Introduction to Bias-Variance Decomposition Theory

Figures from:
Pattern Classification (2nd Edition) by R. Duda, P. Hart, D. Stork (2000)

The Elements of Statistical Learning (2nd edition) by Hastie, Tibshirani and Friedman (2008)

- We want to study the behavior of predictive systems
- We want to find relations between the error and other meaningful concepts
- We will consider the bias, i.e. the error due to the difference between the *true* function and the *model* function that we can represent/compute
- ..and the variance, i.e. the estimation error due to having a finite sample to train out models with

- The expected value or *mean* or *average* of a random variable x is:

$$E[x] = \sum_{x \in \mathcal{X}} x p(x)$$

- The expected value is denoted with the symbol μ
- *If one thinks of probabilities as weights, then the expected value is the center of mass*
- Given a function $f(x)$ we define:

$$E[f(x)] = \sum_{x \in \mathcal{X}} f(x) p(x)$$

Expected Value is a Linear Operator

- The process of computing the expected value is linear
- Given two arbitrary constants α_1 and α_2, it holds that:

$$E[\alpha_1 f_1(x) + \alpha_2 f_2(x)] = \alpha_1 E[f_1(x)] + \alpha_2 E[f_2(x)]$$

- We can think of E as a linear operator

- The second moment is:

$$E[x^2] = \sum_{x \in \mathcal{X}} x^2 p(x)$$

- The variance is:

$$E[(x-\mu)^2] = \sum_{x \in \mathcal{X}} (x-\mu)^2 p(x)$$

- The variance is indicated with σ^2 where σ is the standard deviation
- The variance is also indicated as $Var(x)$

Notes on the standard deviation

- The standard deviation measures how much the values of x tend to differ from their average μ
- For a normal distribution we have:
  - 68% of values are within 1 σ
  - 95% of values are within 2 σ
  - 99.7% of values are within 3 σ
- In the general case a (loose) bound is given by the Chebyshev's inequality

$$p(|x - \mu| > n\sigma) \leq \frac{1}{n^2}$$

Useful Equality

- It holds that:

$$E[(x - E[x])^2] = E[x^2] - (E[x])^2$$

- Proof: let's use the shorthand $\bar{x} = E[x]$

$$\begin{aligned} E[(x-\bar{x})^2] &= E[x^2 - 2x\bar{x} + \bar{x}^2] && (1)\\ &= E[x^2] - 2E[x]\bar{x} + \bar{x}^2 && (2)\\ &= E[x^2] - 2\bar{x}^2 + \bar{x}^2 && (3)\\ &= E[x^2] - \bar{x}^2 && (4) \end{aligned}$$

- and consequently:

$$E[x^2] = E[(x-\bar{x})^2] + \bar{x}^2$$

- Between two random variables it holds that:

$$\sigma(x,y) = E[(x - E[x])(y - E[y])] = E[xy] - E[x]E[y]$$

- $\sigma(x,y)$ is called the *covariance*
- Proof: again we use the shorthand $\bar{x} = E[x]$ and $\bar{y} = E[y]$

$$\begin{aligned} E[(x - E[x])(y - E[y])] &= E[xy - \bar{x}y - x\bar{y} + \bar{x}\bar{y}] \\ &= E[xy] - \bar{x}E[y] - \bar{y}E[x] + \bar{x}\bar{y} \\ &= E[xy] - \bar{x}\bar{y} - \bar{y}\bar{x} + \bar{x}\bar{y} \\ &= E[xy] - \bar{x}\bar{y} \end{aligned}$$

- note that if x and y are independent then $p(xy) = p(x)p(y)$ and hence $E[xy] = E[x]E[y]$ and finally $\sigma(x,y) = 0$

- **Aim:** decompose the error of a predictive system induced from a finite data sample into meaningful components for insight
- **Result:** error $=$ bias^2 $+$ variance $+$ irreducible (Bayes) error

- Assume the true function can be written as:

$$y = f(x) + \epsilon$$

- where $\epsilon = N(0, \sigma^2)$, i.e. ϵ is a random variable normally distributed with zero mean and standard deviation σ
- We are given a set of training examples $S = \{(x_i, y_i)\}$
- From this set we fit $h(\cdot)$, i.e. our model function or hypothesis
- For example:
  - we can choose the class of linear functions $h(x) = x \cdot \beta$
  - ..and as fitting criterion, we can minimize the squared error $\sum_i (y_i - h(x_i))^2$

- We are given a new data point x_0 extracted from the same population from which we extracted the set of training examples
- We observe the corresponding value

$$y_0 = f(x_0) + \epsilon$$

- We want to understand and decompose the expected prediction error

$$E[(y_0 - h(x_0))^2]$$

$$
\begin{aligned}
E[(y_0 - h(x_0))^2] &= E[(y_0 - f(x_0) + f(x_0) - h(x_0))^2] && (5)\\
&= E[(y_0 - f(x_0))^2] + E[(f(x_0) - h(x_0))^2] \\
&\quad +2E[(y_0 - f(x_0))(f(x_0) - h(x_0))] && (6)\\
&= E[(f(x_0) + \epsilon - f(x_0))^2] + E[(f(x_0) - h(x_0))^2] \\
&\quad +2(E[y_0 f(x_0)] - E[y_0 h(x_0)] \\
&\quad -E[f(x_0)^2] + E[f(x_0) h(x_0)]) && (7)\\
&= E[\epsilon^2] + E[(f(x_0) - h(x_0))^2] + 0 && (8)
\end{aligned}
$$

We have to show that:

$$2(E[y_0 f(x_0)] - E[y_0 h(x_0)] - E[f(x_0)^2] + E[f(x_0)h(x_0)]) = 0$$

in fact:
$E[y_0 f(x_0)] = f(x_0)E[y_0] = f(x_0)E[f(x_0) + \epsilon] = f(x_0)^2 + 0$
which cancels out with $-E[f(x_0)^2] = -f(x_0)^2$
Note: $f(x_0)$ is constant and $E[\epsilon] = 0$
finally:
$-E[y_0 h(x_0)] = -E[(f(x_0) + \epsilon)h(x_0)] = -E[f(x_0)h(x_0)] - E[\epsilon h(x_0)]$
where $-E[f(x_0)h(x_0)]$ cancels out with $E[f(x_0)h(x_0)]$
and $-E[\epsilon h(x_0)] = -E[\epsilon]E[h(x_0)] = 0 \cdot E[h(x_0)] = 0$
Note: if two random variables are independent then
$E[ab] = E[a]E[b] + Cov[ab] = E[a]E[b]$ since $Cov[ab] = 0$, and
here the noise is independent from our hypothesis

From eq. (8) we had the term:

$$
\begin{aligned}
E[(f(x_0) - h(x_0))^2] &= E[(f(x_0) - \bar{h}(x_0) + \bar{h}(x_0) - h(x_0))^2] \\
&= E[(f(x_0) - \bar{h}(x_0))^2] + E[(\bar{h}(x_0) - h(x_0))^2] \\
&\quad + 2E[(f(x_0) - \bar{h}(x_0))(\bar{h}(x_0) - h(x_0))] \\
&= E[(f(x_0) - \bar{h}(x_0))^2] + E[(\bar{h}(x_0) - h(x_0))^2] + 0 \\
&= (f(x_0) - \bar{h}(x_0))^2 + E[(\bar{h}(x_0) - h(x_0))^2]
\end{aligned}
$$

where $\bar{h}(x_0) = E[h(x_0)]$

We have to show that:

$$E[(f(x_0) - \bar{h}(x_0))(\bar{h}(x_0) - h(x_0))] = 0$$

$$E[(f(x_0)\bar{h}(x_0)] - E[f(x_0)h(x_0)] - E[\bar{h}(x_0)^2] + E[\bar{h}(x_0)h(x_0)] = 0$$

in fact:
$E[(f(x_0)\bar{h}(x_0)] = f(x_0)\bar{h}(x_0)$, since $f(x_0)$ is constant
which cancels out with
$-E[f(x_0)h(x_0)] = -f(x_0)E[h(x_0)] = -f(x_0)\bar{h}(x_0)$
finally, $E[\bar{h}(x_0)^2] = \bar{h}(x_0)^2$, since $\bar{h}(x_0)$ is constant
which cancels out with $E[\bar{h}(x_0)h(x_0)] = \bar{h}(x_0)E[h(x_0)] = \bar{h}(x_0)^2$

We can finally put everything together:

$$
\begin{aligned}
E[(y_0 - h(x_0))^2] &= E[\epsilon^2] \\
&\quad + (f(x_0) - \bar{h}(x_0))^2 \\
&\quad + E[(h(x_0) - \bar{h}(x_0))^2] && (9) \\
&= \sigma^2 + Bias(h(x_0))^2 + Var(h(x_0)) && (10) \\
& && (11)
\end{aligned}
$$

Expected prediction error = Noise + Bias^2 + Variance

- **Variance:** $E[(h(x_0) - \bar{h}(x_0))^2]$
  it describes the variability of the prediction $h(x_0)$ when different training sets are used to fit the model h
- **Bias:** $(\bar{h}(x_0) - f(x_0))^2$
  it describes the difference between the expected predicted value and the true (but unknown) value
- **Noise:** $E[(y_0 - f(x_0))^2] = \sigma^2$
  it describes how much y_0 can differ from the true $f(x_0)$ due to intrinsic uncertainties

- **Problem:**
  To measure the *expected prediction error* we need to induce predictors from many training sets
- ...unfortunately we generally have only one training set
- **Solution:** simulate multiple training sets by bootstrap replicates

1. Given a set of training examples $S = \{(x_i, y_i)\}$
2. Extract replicate
   $S' = \{x | x \text{ is drawn at random with replacement from } S\}$
3. of identical size $|S'| = |S|$

1. Make B bootstrap replicates of S: $S_1, \ldots, S_B$
2. Use S_b as training set and induce hypothesis h_b
3. Make out of bag set $T_b = S \setminus S_b$
   i.e. all data instances that do not appear in S_b
4. Compute $h_b(x)$ for each x in T_b (indicate with K their number)

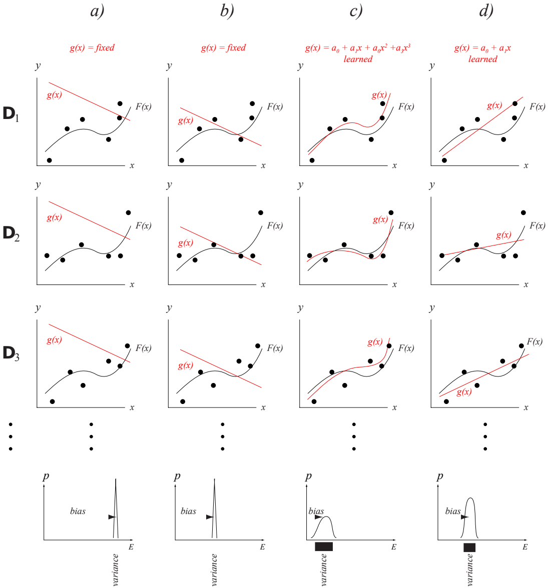
Measuring Bias and Variance

1. Compute expected prediction $\bar{h}(x) = \frac{1}{K}\sum_{b=1}^{K} h_b(x)$
2. Estimate bias^2 as $(\bar{h}(x) - y)^2$
3. Estimate variance as $\frac{1}{K-1}\sum_{b=1}^{K}(\bar{h}(x) - h_b(x))^2$
4. Assume noise is 0

- Note that we are ignoring the noise
- If we have multiple pairs (x_i, y_i) for the same value x_i then we can also estimate the noise
- Alternatively we can estimate it by considering the y values of nearby x

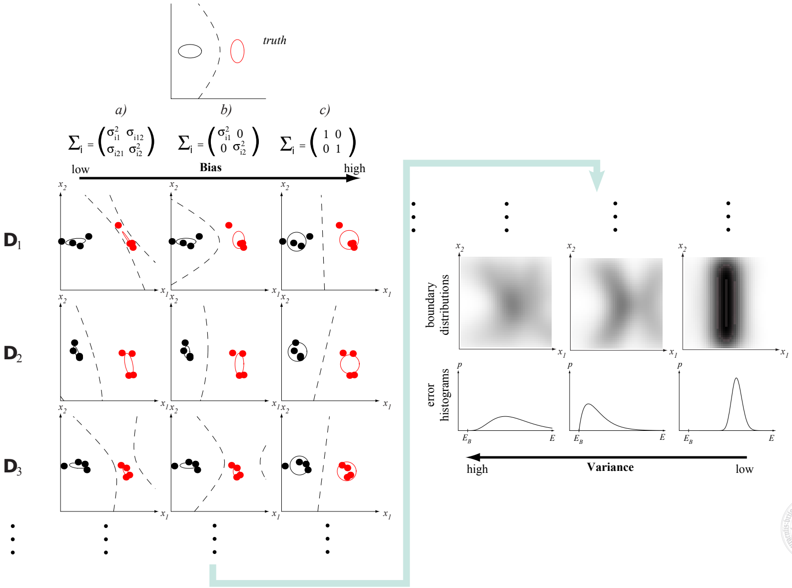
- In the experimental practice we observe an important phenomenon called the bias variance dilemma or *bias variance trade-off*
- Given two classes of hypothesis (e.g. linear models and k-NNs) to fit to some training data set
- ... we observe that the more flexible hypothesis class has a low bias term but a higher variance term
- If we have a parametric family of hypothesis (e.g. k-NN for different values of k), then we can increase the flexibility of the hypothesis (e.g. reducing k) but we still observe the increase of variance

Bias Variance Example 1D



Bias Variance Example 1D

- Each column is a different model: we have two constant functions, a cubic polynomial and a linear model
- Each row is a training set made of 6 points sampled from the same true function (a cubic polynomial) with noise
- Last row shows the error histogram: error in x and the probability of error in y
- **Observation 1:** the constant models have a large bias but zero variance; the second model has a lower bias than the first
- **Observation 2:** the cubic model has the lowest bias but the highest variance
- **Observation 3:** the linear model has a low variance, i.e. the same predictor is obtained from different training sets
- If we had $n \to \infty$ then variance for all models would vanish; however only the bias for the cubic model would diminish (up to the noise level)



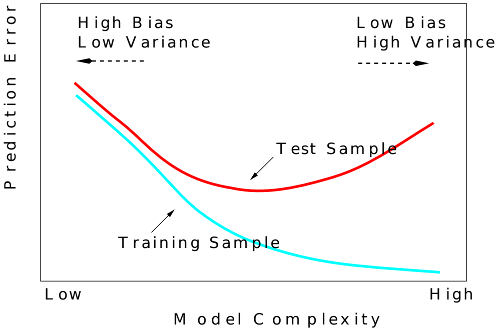
truth
a)
b)
c)
$\Sigma_i = \begin{pmatrix} \sigma_{i1}^2 & \sigma_{i12} \\ \sigma_{i21} & \sigma_{i2}^2 \end{pmatrix}$
$\Sigma_i = \begin{pmatrix} \sigma_{i1}^2 & 0 \\ 0 & \sigma_{i2}^2 \end{pmatrix}$
$\Sigma_i = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$
low
Bias
high
D_1
D_2
D_3
boundary distributions
error histograms
p
E_B
E
high
Variance
low

- Each column is a different model from the same family of functions: we have Gaussian with full, diagonal and unit covariance matrix
- Each row is a training set made of 8 points sampled from the same true function (two Gaussians)
- On the right the decision boundary distribution and the error histogram: error in x and the probability of error in y
- **Observation:** the trade-off between bias and variance is consistent: low bias $\Leftrightarrow$ high variance

Remarks

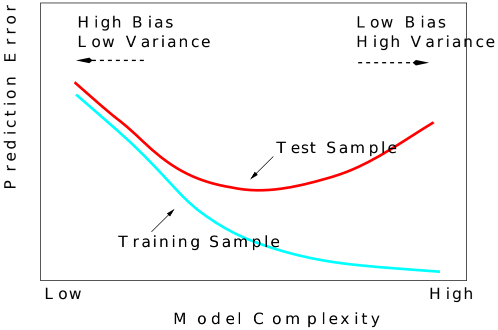
- The expected prediction error is the sum of a bias component and a variance component
- To have a low error it is generally better to prefer low variance to low bias
- For a given bias the variance can be diminished by increasing the size of the training set
- The bias can be reduced increasing the complexity of the model until a perfect match with the true underlying function is achieved
- The error cannot however be reduced below the Bayes Error
- The only way to have zero bias and zero variance is to use the correct true function (by guessing it without any learning)

Expected prediction error estimation



- The expected prediction error (EPE) can be estimated from the error on an independent test set
- The error on the training set instead is a optimistic estimate of EPE as it does not take into account the model complexity (i.e. this error always decreases with higher complexity)

Expected prediction error estimation



- The training error does not allow to estimate the variance component of the error
- A large variance implies a large EPE
- How can we obtain a good estimate of EPE?

- If we had enough data we could set aside a large set to estimate the error
- In practice we have a finite sample of data that we have to split between training and validation data
- If we use a large portion for validation we do not have enough data for training
- If we use a large portion for training we do not estimate the error accurately
- A compromise is to use the K-fold cross-validation technique

Cross-Validation

1. Randomly permute the data
2. Split the data into K roughly equal sized parts with the same distribution of targets as in the whole set
3. Let h^{-i} be the hypothesis fitted to the data set with the i-th part removed
4. The cross-validation estimate of the prediction error is:

$$CV(h) = \frac{1}{N} \sum_{i=1}^{N} L(y_i, h^{-i}(x_i))$$

Cross-Validation

The cross-validation procedure can be used to select the model with lowest expected prediction error

1. Divide the data set as before
2. Let $h(x, \alpha)$ be a hypothesis for point x under parameter α (i.e. α can be the number of neighbors in the k-NN model)
3. Let h^{-i} be the hypothesis fitted to the data set with the i-th part removed
4. The cross-validation estimate of the prediction error of h with parameter α is:

$$CV(h, \alpha) = \frac{1}{N} \sum_{i=1}^{N} L(y_i, h^{-i}(x_i, \alpha))$$

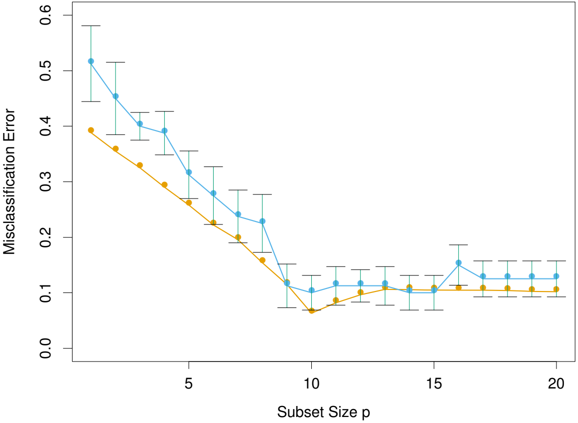
5. Choose the model parameter α^* that minimizes CV

Choice of Cross-Validation parameter K

The estimation of the error by the cross-validation procedure is itself subject to the bias-variance trade-off

- If $K = N$[1] is an unbiased estimator of the true error but has a large variance (because all the training sets are very similar to each other)
- If $K = 5$ the variance is low but the bias can be high (a predictor that overfits a small data will consistently exhibit an optimistically low error)
- $K = 10$ is recommended as a good compromise

[1] This case is also known as Jackknife



Example of the selection of model parameter p with 10-CV.
One can use the *one-standard error rule*: choose the smallest model whose CV error is no more than 1 std above the best.

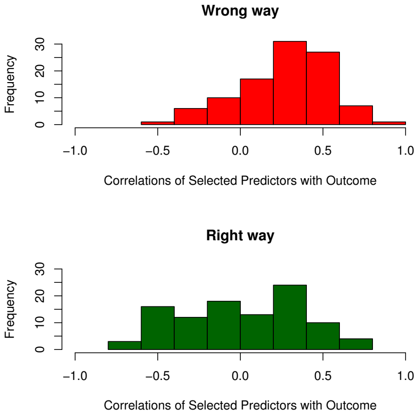
The Wrong and the Right Way of Doing Cross-Validation

- Consider a classification problem with many features (e.g. genomic application)
- This could be a strategy used to build a predictor
  - Filter the features: find a subset of features that correlates strongly with the class label
  - Use only those features to build a predictor
  - Perform cross-validation to estimate the tuning parameters and the prediction error
- Is this procedure correct?

The Wrong and the Right Way of Doing Cross-Validation

- To see why the previous approach is wrong consider this experiment:
  - Take 50 samples of a binary classification problem with $p = 5000$ features
  - The values for each feature are sampled from Gaussian distributions
  - The class label is independent of any feature
  - In this conditions any predictor has a true test error of 50%
  - Choose 100 features with the highest correlation to the class label
  - Use a 1-NN predictor based on these features

- **Q:** If this procedure is repeated 50 times, what will be the average CV error estimate?
- **A:** Surprisingly it can be 3% instead of 50%



The Wrong and the Right Way of Doing Cross-Validation

- The features have been selected looking at all the data
- The information on the class of the test point was available during the training procedure
- The construction of the predictor happens in reality in 2 steps: 1) choice of the features and 2) fitting of the model's parameter
- The CV estimate has to be take into consideration the whole process

The Wrong and the Right Way of Doing Cross-Validation

- What is the correct way of doing cross-validation?
- Divide initially the dataset into the K parts
- In each fold independently:
  - Select the features that correlate best with the target
  - Fit a predictor using those features
  - Use the predictor to classify the instances in the validation fold
- Accumulate the error estimate over the K folds and report the average CV error estimate

Note: *One can correctly use a criterion that does not access the label information to filter the features (e.g. those with highest variance) before doing the K parts split*