Machine Learning

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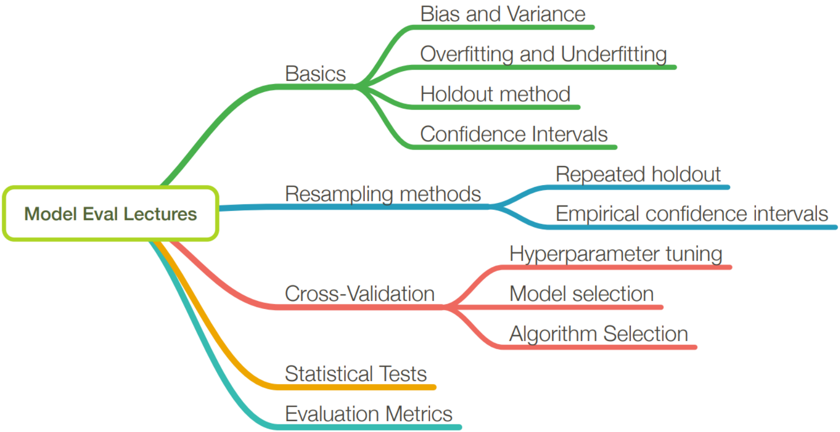
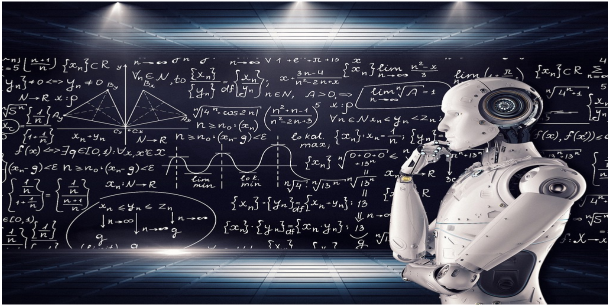
Overview


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



When can we say that the machine has learned?

Generalization Performance

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- When a model to ”generalize” well to unseen data (”high generalization accuracy” or ”low generalization error”)

Overfitting and Underfitting

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Assumptions

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Assumptions

- i.i.d. assumption: inputs are independent, and training and test examples are identically distributed (drawn from the same probability distribution)
- For some random model that has not been fitted to the training set, we expect both the training and test error to be equal
- The training error or accuracy provides an (optimistically) biased estimate of the generalization performance

Overfitting and Underfitting

Model Capacity

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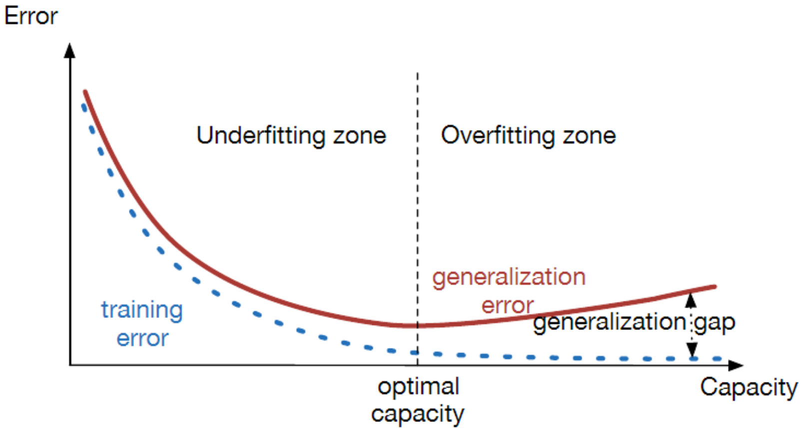
Model Capacity

- Underfitting: both training and test error are large
- Overfitting: gap between training and test error (where test error is higher)
- Large hypothesis space being searched by a learning algorithm
  - high tendency to overfit

Overfitting and Underfitting



Bias-Variance Trade-off

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Bias-Variance Decomposition

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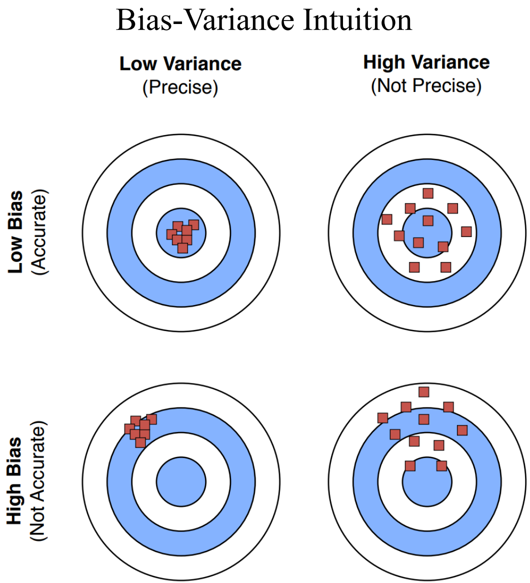
- Decomposition of the loss into bias and variance help us understand learning algorithms, concepts are correlated to underfitting and overfitting
- Helps explain why ensemble methods (last lecture) might perform better than single models

Bias-Variance Trade-off



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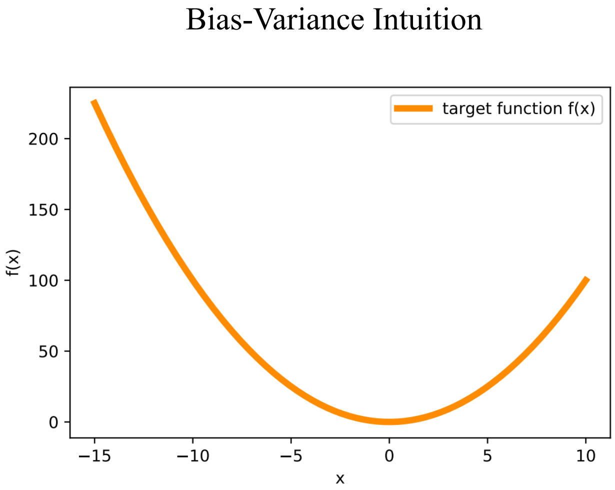
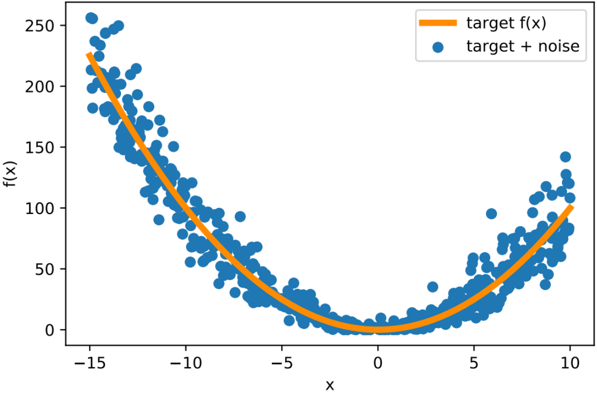


Bias-Variance Trade-off

Bias-Variance Intuition



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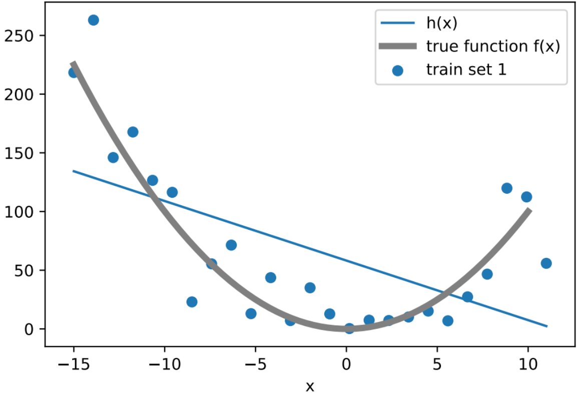

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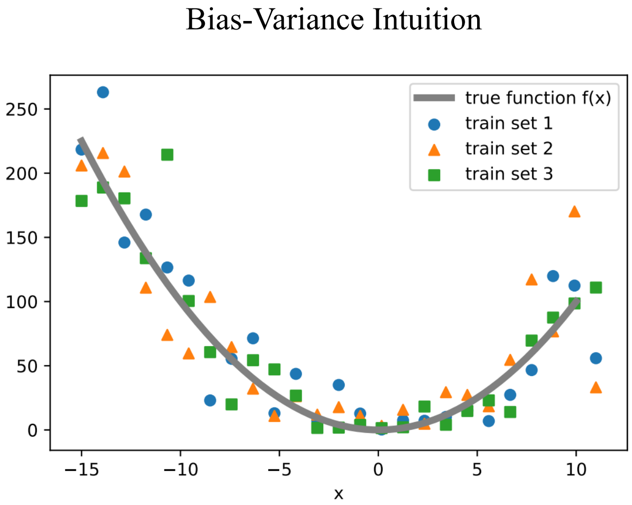

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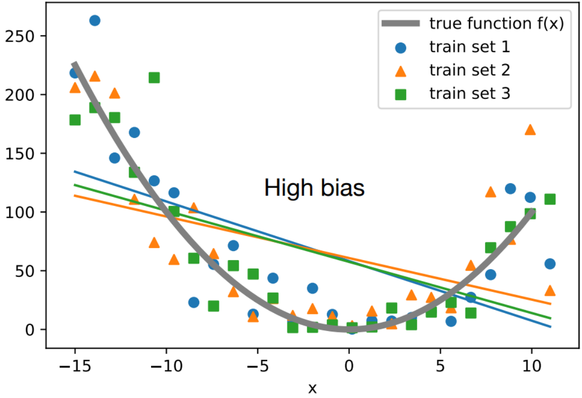

(There are two points where the bias is zero)

Bias-Variance Trade-off

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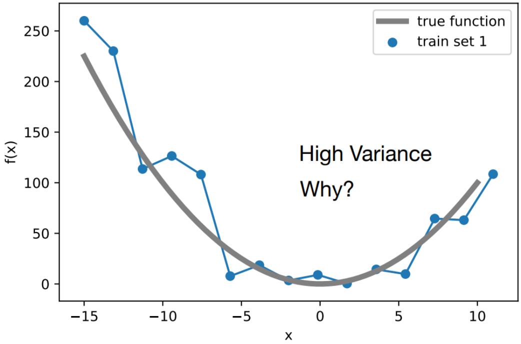

(here, I fit an unpruned decision tree)

Bias-Variance Trade-off

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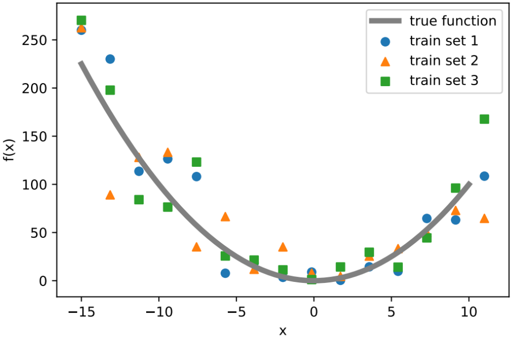
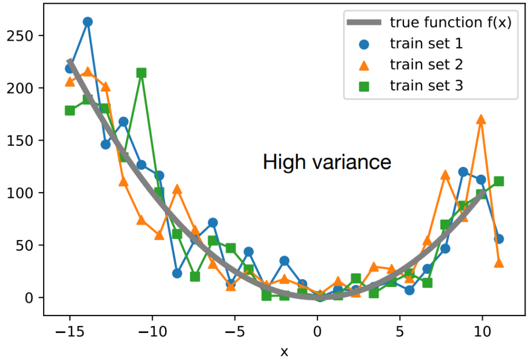


where f(x) is some true (target) function

suppose we have multiple training sets

Bias-Variance Trade-off

Bias-Variance Intuition



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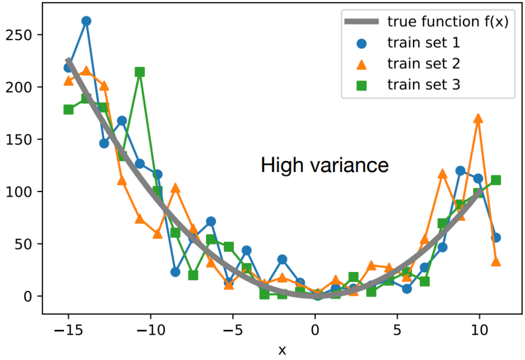

What happens if we take the average?
Does this remind you of something?

Bias-Variance Decomposition

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

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

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

Bias-Variance Decomposition

$$Loss = Bias + Variance + Noise$$

Bias-Variance Decomposition of Squared Error

- the true or target function: $y = f(x)$

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Bias-Variance Decomposition of Squared Error

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- the predicted target value: $\hat{y} = \hat{f}(x) = \hat{h}(x)$
- the squared loss: $S = (y - \hat{y})^2$

(x is a particular data point e.g,. in the test set; the expectation is over training sets)

Bias-Variance Decomposition of Squared Error

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

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

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

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

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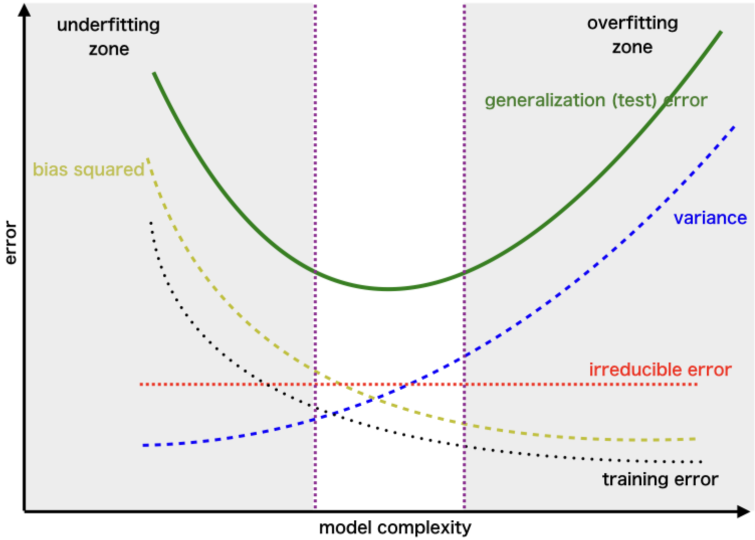
\end{aligned}$$

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

Bias-Variance Trade-off



Thank You!

Any Question?