Lecture 08

Model Evaluation 1:
Introduction to Overfitting and Underfitting

STAT 479: Machine Learning, Fall 2018

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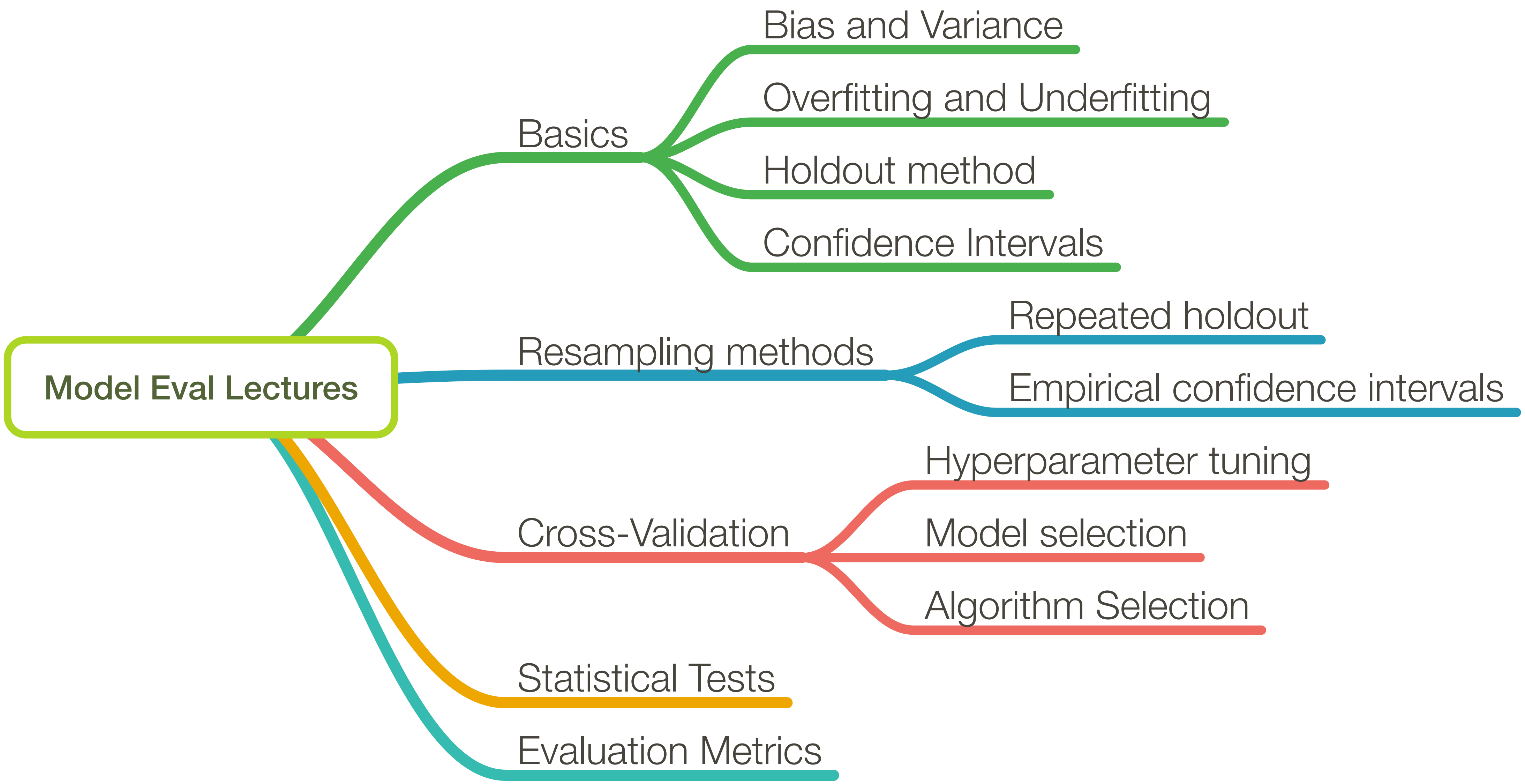
http://stat.wisc.edu/~sraschka/teaching/stat479-fs2018/

Overview



Model Eval Lectures

- Basics
  - Bias and Variance
  - Overfitting and Underfitting
  - Holdout method
  - Confidence Intervals
- Resampling methods
  - Repeated holdout
  - Empirical confidence intervals
- Cross-Validation
  - Hyperparameter tuning
  - Model selection
  - Algorithm Selection
- Statistical Tests
- Evaluation Metrics

Overfitting and Underfitting

Overfitting and Underfitting

"Generalization Performance"

- Goal is to fit a model that performs well on unseen inputs, that is, a model that "generalizes" well to unseen data

- A model that performs well on unseen inputs has a good generalization performance

- We say that a model with a good generalization performance has a "high generalization accuracy" or "low generalization error"

Overfitting and Underfitting

Assumptions

- i.i.d. assumption: inputs are independent, and training and test examples are identically distributed (drawn from the same probability distribution)

- The training error or accuracy provides an (optimistically) biased estimate of the generalization performance

- For some random model that has not been fitted to the training set, we expect both the training and test error to be equal

Overfitting and Underfitting

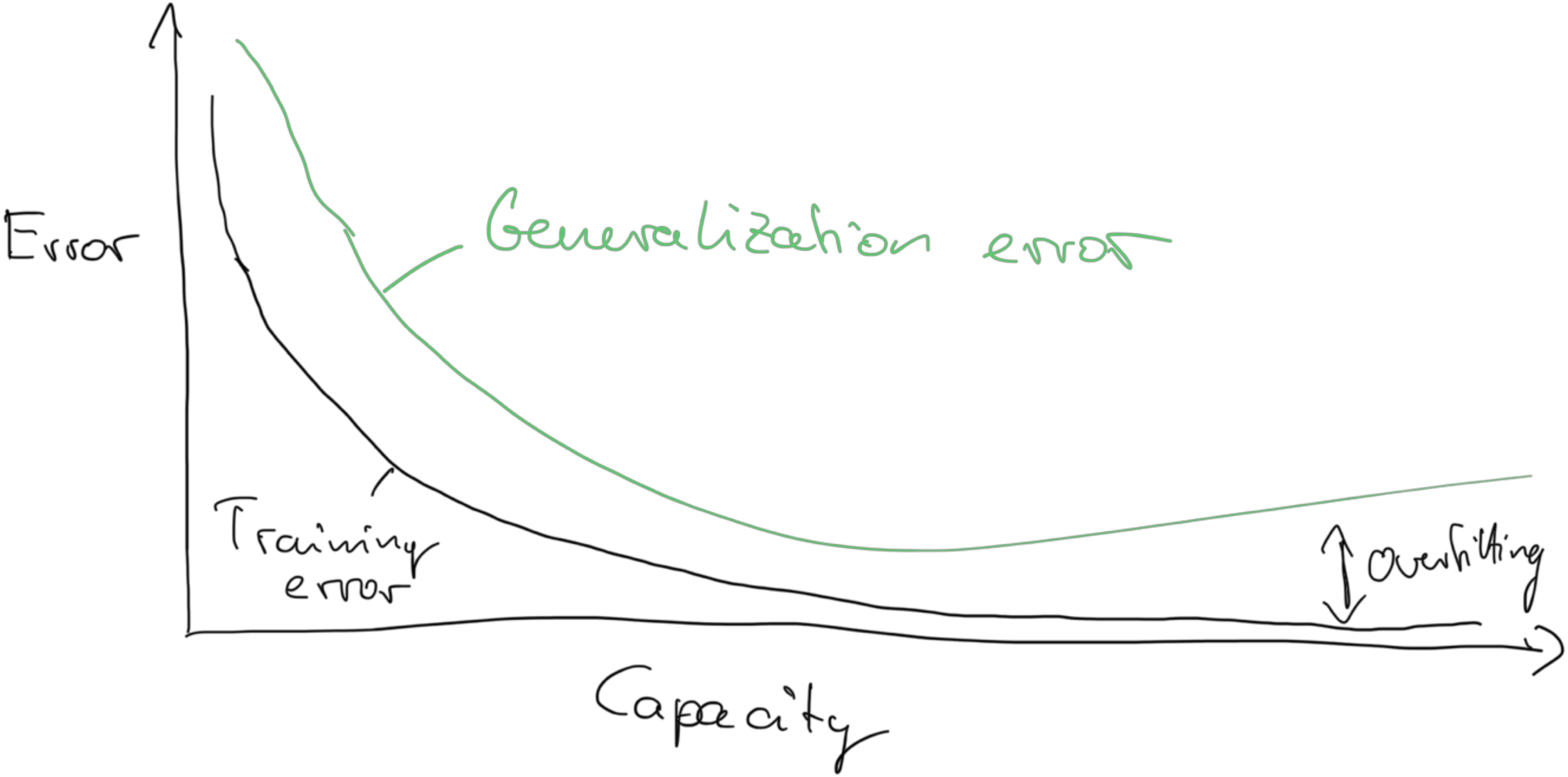
Model Capacity

- Underfitting: both training and test error are large

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

- Generally, the larger the hypothesis space being searched by a learning algorithm, the higher its tendency to overfit (the size of the hypothesis space is related to the so-called "capacity" of a model); vice versa, models with small capacity do not even fit the training set well

Overfitting and Underfitting

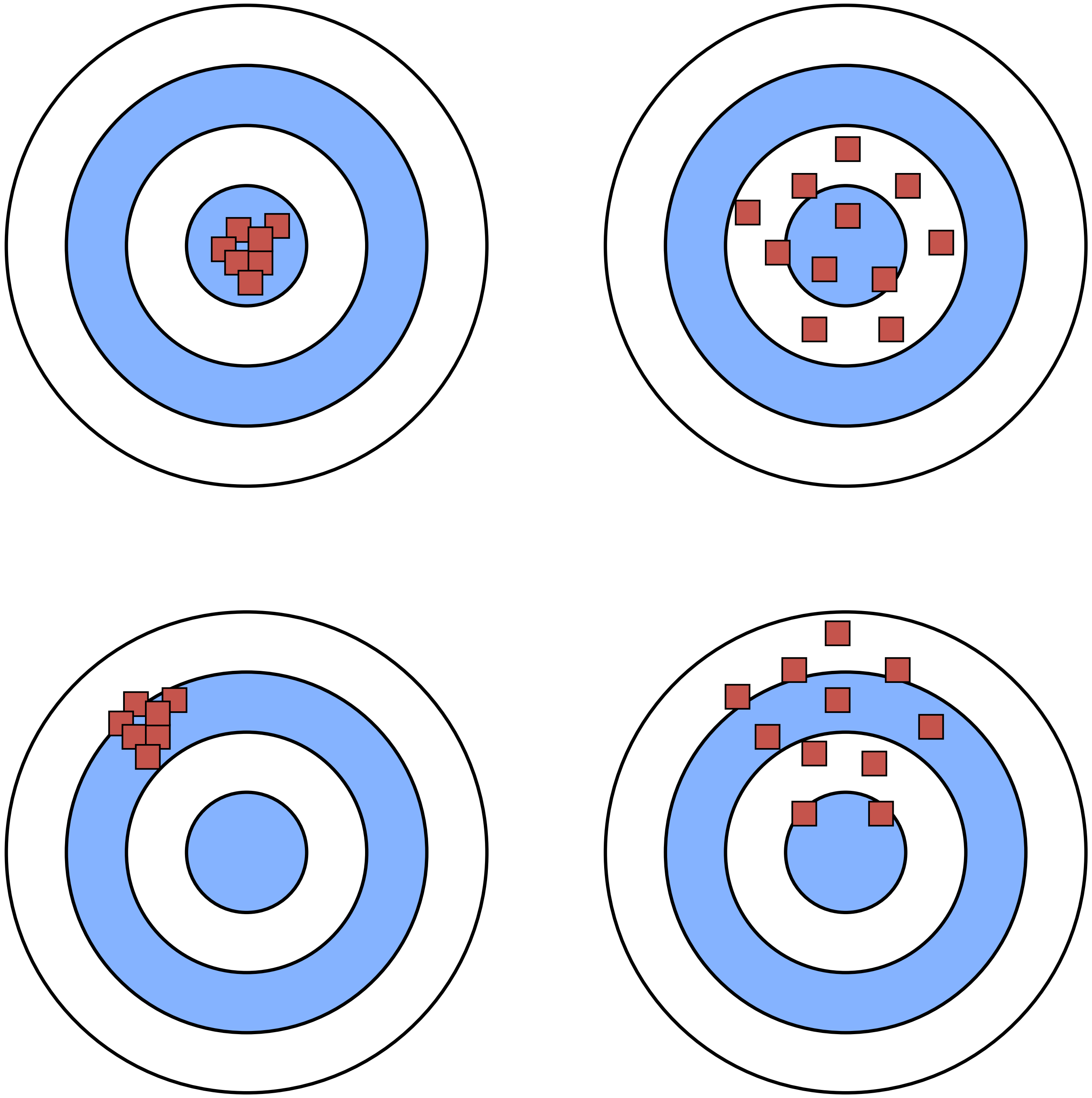


Bias-Variance Decomposition and Trade-off

Bias-Variance Decomposition

- Decomposition of the loss into bias and variance help us understand learning algorithms, concepts are correlated to underfitting and overfitting

Bias-Variance Intuition



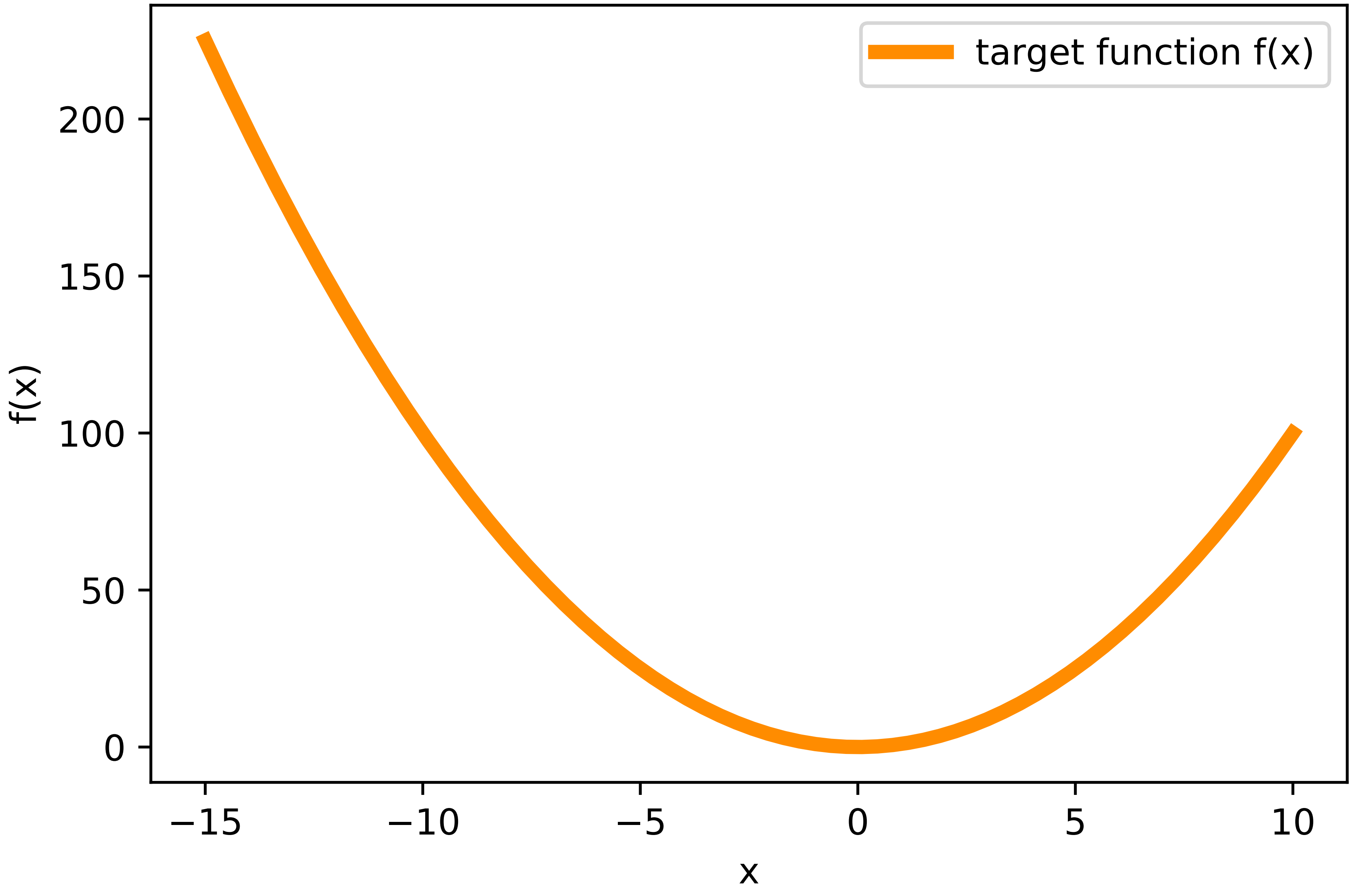
Low Variance
(Precise)

High Variance
(Not Precise)

Low Bias
(Accurate)

High Bias
(Not Accurate)

Bias and Variance Intuition



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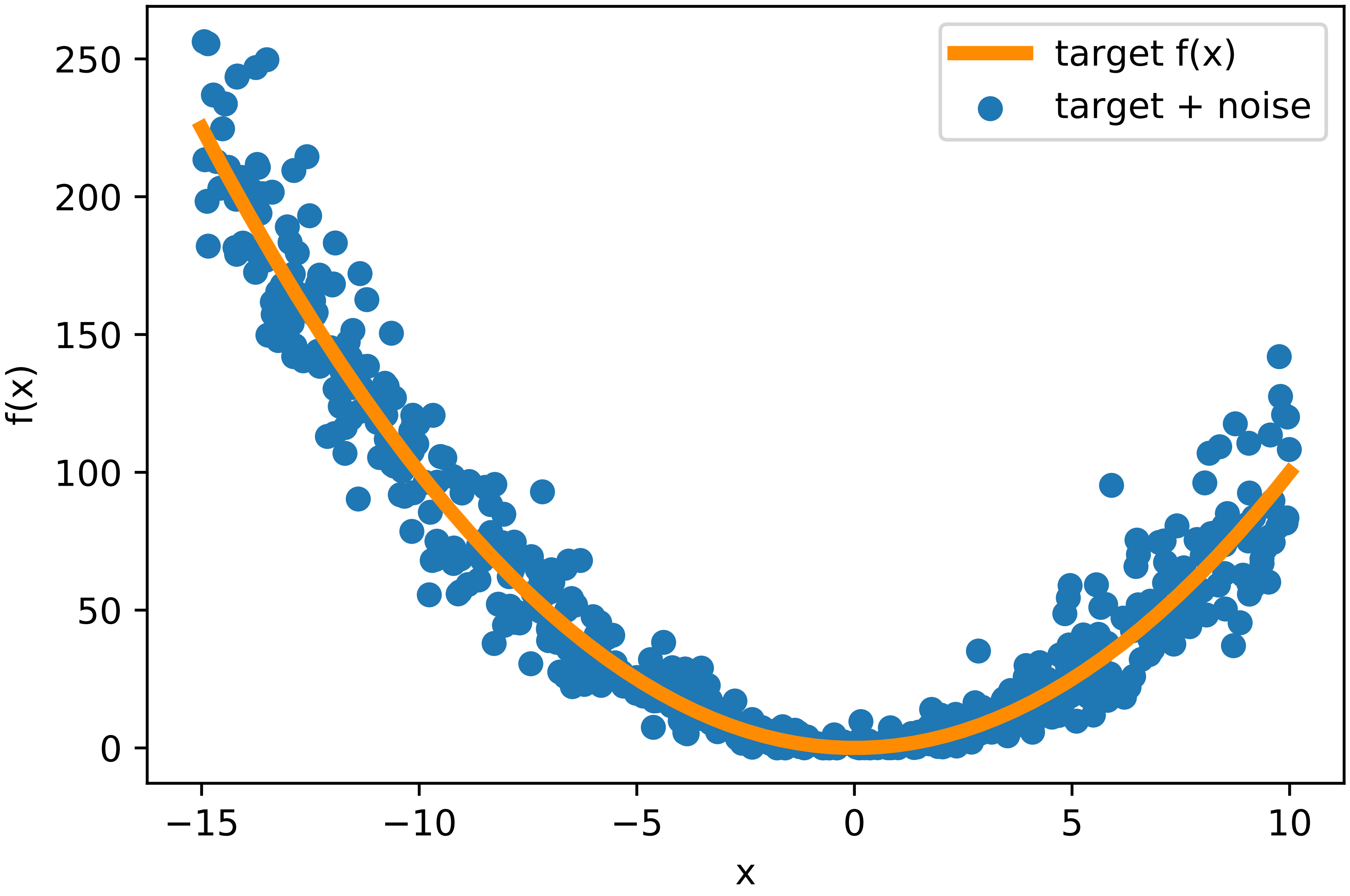

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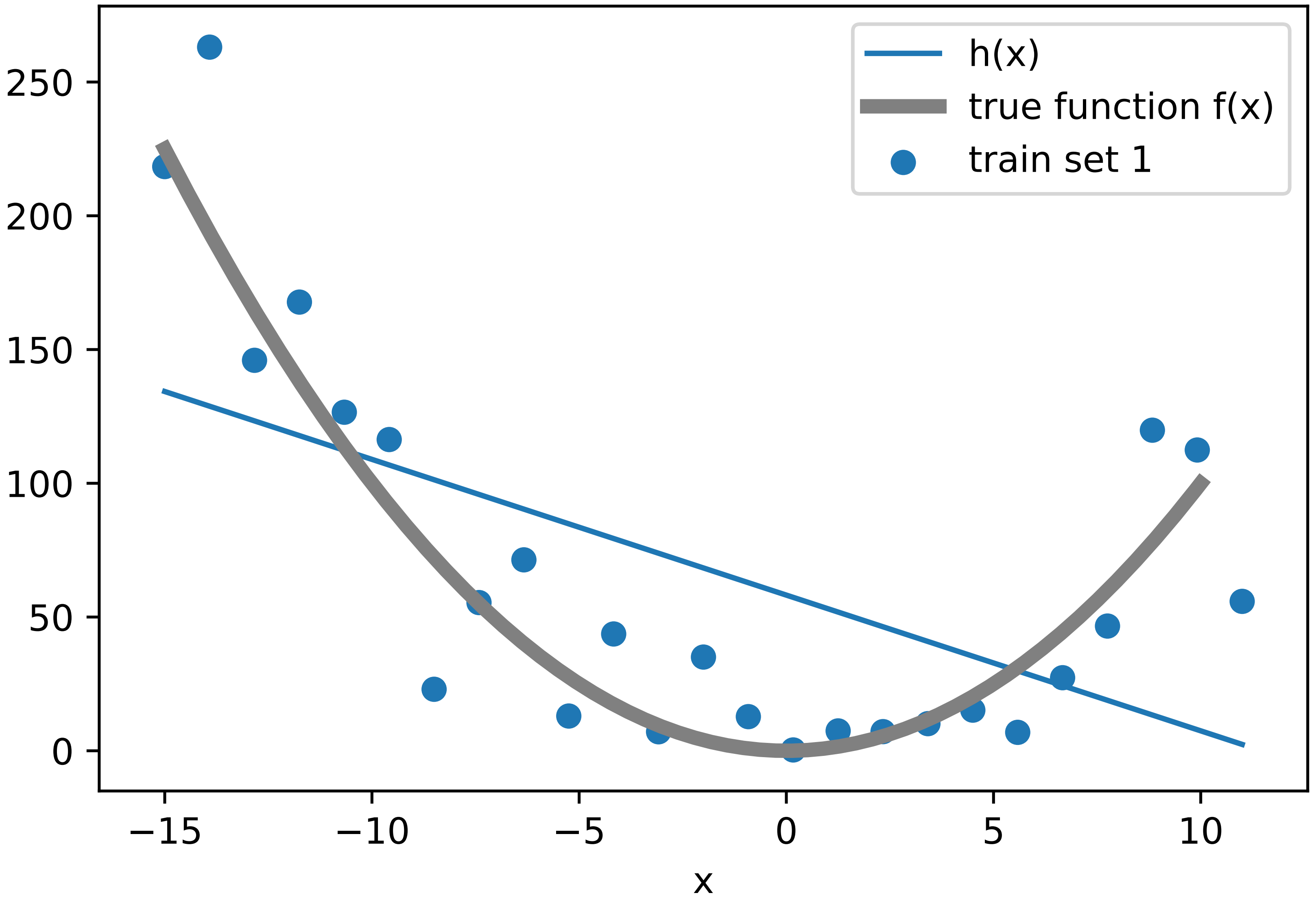

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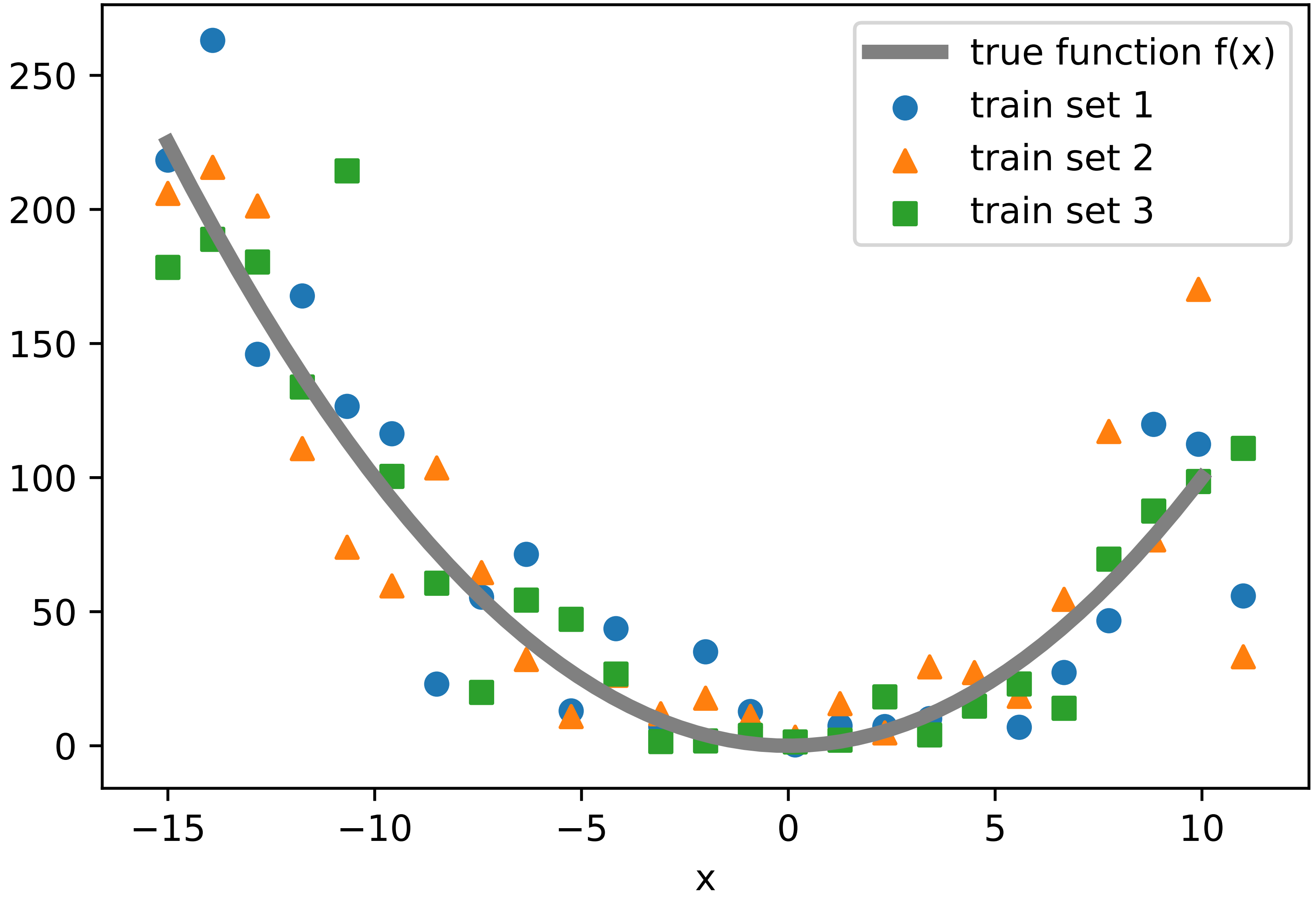

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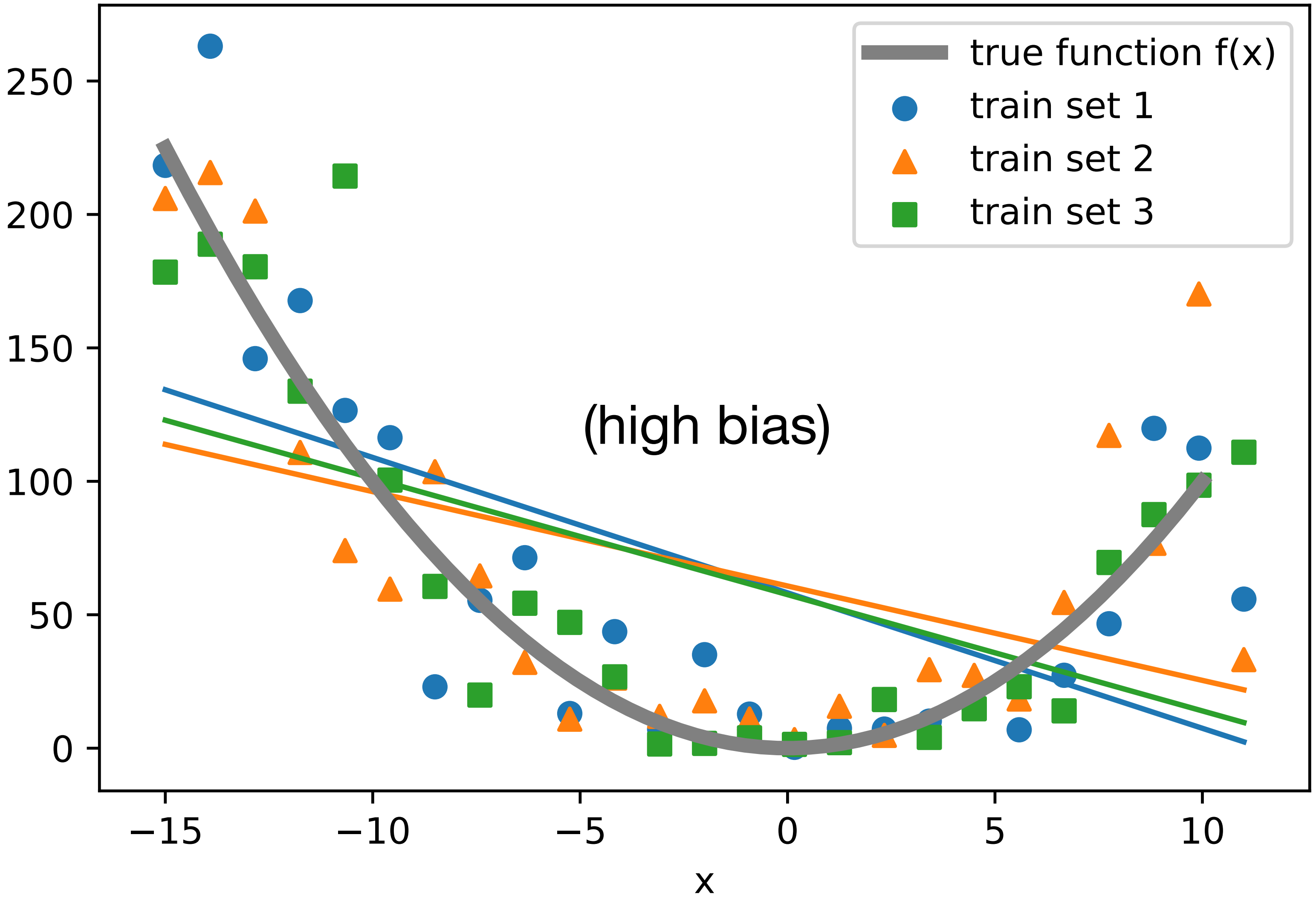
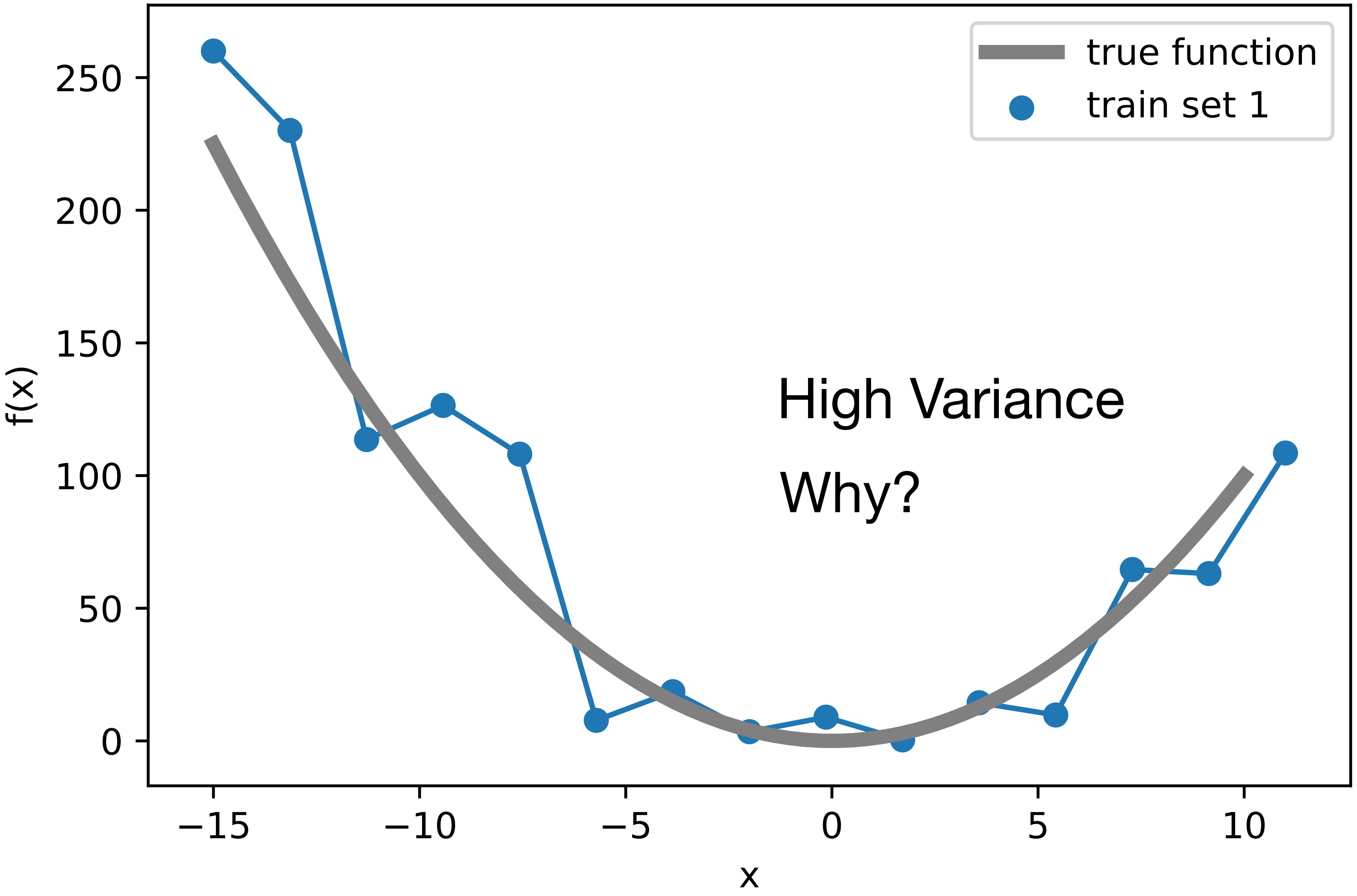
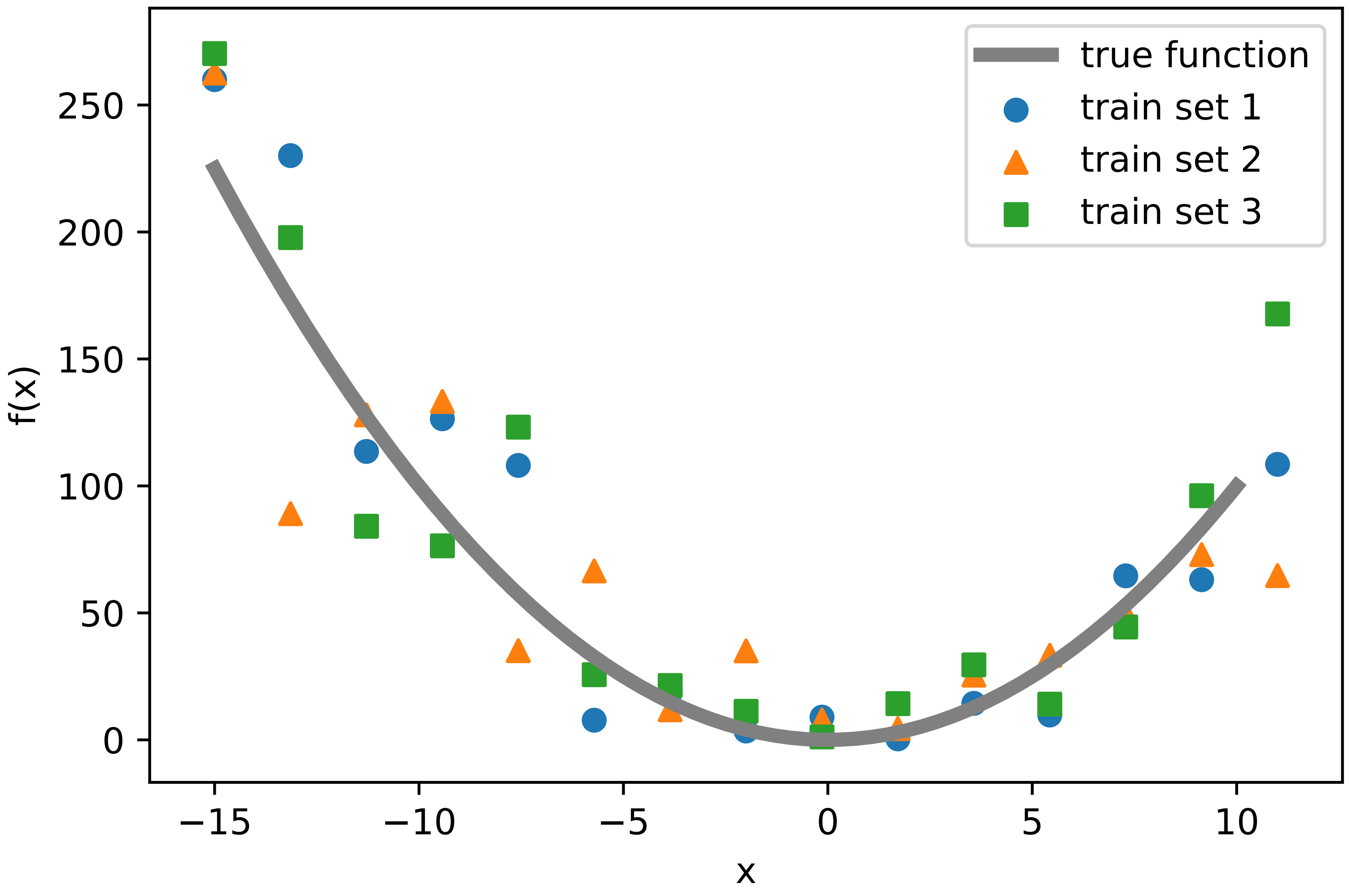


Bias and Variance Intuition



(here, I fit an unpruned decision tree)

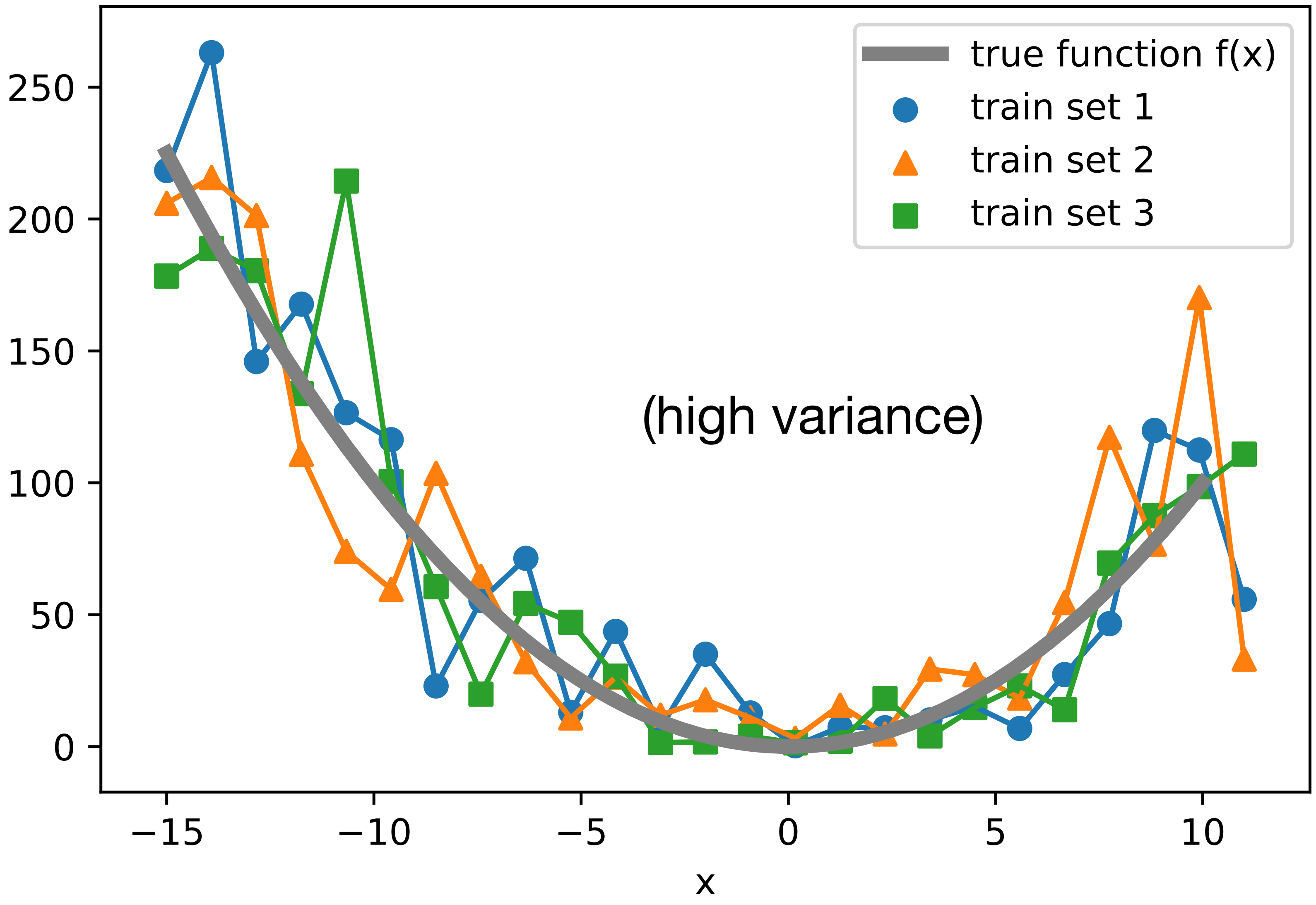
Bias and Variance Example



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

suppose we have multiple training sets

Bias and Variance Example



Bias-Variance Decomposition

Point estimator: $\hat{\theta} = f(x^{[1]}, x^{[2]}, \ldots, x^{[n]})$

of some parameter θ

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

Bias-Variance Decomposition

Point estimator: $\hat{\theta} = f(x^{[1]}, x^{[2]}, \ldots, x^{[n]})$

of some parameter θ

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

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

(the expectation is over the training data, i.e, the average estimator from different training samples)

Bias-Variance Decomposition of Squared Error

General Definition:

Intuition:

$$\textbf{Bias}(\hat{\theta}) = E[\hat{\theta}] - \theta$$

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

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

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

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

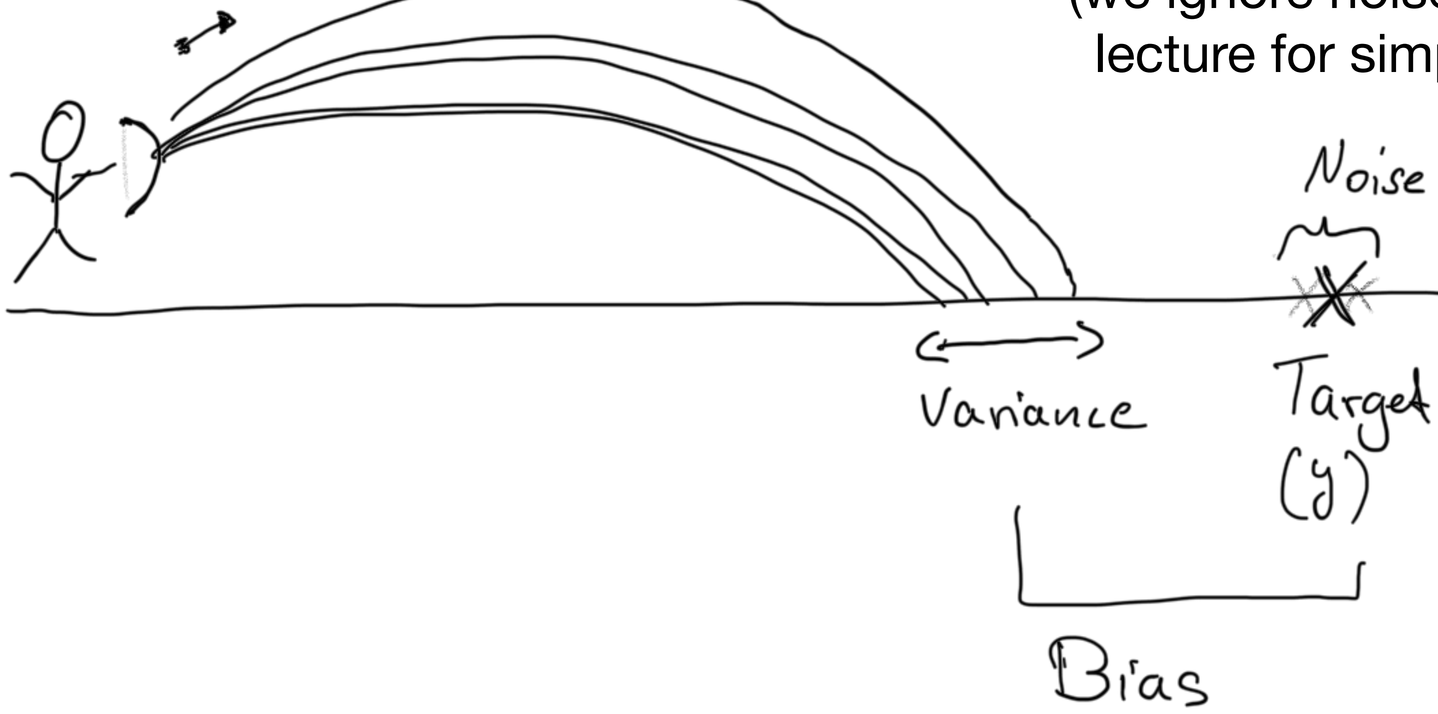
Bias-Variance Decomposition of Squared Error

General Definition:

Intuition:

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

(we ignore noise in this lecture for simplicity)



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

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

Bias-Variance Decomposition of Squared Error

General Definition:

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

"ML notation" for the Squared Error Loss:

$y = f(x)$ (target, target function)

$\hat{y} = \hat{f}(x) = h(x)$

$S = (y - \hat{y})^2$

Bias-Variance Decomposition of Squared Error

"ML notation" for the Squared Error Loss:

$y = f(x)$ (target, target function)

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$S = (y - \hat{y})^2$

$$
\begin{aligned}
S &= (y - \hat{y})^2 \\
(y - \hat{y})^2 &= (y - E[\hat{y}] + E[\hat{y}] - \hat{y})^2 \\
&= (y - E[\hat{y}])^2 + (E[\hat{y}] - y)^2 + 2(y - E[\hat{y}])(E[\hat{y}] - \hat{y})
\end{aligned}
$$

Bias-Variance Decomposition of Squared Error

$$S = (y - \hat{y})^2$$

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

$$\begin{aligned}E[S] &= E[(y - \hat{y})^2] \\ E[(y - \hat{y})^2] &= (y - E[\hat{y}])^2 + E[(E[\hat{y}] - \hat{y})^2] \\ &= \textbf{[Bias of the fit]}^2 + \textbf{Variance of the fit}\end{aligned}$$

Bias-Variance Decomposition of Squared Error

$$S = (y - \hat{y})^2$$

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

$$= (y - E[\hat{y}])^2 + (E[\hat{y}] - y)^2 + \overset{???}{\boxed{2(y - E[\hat{y}])(E[\hat{y}] - \hat{y})}}$$

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Bias-Variance Decomposition of Squared Error

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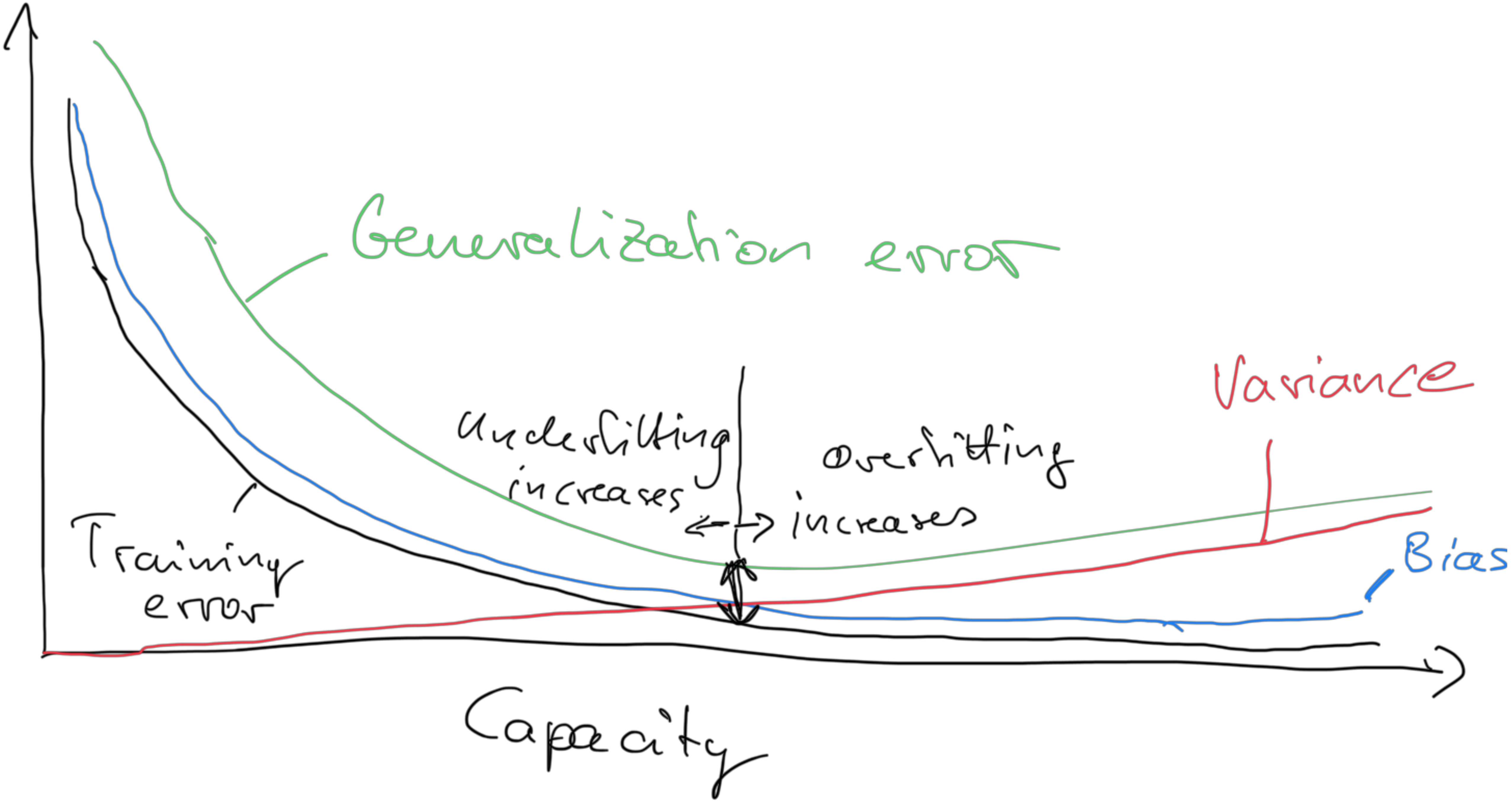
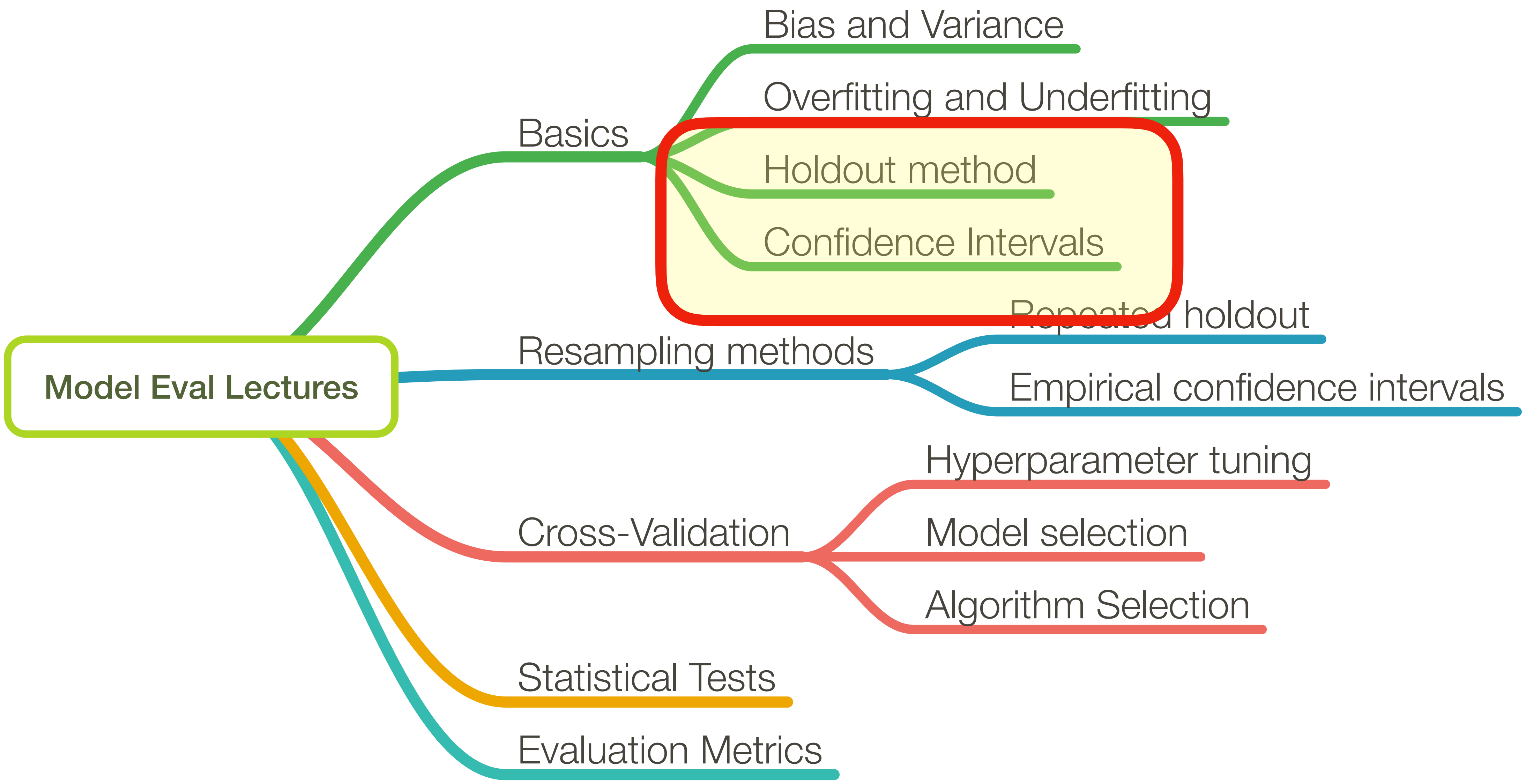
&= (y - E[\hat{y}])^2 + (E[\hat{y}] - y)^2 \overset{???}{\boxed{+\, 2(y - E[\hat{y}])(E[\hat{y}] - \hat{y})}}
\end{aligned}$$

$$\begin{aligned}
E[2(y - E[\hat{y}])(E[\hat{y}] - \hat{y})] &= 2E[(y - E[\hat{y}])(E[\hat{y}] - \hat{y})] \\
&= 2(y - E[\hat{y}])E[(E[\hat{y}] - \hat{y})] \\
&= 2(y - E[\hat{y}])(E[E[\hat{y}]] - E[\hat{y}]) \\
&= 2(y - E[\hat{y}])(E[\hat{y}] - E[\hat{y}]) \\
&= 0
\end{aligned}$$


Generalization error
Variance
underfitting increases
overfitting increases
Bias
Training error
Capacity

to be continued ...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