Machine Learning Basics: Estimators, Bias and Variance

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This is part of lecture slides on Deep Learning:
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Topics in Basics of ML

1. Learning Algorithms
2. Capacity, Overfitting and Underfitting
3. Hyperparameters and Validation Sets
4. Estimators, Bias and Variance
5. Maximum Likelihood Estimation
6. Bayesian Statistics
7. Supervised Learning Algorithms
8. Unsupervised Learning Algorithms
9. Stochastic Gradient Descent
10. Building a Machine Learning Algorithm
11. Challenges Motivating Deep Learning

Topics in Estimators, Bias, Variance

0. Statistical tools useful for generalization
1. Point estimation
2. Bias
3. Variance and Standard Error
4. Bias-Variance tradeoff to minimize MSE
5. Consistency

Statistics provides tools for ML

- The field of statistics provides many tools to achieve the ML goal of solving a task not only on the training set but also to generalize
- Foundational concepts such as
  - Parameter estimation
  - Bias
  - Variance
- They characterize notions of generalization, over- and under-fitting

Point Estimation

- Point Estimation is the attempt to provide the single best prediction of some quantity of interest
  - Quantity of interest can be:
    - A single parameter
    - A vector of parameters
      - E.g., weights in linear regression
    - A whole function

Point estimator or Statistic

- To distinguish estimates of parameters from their true value, a point estimate of a parameter θ is represented by $\hat{\theta}$
- Let $\{\boldsymbol{x}^{(1)}, \boldsymbol{x}^{(2)},..\boldsymbol{x}^{(m)}\}$ be m independent and identically distributed data points
  - Then a *point estimator* or *statistic* is any function of the data

$$\hat{\theta}_m = g(\boldsymbol{x}^{(1)},...\boldsymbol{x}^{(m)})$$

    - Thus a statistic is any function of the data
    - It need not be close to the true θ
  - A good estimator is a function whose output is close to the true underlying θ that generated the data

Function Estimation

- Establishing a relationship between input and target variables can also be point estimation
- Here we predict a variable $\boldsymbol{y}$ given input $\boldsymbol{x}$
- We assume that there is a function $f(\boldsymbol{x})$ that describes the approximate relationship between $\boldsymbol{x}$ and $\boldsymbol{y}$
  - We may assume $\boldsymbol{y}=f(\boldsymbol{x})+\varepsilon$
    - Where ε stands for a part that is not predictable from $\boldsymbol{x}$
  - We are interested in approximating f with a model $\hat{f}$
  - Function estimation is same as estimating a parameter θ; where $\hat{f}$ is a point in function space

Properties of Point Estimators

- Most commonly studied properties of point estimators are:
  1. Bias
  2. Variance
- They inform us about the estimators

1. Bias of an estimator

- The bias of an estimator $\hat{\theta}_m = g(\boldsymbol{x}^{(1)},\ldots\boldsymbol{x}^{(m)})$ for parameter θ is defined as

$$\boxed{\text{bias}\left(\hat{\theta}_m\right) = E\left[\hat{\theta}_m\right] - \theta}$$

- The estimator is unbiased if $\text{bias}(\hat{\theta}_m) = 0$
  - which implies that $\boxed{E\left[\hat{\theta}_m\right] = \theta}$
- An estimator is asymptotically unbiased if

$$\boxed{\lim_{m\to\infty} \text{bias}\left(\hat{\theta}_m\right) = 0}$$

Examples of Estimator Bias

- We look at common estimators of the following parameters to determine whether there is bias:
  - Bernoulli distribution: mean θ
  - Gaussian distribution: mean μ
  - Gaussian distribution: variance σ^2

Estimator of Bernoulli mean

- Bernoulli distribution for binary variable $x\,\varepsilon\{0,1\}$ with mean θ has the form $P(x;\theta)=\theta^x(1-\theta)^{1-x}$
- Estimator for θ given samples $\{\boldsymbol{x}^{(1)},..\boldsymbol{x}^{(m)}\}$ is $\boxed{\hat{\theta}_m=\frac{1}{m}\sum_{i=1}^{m}x^{(i)}}$
- To determine whether this estimator is biased determine

$$\boxed{\begin{aligned}\mathrm{bias}(\hat{\theta}_m) &= E\left[\hat{\theta}_m\right]-\theta\\ &= E\left[\frac{1}{m}\sum_{i-1}^{m}x^{(i)}\right]-\theta\\ &= \frac{1}{m}\sum_{i=1}^{m}E\left[x^{(i)}\right]-\theta\\ &= \frac{1}{m}\sum_{i=1}^{m}\sum_{x^{(i)}=0}^{1}\left(x^{(i)}\theta^{x^{(i)}}(1-\theta)^{(1-x^{(i)})}\right)-\theta\\ &= \frac{1}{m}\sum_{i=1}^{m}(\theta)-\theta=\theta-\theta=0\end{aligned}}$$

  – Since $\mathrm{bias}(\hat{\theta}_m)=0$ we say that the estimator is unbiased

Estimator of Gaussian mean

- Samples $\{\boldsymbol{x}^{(1)},..\boldsymbol{x}^{(m)}\}$ are independently and identically distributed according to $p(\boldsymbol{x}^{(i)})=N(\boldsymbol{x}^{(i)};\mu,\sigma^2)$
  - Sample mean is an estimator of the mean parameter

$$\hat{\mu}_m = \frac{1}{m}\sum_{i=1}^{m} x^{(i)}$$

  - To determine bias of the sample mean:

$$\begin{aligned}
\text{bias}(\hat{\mu}_m) &= \mathbb{E}[\hat{\mu}_m] - \mu \\
&= \mathbb{E}\left[\frac{1}{m}\sum_{i=1}^{m} x^{(i)}\right] - \mu \\
&= \left(\frac{1}{m}\sum_{i=1}^{m} \mathbb{E}\left[x^{(i)}\right]\right) - \mu \\
&= \left(\frac{1}{m}\sum_{i=1}^{m} \mu\right) - \mu \\
&= \mu - \mu = 0
\end{aligned}$$

  - Thus the sample mean is an unbiased estimator of the Gaussian mean

Estimator for Gaussian variance

- The sample variance is $\hat{\sigma}_m^2 = \frac{1}{m}\sum_{i=1}^{m}\left(x^{(i)} - \hat{\mu}_m\right)^2$
- We are interested in computing

$$\text{bias}(\hat{\sigma}_m^2) = E(\hat{\sigma}_m^2) - \sigma^2$$

- We begin by evaluating →

$$\mathbb{E}[\hat{\sigma}_m^2] = \mathbb{E}\left[\frac{1}{m}\sum_{i=1}^{m}\left(x^{(i)} - \hat{\mu}_m\right)^2\right] = \frac{m-1}{m}\sigma^2$$

- Thus the bias of $\hat{\sigma}_m^2$ is $-\sigma^2/m$
- Thus the sample variance is a biased estimator
- The unbiased sample variance estimator is

$$\hat{\sigma}_m^2 = \frac{1}{m-1}\sum_{i=1}^{m}\left(x^{(i)} - \hat{\mu}_m\right)^2$$

2. Variance and Standard Error

- How much we expect the estimator to vary as a function of the data sample
- Just as we computed the expectation of the estimator to determine its bias, we can compute its variance
- The variance of an estimator is simply $\mathrm{Var}(\hat{\theta})$ where the random variable is the training set
- The square root of the the variance is called the Standard Error, denoted $\mathrm{SE}(\hat{\theta})$

Importance of Standard Error

- It measures how we would expect the estimate to vary as we obtain different samples from the same distribution
- The standard error of the mean is given by

$$SE(\hat{\mu}_m) = \sqrt{Var\left[\frac{1}{m}\sum_{i=1}^{m} x^{(i)}\right]} = \frac{\sigma}{\sqrt{m}}$$

  - where σ^2 is the true variance of the samples $\boldsymbol{x}^{(i)}$
  - Standard error often estimated using estimate of σ
    - Although not unbiased, approximation is reasonable
      - The standard deviation is less of an underestimate than variance

Standard Error in Machine Learning

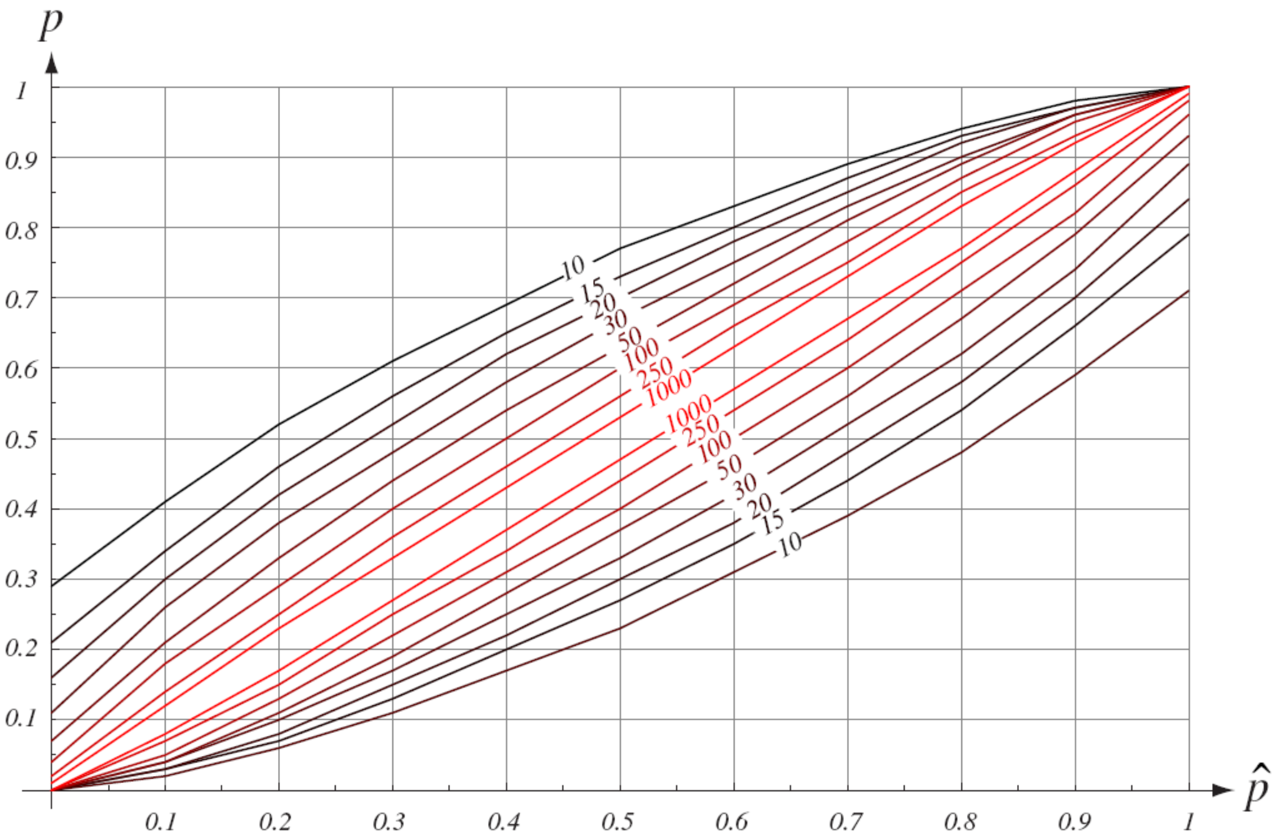
- We often estimate generalization error by computing error on the test set
  - No of samples in the test set determine its accuracy
  - Since mean will be normally distributed, (according to Central Limit Theorem), we can compute probability that true expectation falls in any chosen interval
    - Ex: 95% confidence interval centered on mean $\hat{\mu}_m$ is

$$\boxed{\left(\hat{\mu}_m - 1.96SE\left(\hat{\mu}_m\right), \hat{\mu}_m + 1.96SE\left(\hat{\mu}_m\right)\right)}$$

- ML $\mathrm{algorithm\ A}$ is better than ML $\mathrm{algorithm\ B}$ if
  - upperbound of A is less than lower bound of B

Confidence Intervals for error

95% confidence intervals for error estimate

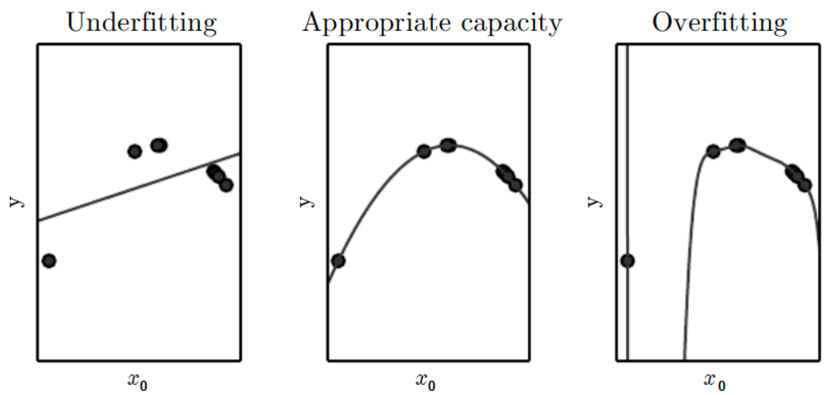


Trading-off Bias and Variance

- Bias and Variance measure two different sources of error of an estimator
- Bias measures the expected deviation from the true value of the function or parameter
- Variance provides a measure of the expected deviation that any particular sampling of the data is likely to cause

Negotiating between bias - tradeoff

- How to choose between two algorithms, one with a large bias and another with a large variance?



  - Most common approach is to use cross-validation
  - Alternatively we can minimize Mean Squared Error which incorporates both bias and variance

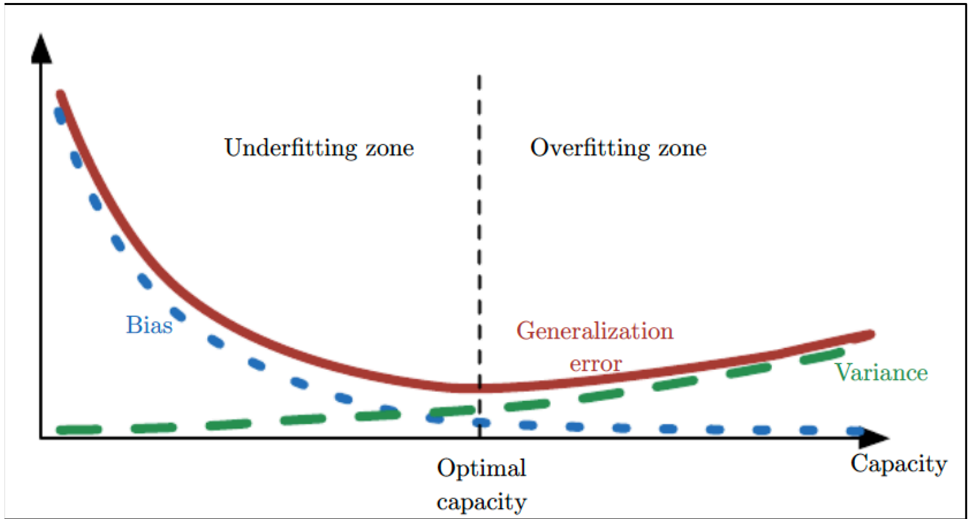
Mean Squared Error

- Mean Squared Error of an estimate is

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

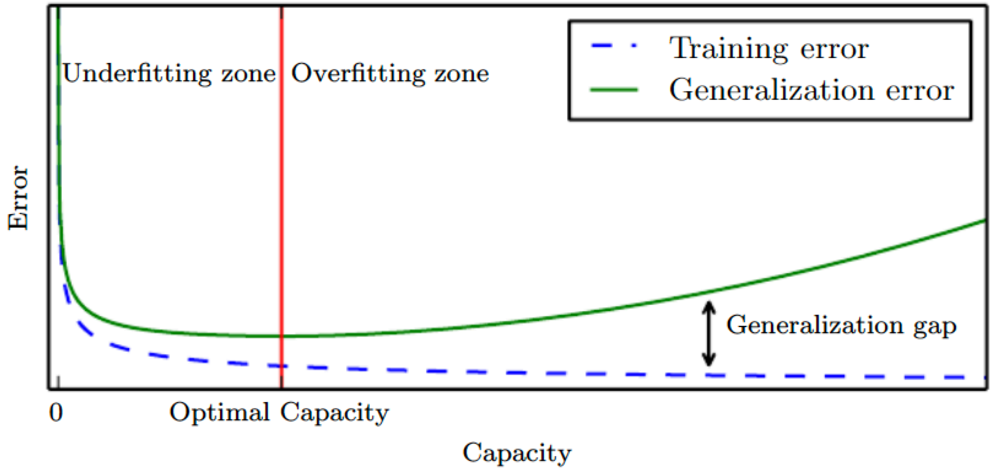
$$= \mathrm{Bias}\left(\hat{\theta}_m\right)^2 + \mathrm{Var}\left(\hat{\theta}_m\right)$$

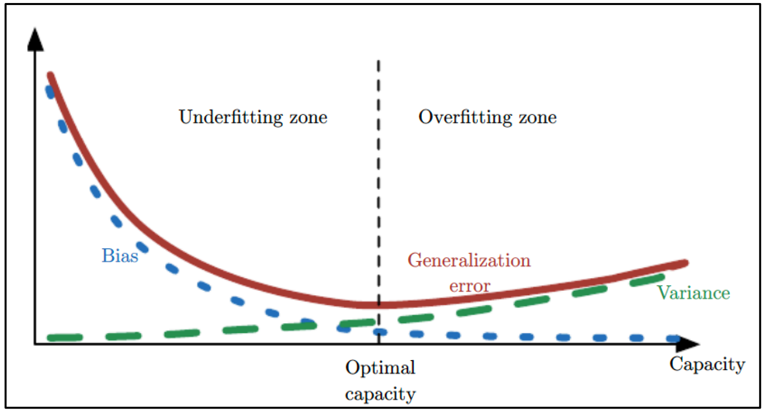
- Minimizing the MSE keeps both bias and variance in check



Underfit-Overfit : Bias-Variance

Both have a U-shaped curve of generalization Error as a function of capacity





Consistency

- So far we have discussed behavior of an estimator for a fixed training set size
- We are also interested with the behavior of the estimator as training set grows
- As the no. of data points m in the training set grows, we would like our point estimates to converge to the true value of the parameters:

$$\text{plim}_{m\to\infty}\hat{\theta}_m = \theta$$

  - plim, known as consistency, is probability in the limit
    - Also known as weak consistency
  - Consistency ensures that bias decreases with m