CIE 555
Neural Networks and Deep Learning

Machine Learning Basics

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Overview

- Review of some Linear Algebra basics (selected sections – see next slide)
- Review of the basics of Probability and Information Theory (selected sections – see next slide)
- Capacity, Overfitting and Underfitting (section 5.2)
- Hyperparameters and Validation Sets (section 5.3)
- Estimators, Bias and Variance (section 5.4)
- Consistency (section 5.4.5)

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Review

- Review of some Linear Algebra basics. In particular we discussed
  - Scalars, Vectors, Matrices and Tensors (section 2.1)
  - Norms (section 2.5)
  - Other concepts will be introduced in upcoming lectures where needed
- Review of the basics of Probability and Information Theory
  - Random Variables (section 3.2)
  - Probability Distributions (section 3.3)
  - Marginal Probability (section 3.4)
  - Conditional Probability (section 3.5)
  - The Chain Rule of Conditional Probabilities (section 3.6)
  - Independence and Conditional Independence (section 3.7)
  - Expectation and Variance (section 3.8)
  - Bayes' Rule (section 3.11)

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Machine Learning

- "A computer program is said to learn from experience *E* with respect to some class of tasks *T* and performance measure *P* , if its performance at tasks in *T* , as measured by *P* , improves with experience *E*." Mitchell (1997)
- **Tasks:** described in terms of how the machine learning system should process an **example** (a collection of features that have been quantitatively measured from some object or event).
- Example tasks: classification, regression, transcription, machine translation, anomaly detection, etc.
- **Performance:** specific to the *task T* (e.g. accuracy, error rate)
- **The Experience, *E:*** Most machine learning algorithms simply experience a dataset.

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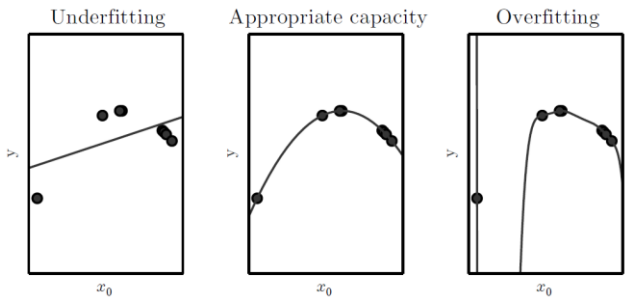
Capacity, Overfitting and Underfitting

- **Underfitting:** occurs when the model is not able to obtain a sufficiently low error value on the training set.
- **Overfitting:** occurs when the gap between the training error and test error is too large.
- We can control whether a model is more likely to overfit or underfit by altering its **capacity** (Informally, a model's capacity is its ability to fit a wide variety of functions.).



Underfitting and Overfitting in Polynomial Estimation

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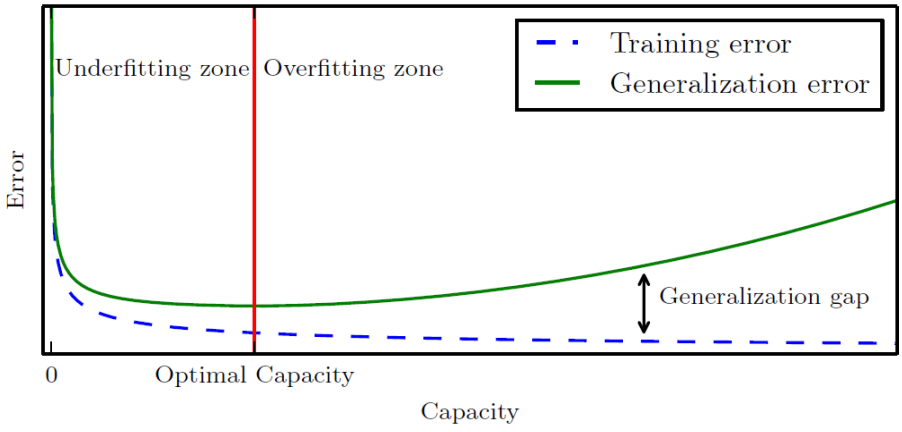
Capacity, Overfitting and Underfitting



Generalization and Capacity

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Non-parametric models

- Parametric models learn a function described by a parameter vector whose size is ***finite and fixed*** before any data is observed.
- Non-parametric models have no such limitation.
- However, we can also design practical non-parametric models by making their complexity a function of the training set size (example: nearest neighbor regression).
- When asked to classify a test point x , the model looks up the nearest entry in the training set and returns the associated regression target.
- While simpler functions are more likely to generalize (to have a small gap between training and test error) we must still choose a sufficiently complex hypothesis to achieve low training error.

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Hyperparameters and Validation Sets

- **Hyperparameters**: settings that designers use to control the behavior of the learning algorithm.
  - In polynomial regression: the degree of the polynomial is a hyperparameter (capacity hyperparmeter)
  - The learning rate λ
- Typically, it is inappropriate to learn hyperparameters on the training set. Why?
  - We need a **validation set**
  - no example from the test set can be used in the validation set. (why?)
  - we always construct the validation set from the *training data* (split training dataset into two disjoint subsets).
  - Typically, one uses about 80% of the training data for training and 20% for validation.
  - the validation set error will *underestimate* the generalization error, though typically by a smaller amount than the training error.

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Cross-Validation

- Dividing the dataset into a fixed training set and a fixed test set can be problematic if it results in the test set being small.
- A small test set implies *statistical uncertainty* around the *estimated average validation error*, making it difficult to claim that algorithm *A* works better than algorithm *B* on the given task.
- When the dataset is too small, are alternative procedures enable one to *use all of the examples in the estimation of the mean test error*, at the price of increased computational cost.
- These procedures are based on the idea of *repeating the training and testing computation on different randomly chosen subsets or splits of the original dataset*.

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Cross-Validation

- The most common of these is *the k-fold cross-validation procedure*, in which a partition of the dataset is formed by splitting it into k non-overlapping subsets.
- The test error may then be estimated by taking the average test error across *k* trials.
- One problem is that there exist no unbiased estimators of the variance of such average error estimators (Bengio and Grandvalet, 2004), but approximations are typically used.

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Estimators, Bias and Variance

- Estimation
  - E.g. estimating the weights in the linear regression example
  - Let $\{x^{(1)}, \ldots, x^{(m)}\}$ be a set of *m* independent and identically distributed data points
  - A point estimator is any function $\hat{\theta}_m = g(x^{(1)}, \ldots, x^{(m)})$
  - a good estimator is a function whose output is close to the true underlying function θ that generated the training data.

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Bias

- Bias
  - measures the expected deviation from the true value of the function or parameter.
  - Defined as: $bias(\hat{\theta}_m) = \mathbb{E}(\hat{\theta}_m) - \theta$ where $\mathbb{E}(\hat{\theta}_m)$: expectation over the data
  - An estimator $\hat{\theta}_m$ is *unbiased* when $bias(\hat{\theta}_m) = 0$
  - An estimator $\hat{\theta}_m$ is said to be **asymptotically unbiased** if $\lim_{m\to\infty} bias(\hat{\theta}_m) = 0$ $(i.e. \lim_{m\to\infty} \mathbb{E}(\hat{\theta}_m) = \theta)$
  - *Asymptotically unbiased estimators:* estimators whose bias goes to 0 as the sample size goes to infinity.

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Variance and Standard Error

- Measures how we would expect the estimate we compute from data to vary as we independently resample the dataset from the underlying data generating process.
- Simply the variance $Var(\hat{\theta})$
- *Standard error:* the square root of the variance.

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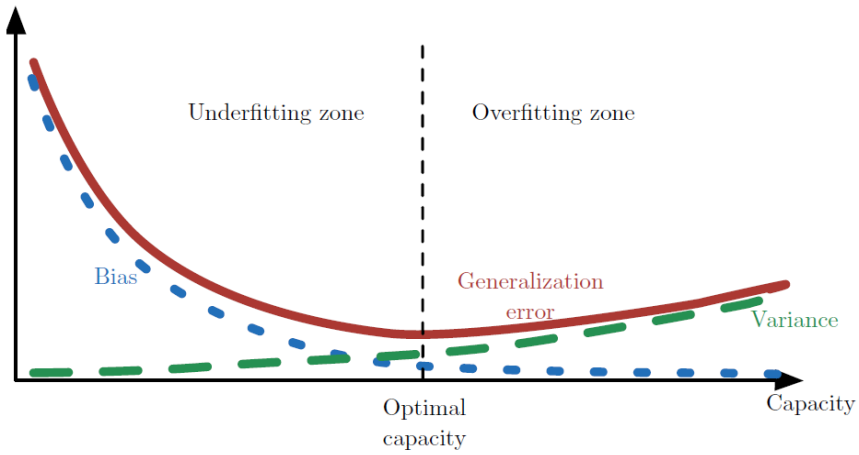
Trading off Bias and Variance

- tightly linked to the concepts of capacity, underfitting and overfitting
- increasing capacity tends to increase variance and decrease bias



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Consistency

- *Consistency* ensures that the bias and variance induced by the estimator diminishes as the number of data examples grows.
- We would like that $\operatorname{plim}_{m \to \infty} \hat{\theta}_m = \theta$ (plim: indicates convergence in probability)
- meaning that for any $\in > 0$, $P(\left|\hat{\theta}_m - \theta\right| > \in) \rightarrow 0$ as m $\rightarrow \infty$
- The estimator will be consistent if it is asymptotically unbiased, ***and*** its variance $\rightarrow 0$ as m $\rightarrow \infty$.

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