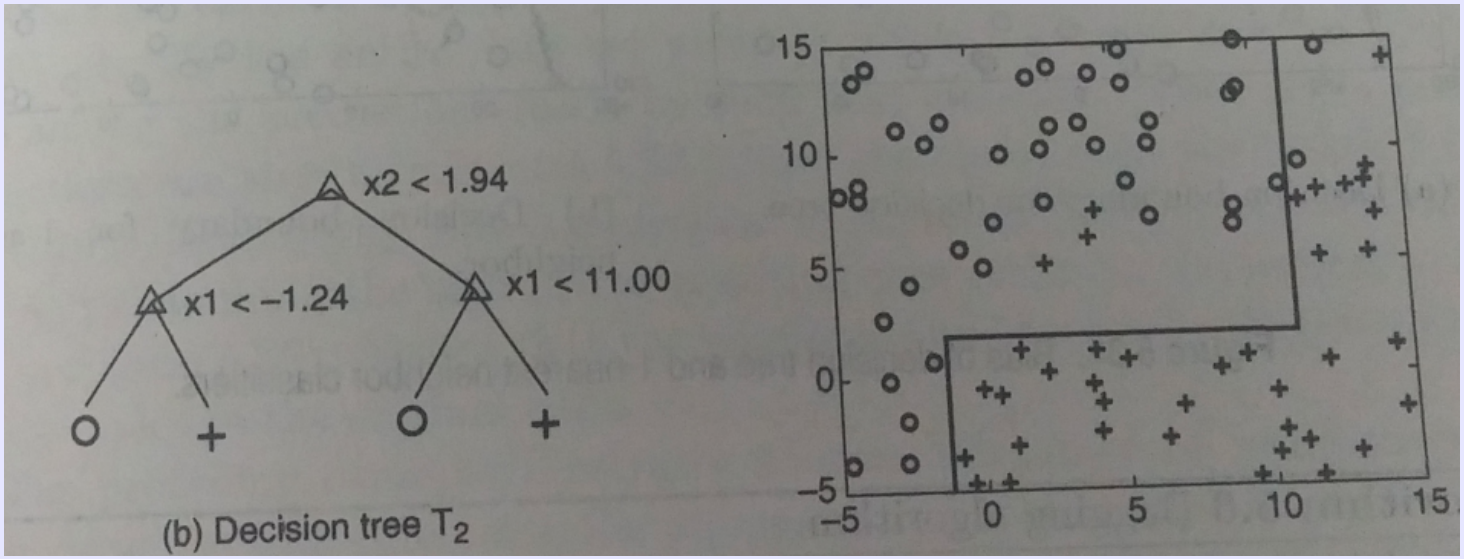


CS 422: Data Mining
Vijay K. Gurbani, Ph.D.,
Illinois Institute of Technology

Bias-variance tradeoff

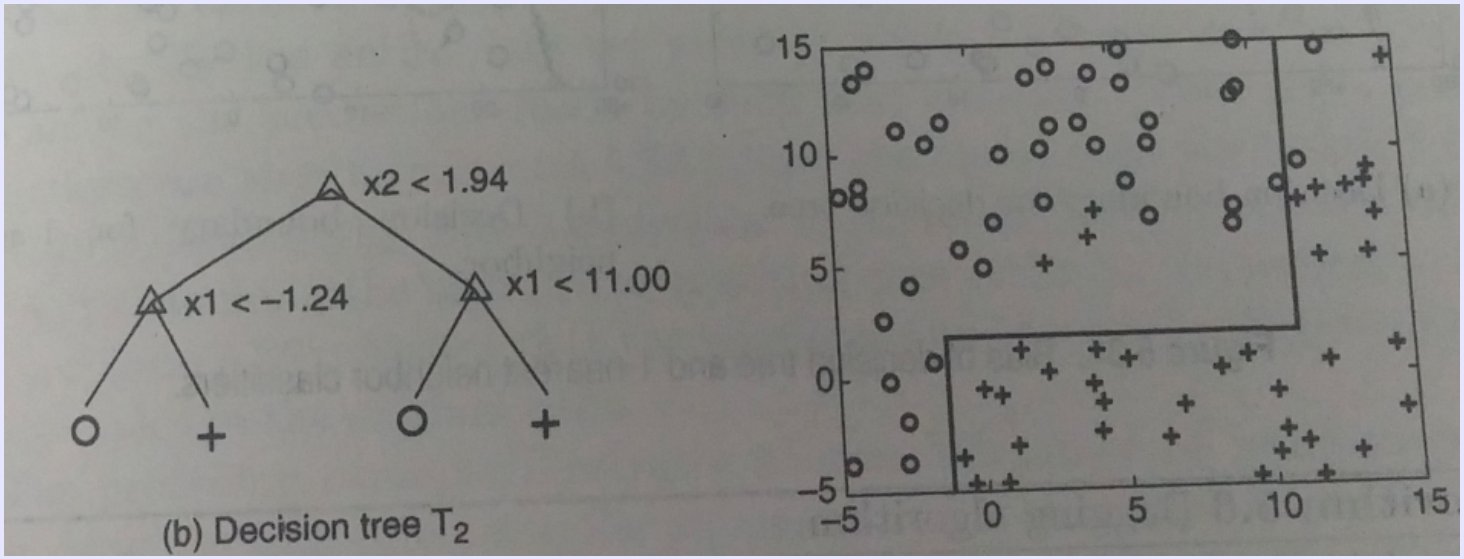
Bias, Variance, Under/Over-fitting

High Bias

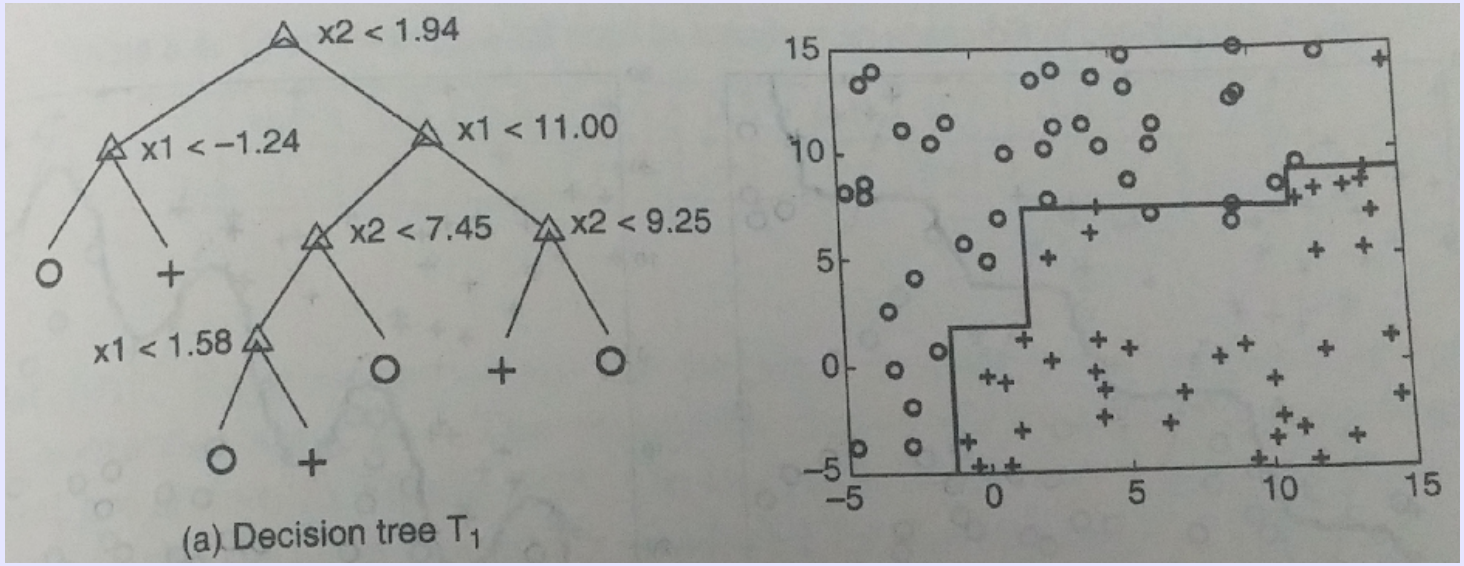


Bias, Variance, Under/Over-fitting

High Bias

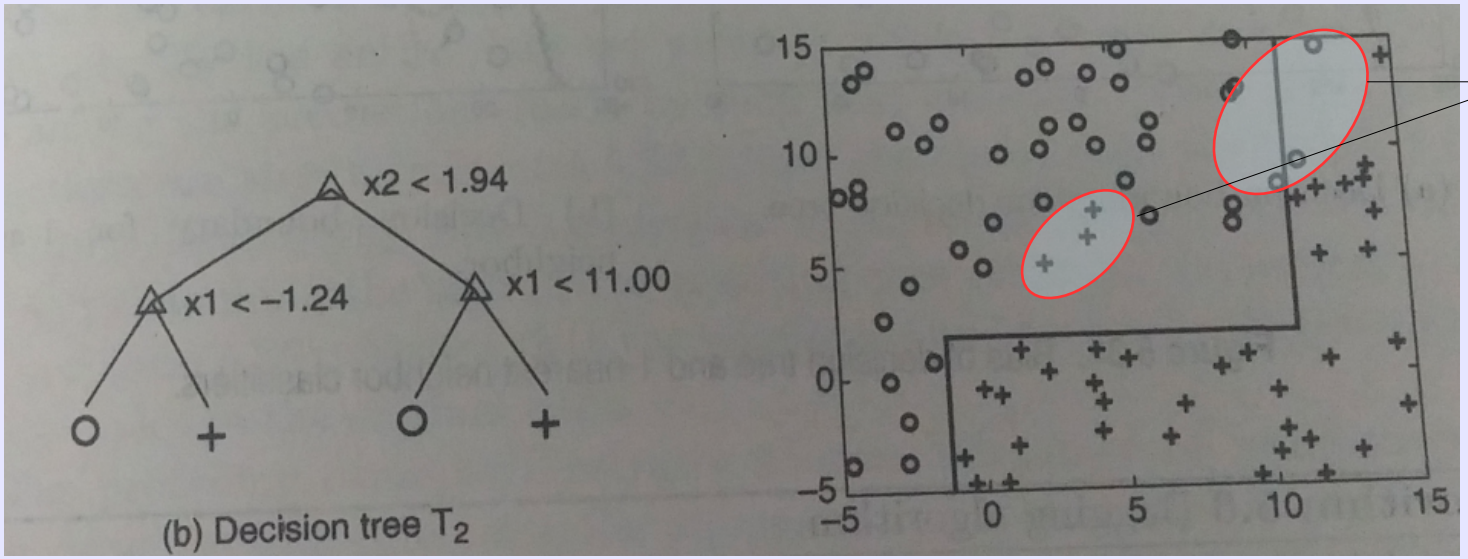


Low Bias



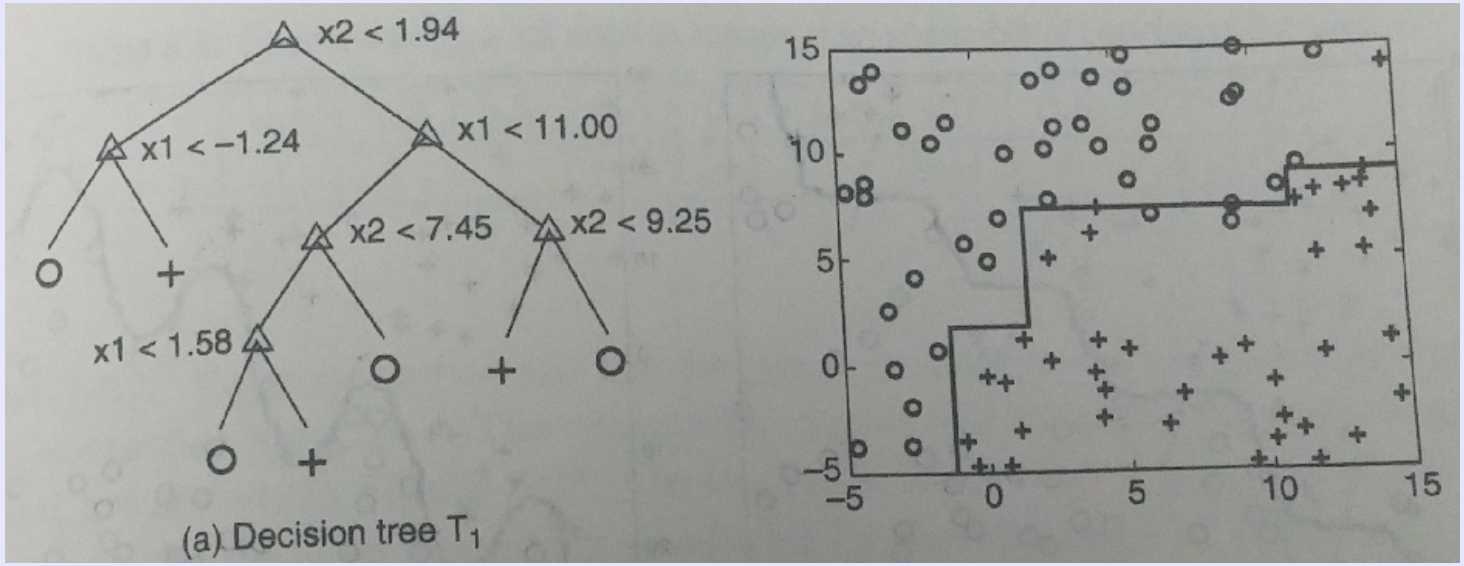
Bias, Variance, Under/Over-fitting

High Bias



Mis-classified

Low Bias



Overfit?

Bias, Variance, Under/Over-fitting

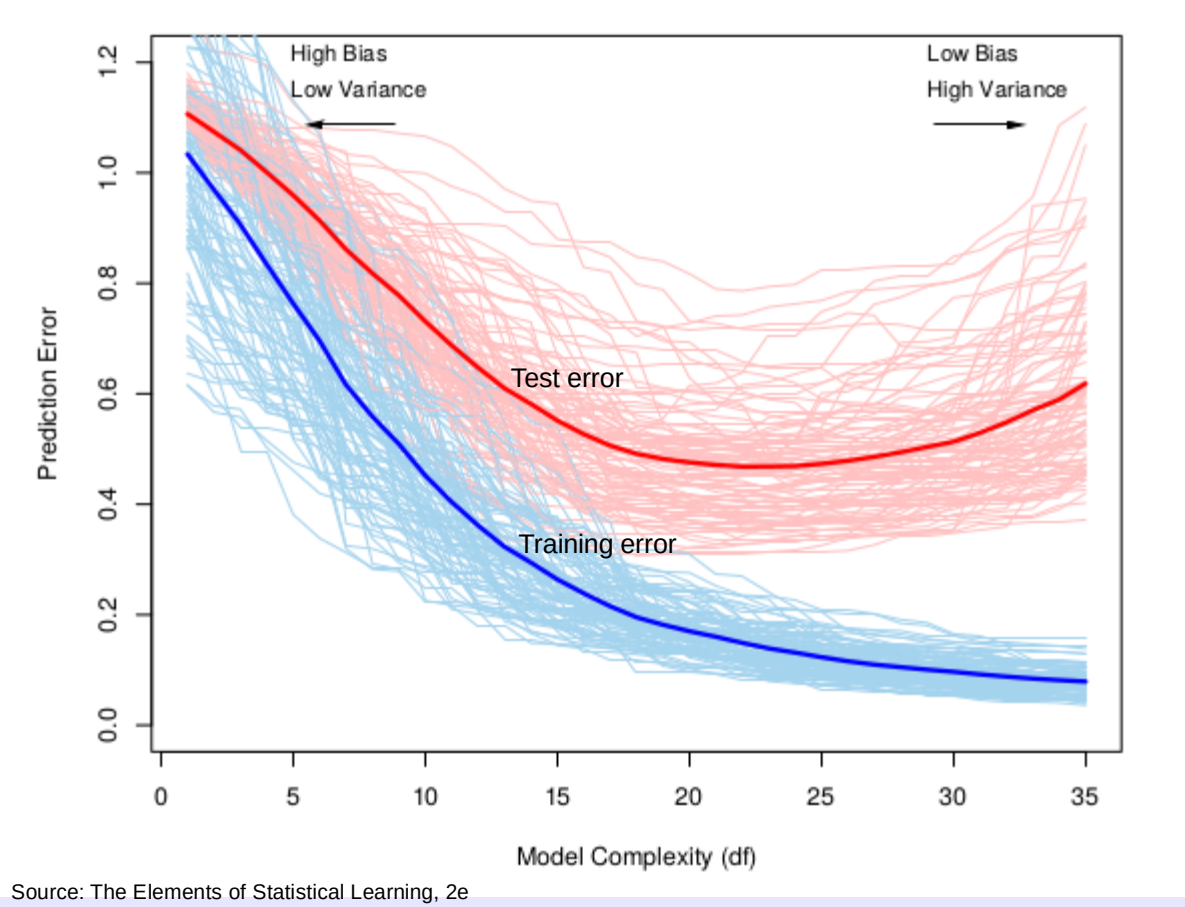
- Bias is how far a model's predictions are from the target.
  - $\text{bias}(\hat{\theta}) = E(\hat{\theta}) - \theta$
- Variance, on the other hand, is how your model reacts to changes in the training data.
  - $\text{variance}(\hat{\theta}) = E(\hat{\theta} - E(\hat{\theta}))^2$
- As the model becomes more complex, it picks up patterns in the training data, thus making it less generalizable.
  - A different training dataset (drawn from the same distribution) may induce results that vary from before.

Bias, Variance, Under/Over-fitting

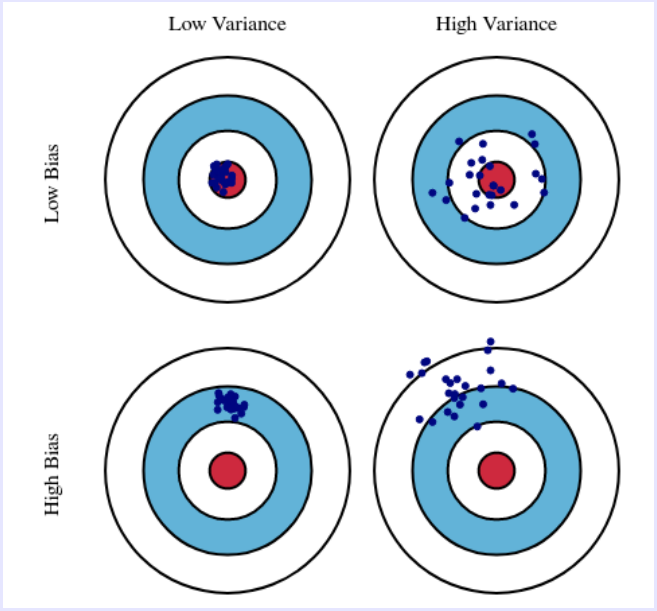
- Let’s play a game!

Photo by JESHOOTS.COM on Unsplash (https://unsplash.com)

Bias, Variance, Under/Over-fitting



Source: The Elements of Statistical Learning, 2e



A model with many predictive attributes will exhibit **low bias, high variance**.
A model with too few predictive attributes will exhibit **low variance, but may be quite biased**.

Informally: **bias** is how far a model's predictions are from target (underfitting), and **variance** is the degree to which these predictions vary between model iterations (overfitting).

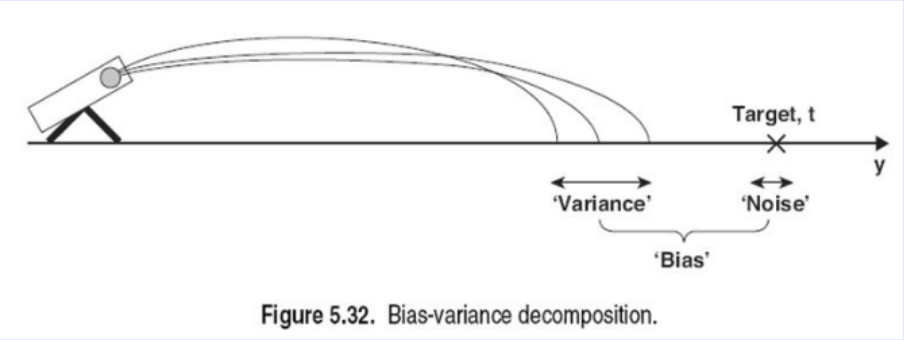
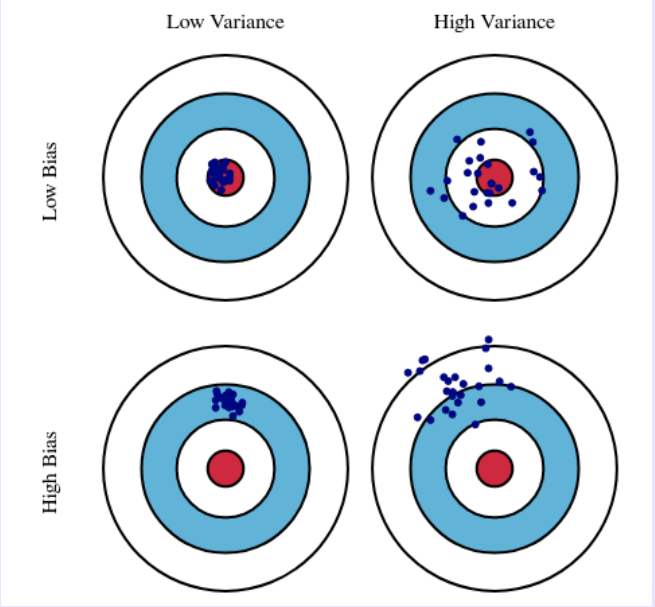


Figure 5.32. Bias-variance decomposition.

Bias, Variance, Under/Over-fitting

Informally: **bias** is how far a model's predictions are from target (underfitting), and **variance** is the degree to which these predictions vary between model iterations (overfitting).



Mathematically,

$$\mathrm{Err}(\hat{\theta}) = \mathrm{bias}(\hat{\theta})^2 + \mathrm{variance}(\hat{\theta}) + \epsilon, \text{where } \epsilon \text{ is the irreducible error}$$

Proof follows. Recall that:

1) E[X+Y] = E[X]+E[Y] (Linearity of expectation)
2) E[XY] = E[X] * E[Y] iff X and Y are iid
3) E[E[X]] = E[X]

Bias, Variance, Under/Over-fitting

$\text{Err}(\hat{\theta}) = \text{bias}(\hat{\theta})^2 + \text{variance}(\hat{\theta}) + \epsilon$, where ϵ is the irreducible error

The mean squared error of an estimator $\hat{\theta} = f(D;\theta)$ can be defined as:
$\text{mse}(\hat{\theta}) = E[(\hat{\theta} - \theta)^2|\theta]$

Proposition: $\text{mse}(\hat{\theta}) = \text{bias}(\hat{\theta})^2 + \text{variance}(\hat{\theta})$

Bias, Variance, Under/Over-fitting

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Proof: $\text{mse}(\hat{\theta}) = E(\hat{\theta} - \theta)^2 = E[\hat{\theta} - E(\hat{\theta}) + E(\hat{\theta}) - \theta]^2$

Bias, Variance, Under/Over-fitting

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

Bias, Variance, Under/Over-fitting

$\text{Err}(\hat{\theta}) = \text{bias}(\hat{\theta})^2 + \text{variance}(\hat{\theta}) + \epsilon$, where ϵ is the irreducible error

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Proposition: $\text{mse}(\hat{\theta}) = \text{bias}(\hat{\theta})^2 + \text{variance}(\hat{\theta})$

Proof:
$$\begin{aligned}\text{mse}(\hat{\theta}) = E(\hat{\theta} - \theta)^2 &= E[\hat{\theta} - E(\hat{\theta}) + E(\hat{\theta}) - \theta]^2 \\ &= E[(\hat{\theta} - E(\hat{\theta})) + (E(\hat{\theta}) - \theta)]^2 \\ &= E[(\hat{\theta} - E(\hat{\theta}))^2 + 2(\hat{\theta} - E(\hat{\theta}))(E(\hat{\theta}) - \theta)) + (E(\hat{\theta}) - \theta)^2]\end{aligned}$$

Bias, Variance, Under/Over-fitting

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$$\begin{aligned}\text{mse}(\hat{\theta}) = E(\hat{\theta} - \theta)^2 &= E[\hat{\theta} - E(\hat{\theta}) + E(\hat{\theta}) - \theta]^2 \\ &= E[(\hat{\theta} - E(\hat{\theta})) + (E(\hat{\theta}) - \theta)]^2 \\ &= E[(\hat{\theta} - E(\hat{\theta}))^2 + 2(\hat{\theta} - E(\hat{\theta}))(E(\hat{\theta}) - \theta)) + (E(\hat{\theta}) - \theta)^2]\end{aligned}$$

0

Bias, Variance, Under/Over-fitting

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Proof:

$$\begin{aligned}
\text{mse}(\hat{\theta}) = E(\hat{\theta} - \theta)^2 &= E[\hat{\theta} - E(\hat{\theta}) + E(\hat{\theta}) - \theta]^2 \\
&= E[(\hat{\theta} - E(\hat{\theta})) + (E(\hat{\theta}) - \theta)]^2 \\
&= E[(\hat{\theta} - E(\hat{\theta}))^2 + 2(\hat{\theta} - E(\hat{\theta}))(E(\hat{\theta}) - \theta)) + (E(\hat{\theta}) - \theta)^2] \\
&= E(\hat{\theta} - E(\hat{\theta}))^2 + E(E(\hat{\theta}) - \theta)^2
\end{aligned}$$

0

Variance

Bias, Variance, Under/Over-fitting

$\text{Err}(\hat{\theta}) = \text{bias}(\hat{\theta})^2 + \text{variance}(\hat{\theta}) + \epsilon$, where ϵ is the irreducible error

The mean squared error of an estimator $\hat{\theta} = f(D;\theta)$ can be defined as:
$\text{mse}(\hat{\theta}) = E[(\hat{\theta} - \theta)^2 | \theta]$

Proposition: $\text{mse}(\hat{\theta}) = \text{bias}(\hat{\theta})^2 + \text{variance}(\hat{\theta})$

Proof:

$$\begin{aligned}
\text{mse}(\hat{\theta}) = E(\hat{\theta} - \theta)^2 &= E[\hat{\theta} - E(\hat{\theta}) + E(\hat{\theta}) - \theta]^2 \\
&= E[(\hat{\theta} - E(\hat{\theta})) + (E(\hat{\theta}) - \theta)]^2 \\
&= E[(\hat{\theta} - E(\hat{\theta}))^2 + 2(\hat{\theta} - E(\hat{\theta}))(E(\hat{\theta}) - \theta)) + (E(\hat{\theta}) - \theta)^2] \\
&= E(\hat{\theta} - E(\hat{\theta}))^2 \\
&\quad + E(E(\hat{\theta}) - \theta)^2 \\
&\quad + (E(\hat{\theta}) - \theta)^2
\end{aligned}$$

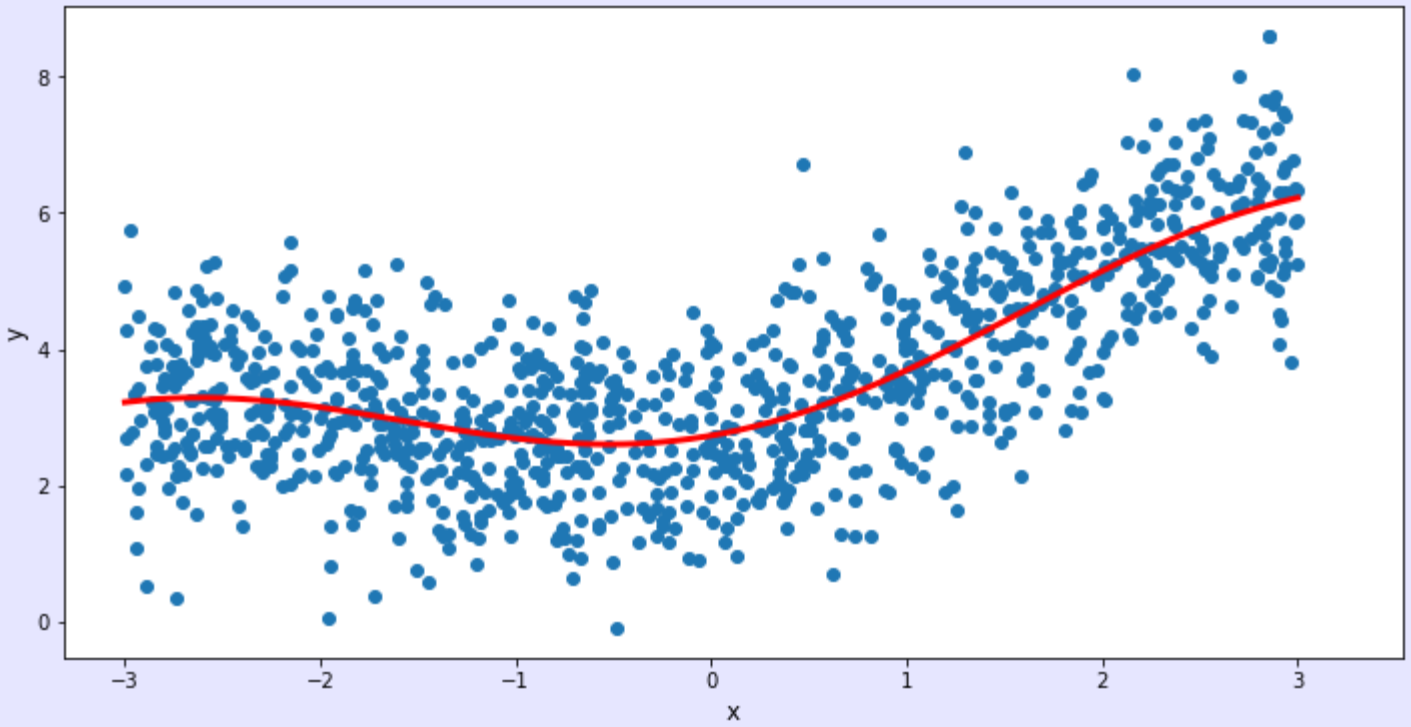
0

Variance

Bias^2

Bias, Variance, Under/Over-fitting

Example: $f(x) = \frac{1}{2}x + \sqrt{\max(x, 0)} - cosx + 2$



- Noise is $\mathcal{N}(0, 1)$.
- 1,000 points.
- Red curve: true f(x)

Note: f(x) follows a non-linear pattern due to square root and cosine in its definition.

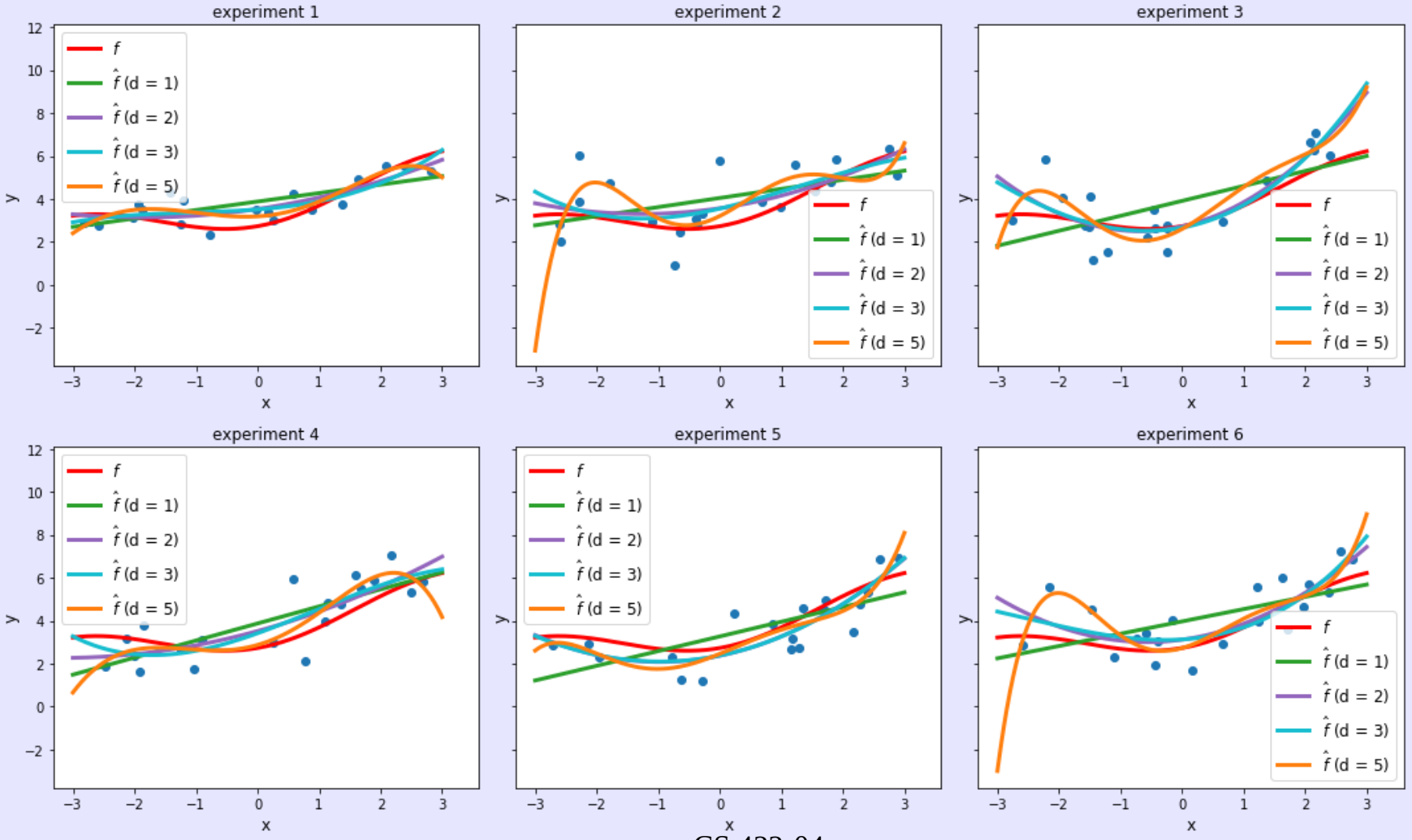
Task: To predict f(x), model the problem with polynomial regression of varying degrees:

$$\hat{f}(x) = w_0 + w_1 x + w_2 x^2 + \ldots + w_d x^d$$

Source: "The bias-variance tradeoff," Giorgos Oaoachristoudis, Nov 2019.

Bias, Variance, Under/Over-fitting

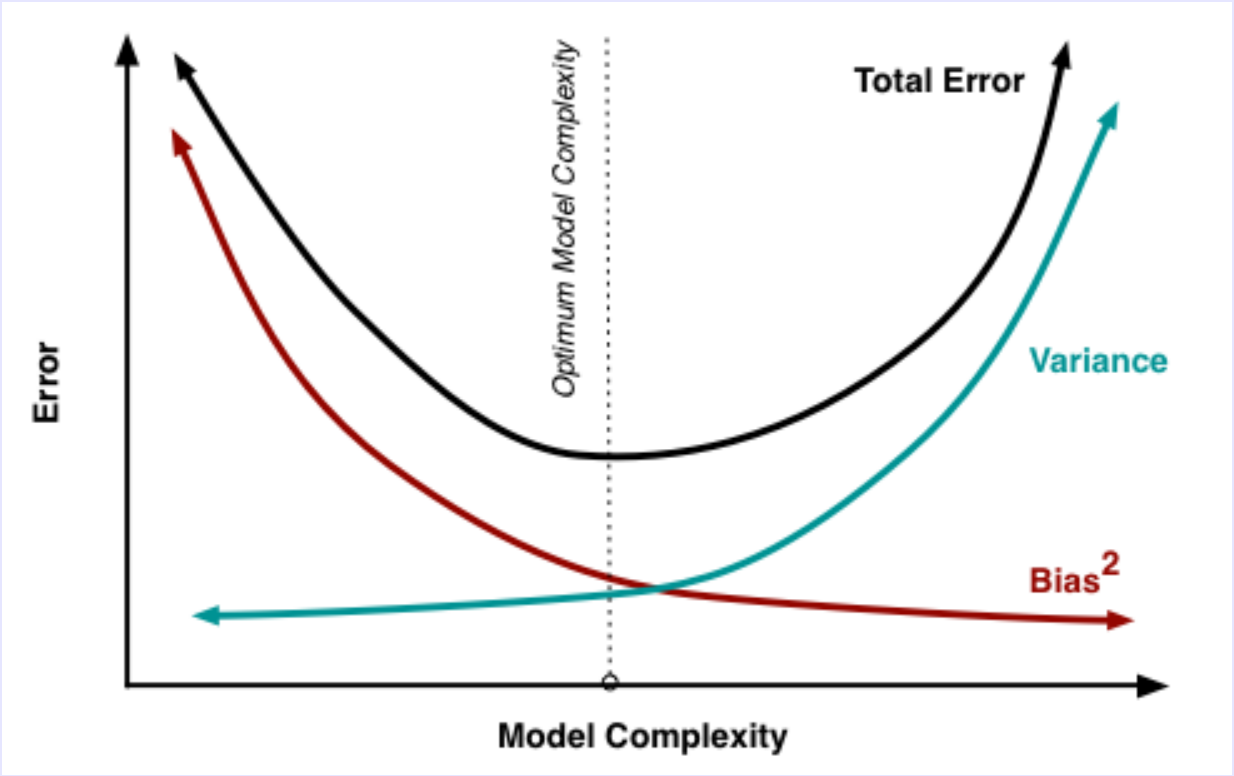
Example: 20 random points chosen for training in 6 different experiments. Different degree regression models (d = 1, 2, 3, 5); note the variance: complex models have high variance.



Source: "The bias-variance tradeoff," Giorgos Oaoachristoudis, Nov 2019.

Bias, Variance, Under/Over-fitting

- At its heart, bias and variance is really about dealing with underfitting (bias) and overfitting (variance).



Graphic source: Scott Fortman
http://scott.fortmann-roe.com/docs/BiasVariance.html

Bias, Variance, Under/Over-fitting

A model with many predictive attributes will exhibit **low bias, high variance**. A model with too few predictive attributes will exhibit **low variance, but may be quite biased**.

- Mitigation approaches
  - Dimensionality reduction and feature selection can reduce variance by simplifying models.
  - Regularization can help reduce variance.
  - If you cannot reduce dimensions or engage in feature selection, a larger training set may decrease variance.
  - Adding features decreases bias, at the expense of additional variance.