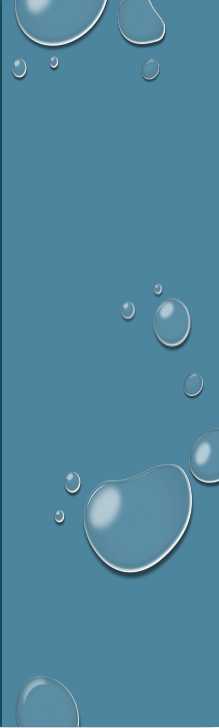


WEEK 12 LECTURE

RESAMPLING METHODS



OBJECTIVES

- Cross validation
- Bootstrap

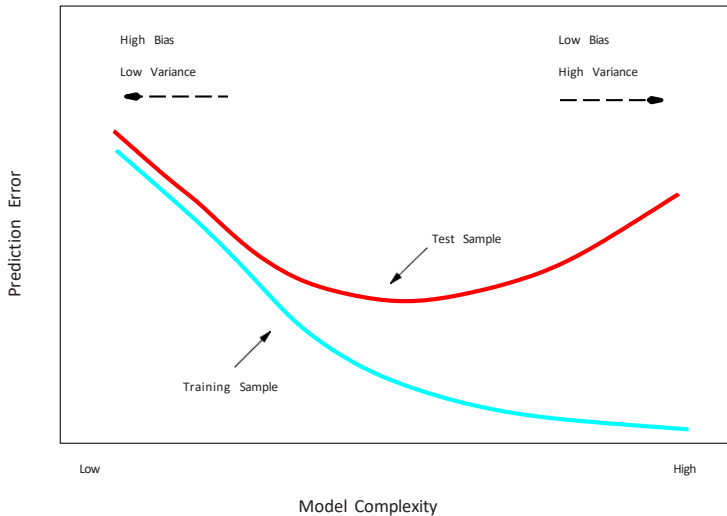
OVERVIEW

- In the section we discuss two *resampling* methods: cross-validation and the bootstrap.
- These methods refit a model of interest to samples formed from the training set, in order to obtain additional information about the fitted model.
- For example, they provide estimates of test-set prediction error, and the standard deviation and bias of our parameter estimates

TRAINING ERROR VERSUS TEST ERROR

- Recall the distinction between the *test error* and the *training error*:
- The *test error* is the average error that results from using a statistical learning method to predict the response on a new observation, one that was not used in training the method.
- In contrast, the *training error* can be easily calculated by applying the statistical learning method to the observations used in its training.
- But the training error rate often is quite different from the test error rate, and in particular the former can *dramatically underestimate* the latter.

TRAINING- VERSUS TEST-SET PERFORMANCE



MORE ON PREDICTION-ERROR ESTIMATES

- Best solution: a large designated test set. OFTEN NOT available
- Some methods make a mathematical adjustment to the training error rate in order to estimate the test error rate.
- Here we instead consider a class of methods that estimate the test error by holding out a subset of the training observations from the fitting process, and then applying the statistical learning method to those held out observations

VALIDATION-SET APPROACH

- Here we randomly divide the available set of samples into two parts: a *training set* and a *validation* or *hold-out set*.
- The model is fit on the training set, and the fitted model is used to predict the responses for the observations in the validation set.
- The resulting validation-set error provides an estimate of the test error. This is typically assessed using MSE in the case of a quantitative response and misclassification rate in the case of a qualitative (discrete) response.

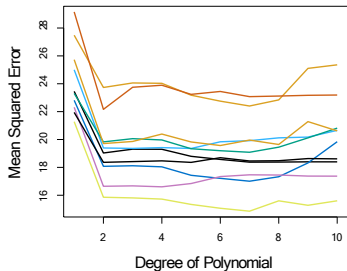
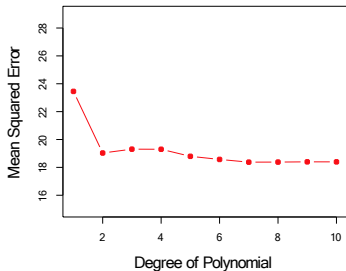
THE VALIDATION PROCESS



A random splitting into two halves: left part is training set, right part is validation set

EXAMPLE: AUTOMOBILE DATA

- Want to compare linear vs higher-order polynomial terms in a linear regression
- We randomly split the 392 observations into two sets, a training set containing 196 of the data points, and a validation set containing the remaining 196 observations.



Left panel shows single split; right panel shows multiple splits

DRAWBACKS OF VALIDATION SET APPROACH

- The validation estimate of the test error can be highly variable, depending on precisely which observations are included in the training set and which observations are included in the validation set.
- In the validation approach, only a subset of the observations — those that are included in the training set rather than in the validation set — are used to fit the model.
- This suggests that the validation set error may tend to *overestimate* the test error for the model fit on the entire data set.

K - FOLD CROSS-VALIDATION

- *Widely used approach* for estimating test error.
- Estimates can be used to select best model, and to give an idea of the test error of the final chosen model.
- Idea is to randomly divide the data into K equal-sized parts. We leave out part k , fit the model to the other $K - 1$ parts (combined), and then obtain predictions for the left-out k th part.
- This is done in turn for each part $k = 1, 2, \dots, K$, and then the results are combined.

K - FOLD CROSS-VALIDATION

Divide data into K roughly equal-sized parts ($K = 5$ here)

1 2 3 4 5

Validation	Train	Train	Train	Train
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K - FOLD CROSS-VALIDATION

- Let the K parts be C_1, C_2, \dots, C_K , where C_k denotes the indices of the observations in part k . There are n_k observations in part k : if N is a multiple of K , then $n_k = n/K$.

- Compute
$$CV_K = \sum_{k=1}^K \frac{n_k}{n} MSE_k$$

where $MSE_k = \sum_{i \in C_k} (y_i - \hat{y}_i)^2 / n_k$, and \hat{y}_i is the fit for observation i , obtained from the data with part k removed.

- Setting $K = n$ yields n -fold or leave-one out cross-validation (LOOCV).

A special case!

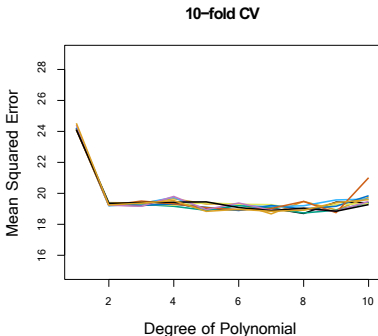
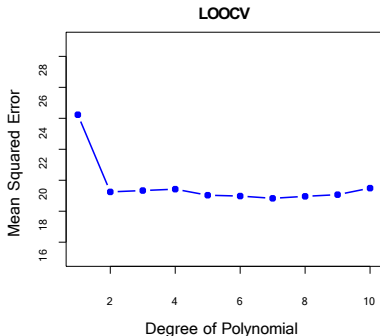
- With least-squares linear or polynomial regression, an amazing shortcut makes the cost of LOOCV the same as that of a single model fit. The following formula holds.

$$CV_n = \frac{1}{n} \sum_{i=1}^n \left(\frac{y_i - \hat{y}_i}{1 - h_i} \right)^2$$

where \hat{y}_i is the i^{th} fitted value from the original least squares fit, and h_i is the leverage (diagonal of the “hat” matrix; see book for details.) This is like the ordinary MSE, except the i th residual is divided by $1 - h_i$.

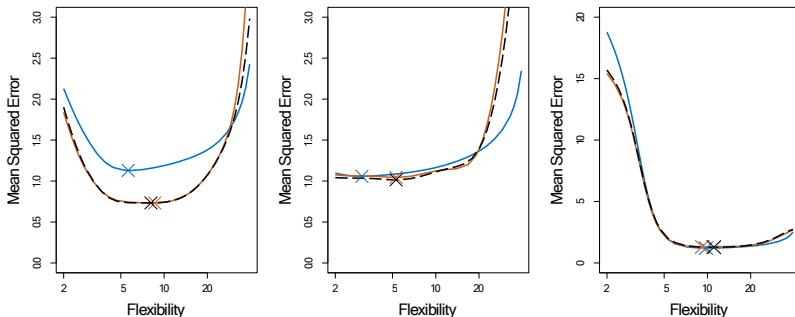
- LOOCV sometimes useful, but typically doesn't *shake up* the data enough. The estimates from each fold are highly correlated and hence their average can have high variance.
- A better choice is $K = 5$ or 10 .

Example



Left: *The LOOCV error curve.* Right: *10-fold CV was run nine separate times, each with a different random split of the data into ten parts. The figure shows the nine slightly different CV error curves.*

True and estimated test MSE for the simulated data



True and estimated test MSE for the simulated data sets in Figures 2.9 (left), 2.10 (center), and 2.11 (right). The true test MSE is shown in blue, the LOOCV estimate is shown as a black dashed line, and the 10-fold CV estimate is shown in orange. The crosses indicate the minimum of each of the MSE curves.

OTHER ISSUES WITH CROSS-VALIDATION

- Since each training set is only $(K-1)/K$ as big as the original training set, the estimates of prediction error will typically be biased upward.
- This bias is minimized when $K = n$ (LOOCV), but this estimate has high variance, as noted earlier.
- $K = 5$ or 10 provides a good compromise for this bias-variance tradeoff.

CROSS-VALIDATION FOR CLASSIFICATION PROBLEMS

- We divide the data into K roughly equal-sized parts C_1, C_2, \dots, C_K . C_k denotes the indices of the observations in part k . There are n_k observations in part k : if n is a multiple of K , then $n_k = n/K$.
- Compute

$$CV_K = \sum_{k=1}^K \frac{n_k}{n} \text{Err}_k$$

where $\text{Err}_k = \sum_{i \in C_k} I(y_i \neq \hat{y}_i) / n_k$.

- The estimated standard deviation of CV_K is

$$\widehat{\text{SE}}(CV_K) = \sqrt{\frac{1}{K} \sum_{k=1}^K \frac{(\text{Err}_k - \overline{\text{Err}})^2}{K-1}}$$

- This is a useful estimate, but strictly speaking, not quite valid.

THE BOOTSTRAP

- The *bootstrap* is a flexible and powerful statistical tool that can be used to quantify the uncertainty associated with a given estimator or statistical learning method.
- For example, it can provide an estimate of the standard error of a coefficient, or a confidence interval for that coefficient.

A simple example

- Suppose that we wish to invest a fixed sum of money in two financial assets that yield returns of X and Y , respectively, where X and Y are random quantities.
- We will invest a fraction α of our money in X , and will invest the remaining $1 - \alpha$ in Y .
- We wish to choose α to minimize the total risk, or variance, of our investment. In other words, we want to minimize $\text{Var}(\alpha X + (1 - \alpha)Y)$.
- One can show that the value that minimizes the risk is given by

$$\alpha = \frac{\sigma_Y^2 - \sigma_{XY}}{\sigma_X^2 + \sigma_Y^2 - 2\sigma_{XY}},$$

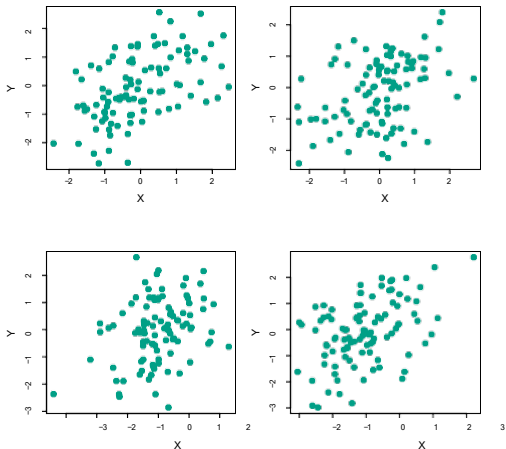
where $\sigma_X^2 = \text{Var}(X)$, $\sigma_Y^2 = \text{Var}(Y)$, and $\sigma_{XY} = \text{Cov}(X, Y)$.

Example continued

- But the values of σ_X^2 , σ_Y^2 , and σ_{XY} are unknown.
- We can compute estimates for these quantities, $\hat{\sigma}_X^2$, $\hat{\sigma}_Y^2$, and $\hat{\sigma}_{XY}$, using a data set that contains measurements for X and Y .
- We can then estimate the value of α that minimizes the variance of our investment using

$$\hat{\alpha} = \frac{\hat{\sigma}_Y^2 - \hat{\sigma}_{XY}}{\hat{\sigma}_X^2 + \hat{\sigma}_Y^2 - 2\hat{\sigma}_{XY}}.$$

Example continued



Each panel displays 100 simulated returns for investments X and Y . From left to right and top to bottom, the resulting estimates for α are 0.576, 0.532, 0.657, and 0.651.

Example continued

- To estimate the standard deviation of $\hat{\alpha}$, we repeated the process of simulating 100 paired observations of X and Y , and estimating α 1,000 times.
- We thereby obtained 1,000 estimates for α , which we can call $\hat{\alpha}_1, \hat{\alpha}_2, \dots, \hat{\alpha}_{1000}$.
- For these simulations the parameters were set to

$\sigma_X^2 = 1, \sigma_Y^2 = 1.25$, and $\sigma_{XY} = 0.5$, and so we know that the true value of α is 0.6 (indicated by the red line).

Example continued

- The mean over all 1,000 estimates for α is

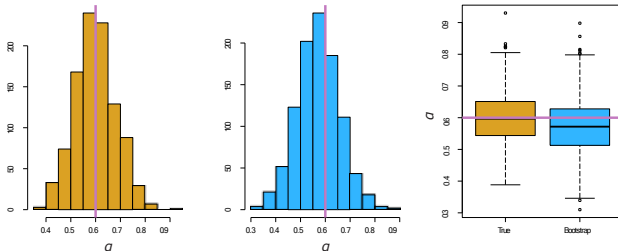
$$\bar{\alpha} = \frac{1}{1000} \sum_{r=1}^{1000} \hat{\alpha}_r = 0.5996$$

very close to $\alpha = 0.6$, and the standard deviation of the estimates is

$$\sqrt{\frac{1}{1000 - 1} \sum_{r=1}^{1000} (\hat{\alpha}_r - \bar{\alpha})^2} = 0.083.$$

- This gives us a very good idea of the accuracy of $\hat{\alpha}$: $SE(\hat{\alpha}) \approx 0.083$.
- So roughly speaking, for a random sample from the population, we would expect $\hat{\alpha}$ to differ from α by approximately 0.08, on average.

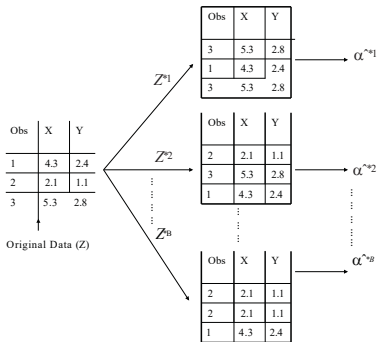
RESULTS



Left: A histogram of the estimates of α obtained by generating 1,000 simulated data sets from the true population. *Center:* A histogram of the estimates of α obtained from 1,000 bootstrap samples from a single data set. *Right:* The estimates of α displayed in the left and center panels are shown as boxplots. In each panel, the pink line indicates the true value of α .

- The procedure outlined above cannot be applied, because for real data we cannot generate new samples from the original population.
- However, the bootstrap approach allows us to use a computer to mimic the process of obtaining new data sets, so that we can estimate the variability of our estimate without generating additional samples.
- Rather than repeatedly obtaining independent data sets from the population, we instead obtain distinct data sets by repeatedly sampling observations from the original data set *with replacement*.
- Each of these “bootstrap data sets” is created by sampling *with replacement*, and is the *same size* as our original dataset. As a result some observations may appear more than once in a given bootstrap data set and some not at all.

Example with just 3 observations



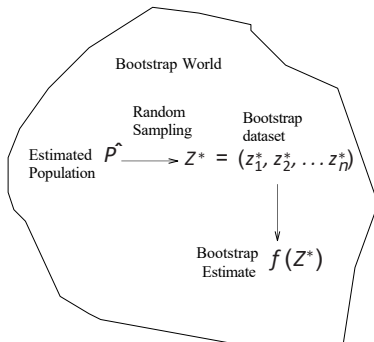
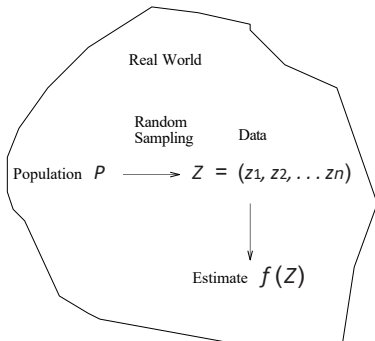
A graphical illustration of the bootstrap approach on a small sample containing $n = 3$ observations. Each bootstrap data set contains n observations, sampled with replacement from the original data set. Each bootstrap data set is used to obtain an estimate of α .

- Denoting the first bootstrap data set by Z^{*1} , we use Z^{*1} to produce a new bootstrap estimate for α , which we call $\hat{\alpha}^{*1}$
- This procedure is repeated B times for some large value of B (say 100 or 1000), in order to produce B different bootstrap data sets, $Z^{*1}, Z^{*2}, \dots, Z^{*B}$, and B corresponding α estimates, $\hat{\alpha}^{*1}, \hat{\alpha}^{*2}, \dots, \hat{\alpha}^{*B}$.
- We estimate the standard error of these bootstrap estimates using the formula

$$SE_B(\hat{\alpha}) = \sqrt{\frac{1}{B-1} \sum_{r=1}^B (\hat{\alpha}^{*r} - \bar{\hat{\alpha}}^*)^2}.$$

- This serves as an estimate of the standard error of $\hat{\alpha}$ estimated from the original data set. Bootstrap results are in blue. For this example $SE_B(\hat{\alpha}) = 0.087$.

A GENERAL PICTURE FOR THE BOOTSTRAP



THE BOOTSTRAP IN GENERAL

- In more complex data situations, figuring out the appropriate way to generate bootstrap samples can require some thought.
- For example, if the data is a time series, we can't simply sample the observations with replacement.
- We can instead create blocks of consecutive observations, and sample those with replacements. Then we paste together sampled blocks to obtain a bootstrap dataset.