

Machine Learning

Lecture 05: The Bias-Variance decomposition

Nevin L. Zhang

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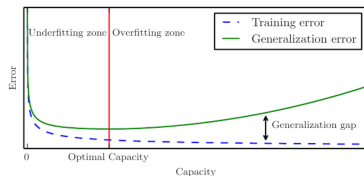
Department of Computer Science and Engineering
The Hong Kong University of Science and Technology

This set of notes is based on internet resources and
Andrew Ng. Lecture Notes on Machine Learning. Stanford.

Outline

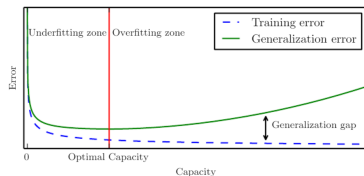
- 1 Introduction
- 2 The Bias-Variance Decomposition
- 3 Illustrations
- 4 Ensemble Learning

Introduction



- Earlier, we have learned that
 - Training error always decreases with model capacity, while
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 - Training error always decreases with model capacity, while
 - Generalization error decreases with model capacity model initially, and increases with it after a certain point.
- Model selection: Choose a model of appropriate capacity so as to minimize the generalization error.

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- Objective of this lecture:
 - Point out that generalization error has two sources: **bias** and **variance**.
 - Use the decomposition to explain the dependence of generalization error on model capacity.

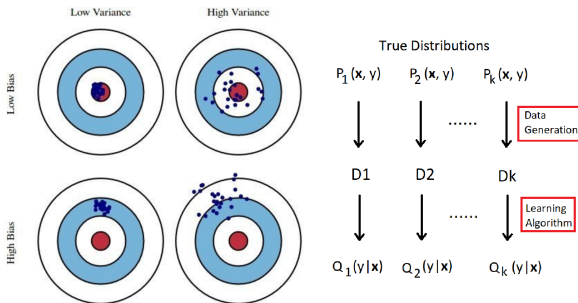
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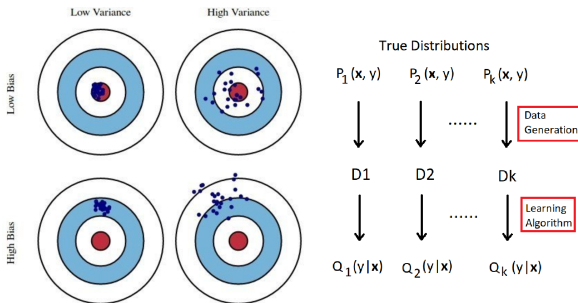
- Objective of this lecture:
 - Point out that generalization error has two sources: **bias** and **variance**.
 - Use the decomposition to explain the dependence of generalization error on model capacity.
 - Model selection: Trade-off between bias and variance.
- The bias-variance decomposition will be derived in the context of regression, but the bias-variance trade-off applies to classification also.

Bias and Variance: The Concept



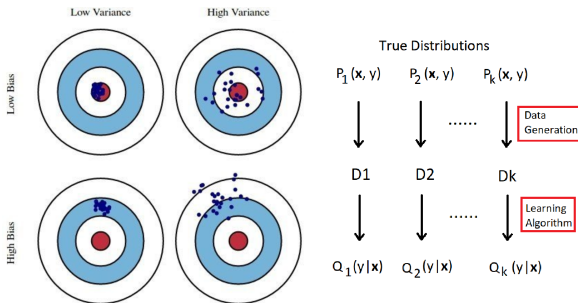
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Bias and Variance: The Concept



- An algorithm is to be applied on different occasions.
- **High bias:** Poor performances on most occasions.
 - Cause: Erroneous assumptions in the learning algorithm.
- **High variance:** Different performances on different occasions.
 - Cause: Fluctuations in the training set.

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Training and Training Error

- The training/empirical error of a hypothesis h is calculated on the training set $S = \{(\mathbf{x}_i, y_i)\}_{i=1}^m$

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- The **training error** is: $\hat{\epsilon}(\hat{h})$

Random Fluctuations in Training Set

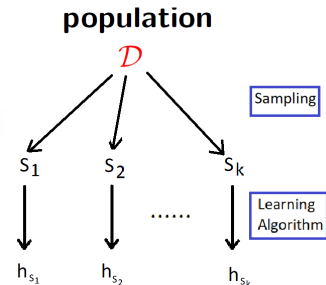
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- We assume that the training set consist of i.i.d samples from a **population** (i.e., true distribution) \mathcal{D} .
- Obviously, the learned function \hat{h} depends on the particular training set used. So, we denote it as h_S .
- The learning algorithm is to be applied in the future. There are multiple ways in which the sampling can turn out. In other words, the training set we will get is only one of many possible training sets.



The Generalization Error

- The **generalization error** of the learned function h_S is

$$\epsilon(h_S) = E_{(\mathbf{x}, y) \sim \mathcal{D}}[(y - h_S(\mathbf{x}))^2]$$

- The difference between the generalization error and the training error is called the **generalization gap**:

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- Error decomposition:

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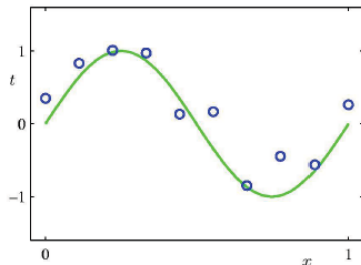
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- The bias is an error from **erroneous assumptions** in the learning algorithm. High bias can cause an algorithm to miss the relevant relations between features and target outputs (underfitting).
- The variance is an error from **sensitivity to small fluctuations in the training set**. High variance can cause an algorithm to model the random noise in the training data, rather than the intended outputs (overfitting).

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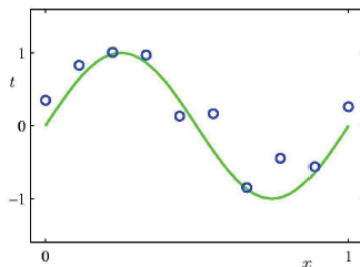
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Bias-Variance Decomposition: Illustration



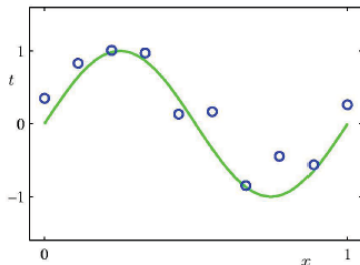
- Suppose the green curve is the true function.

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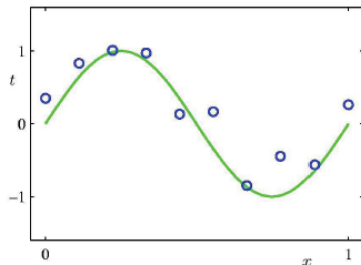
- Suppose the green curve is the true function.
- We randomly sample 10 training points (blue) from the function.

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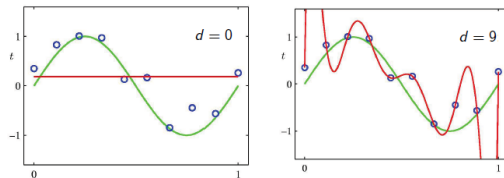
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- Consider learning a polynomial function $y = h(x)$ of order d from the data.

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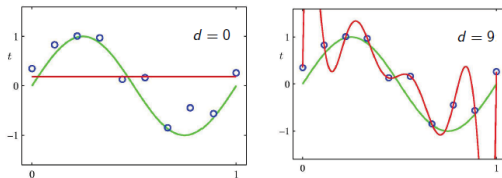
- Suppose the green curve is the true function.
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- Consider learning a polynomial function $y = h(x)$ of order d from the data.
- We the above multiple times.

Bias-Variance Tradeoff: Illustration



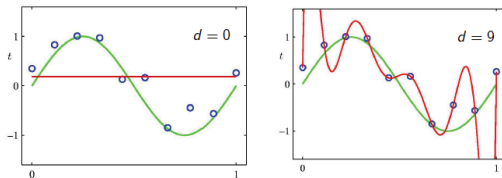
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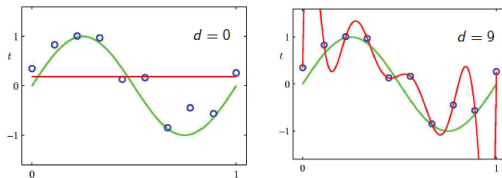
- If we choose $d = 0$, then we have
 - **Low variance:**

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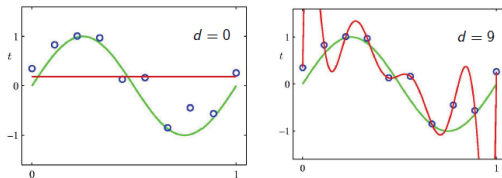
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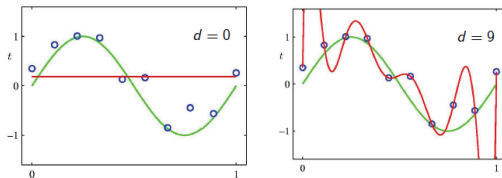
- If we choose $d = 0$, then we have
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 - **High bias:** While the hypothesis is linear, the true function is not.

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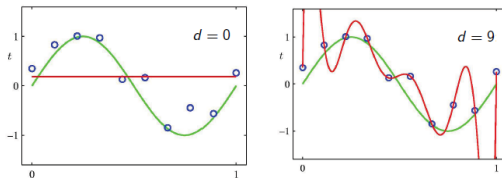
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 - **High bias:** While the hypothesis is linear, the true function is not. If we sample a large number of training sets from the true function and learn a function from each of them, *the average will still be very different from the true function*.

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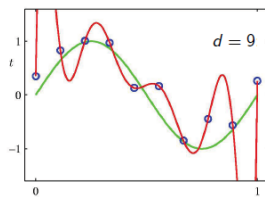
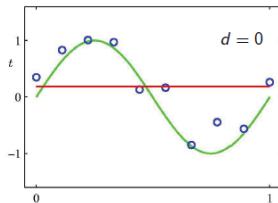
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 - In this case, the generalization would be high.

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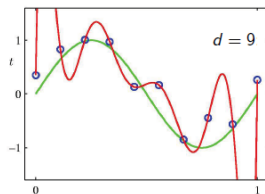
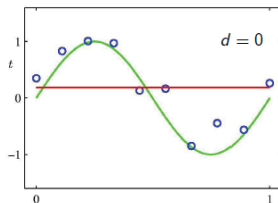
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 - **Low variance:** If there is another training set sampled from the true function (blue) and we run the learning algorithm on it, we will get **roughly the same function**.
 - **High bias:** While the hypothesis is linear, the true function is not. If we sample a large number of training sets from the true function and learn a function from each of them, **the average will still be very different from the true function**.
 - In this case, the generalization would be high. And it is due to **underfitting**: hypothesis function too rigid to fit the data points.

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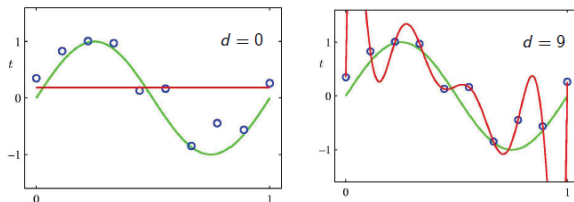
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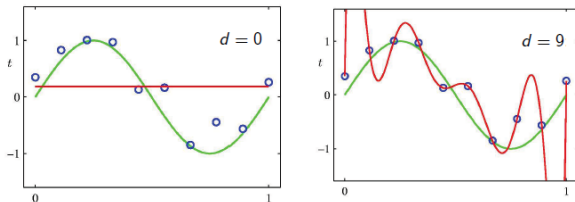
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Bias-Variance Tradeoff: Illustration



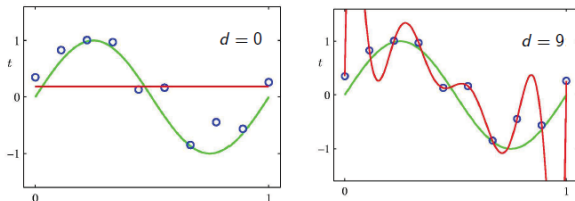
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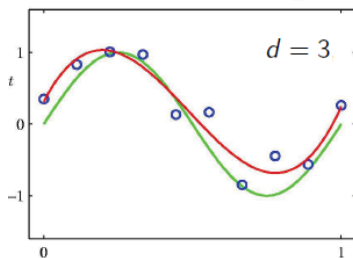
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 - **Low bias:** If we sample a large number of training sets from the true function and learn a function from each of them, **the average will still approximate the true function well**.
 - In this case, the generalization would be high. It is due to **overfitting**: hypothesis too soft, fit the data points too much.

Bias-Variance Tradeoff: Illustration

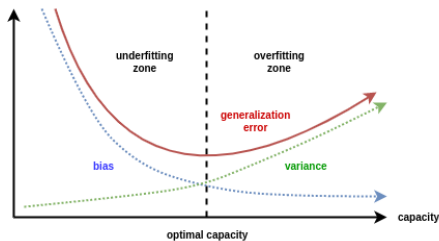
Bias-Variance Tradeoff: Illustration



- If we choose $d = 3$, we get low generalization error
 - not too much variance and not too much bias
 - the hypothesis fit the data just right

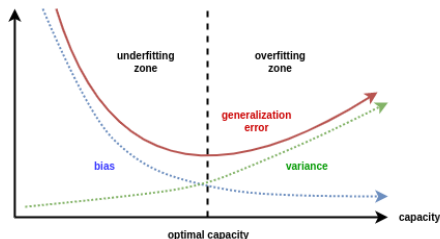
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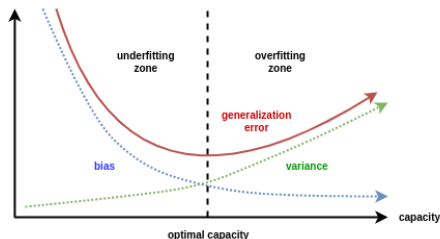
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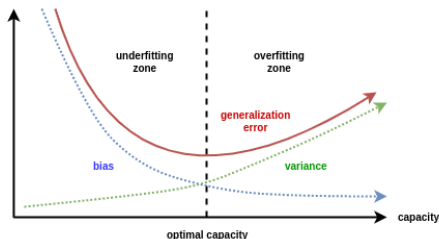
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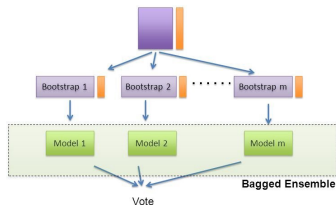
- The bias-variance decomposition was originally formulated for least-squares regression.
- For the case of classification under the 0-1 loss, it's possible to find a similar decomposition.
- If the classification problem is phrased as probabilistic classification, then the expected squared error of the predicted probabilities with respect to the true probabilities can be decomposed in a similar fashion.

Outline

- 1 Introduction
- 2 The Bias-Variance Decomposition
- 3 Illustrations
- 4 Ensemble Learning**

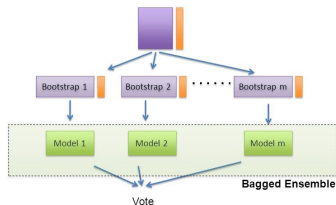
Bagging (Bootstrap Aggregation) for Variance Reduction

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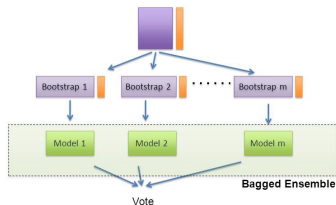
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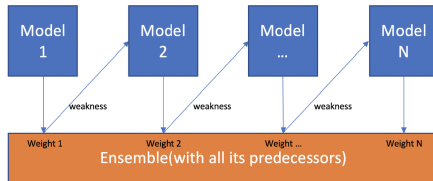
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 - Estimate average income of HKer by randomly interviewing 10 people.
 - Variance is reduced if do it multiple times and take average.
- In HW2, we will analyze this mathematically.

Boosting for Bias Reduction



- Assign equal weights to all the training examples and choose a base algorithm.
- At each step of iteration, we apply the base algorithm to the training set and increase the weights of the incorrectly classified examples.
- We iterate n times, each time applying base learner on the training set with updated weights.
- The final model is the weighted sum of the n learners.