Cross-validation and the Bootstrap

Remuestreo
Validación de modelos

- 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

Note: Section 5.1.5, Cross-Validation on Classification Problems, is ommited.

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.

• Test error, Training error: Capítulo 2.
• Recuérdese:
MSE= mean squared error=error cuadrático medio
= ∑(y_i-f(x_i))^2/n

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. These include the *Cp statistic*, *AIC* and *BIC*. They are discussed elsewhere in this course
- 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

K-fold Cross-validation

Validación cruzada de K iteraciones

- *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 kth part.
- This is done in turn for each part $k = 1, 2, \ldots K$, and then the results are combined.

K-fold Cross-validation in detail

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

	1	2	3	4	5
k=1:	Validation	Train	Train	Train	Train

datos de prueba

datos de entrenamiento

The details

- Let the K parts be $C_1, C_2, \ldots C_K$, 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

$$\mathrm{CV}_{(K)} = \sum_{k=1}^{K} \frac{n_k}{n} \mathrm{MSE}_k$$

  where $\mathrm{MSE}_k = \sum_{i \in C_k} (y_i - \hat{y}_i)^2 / n_k$, 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 nice 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:

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

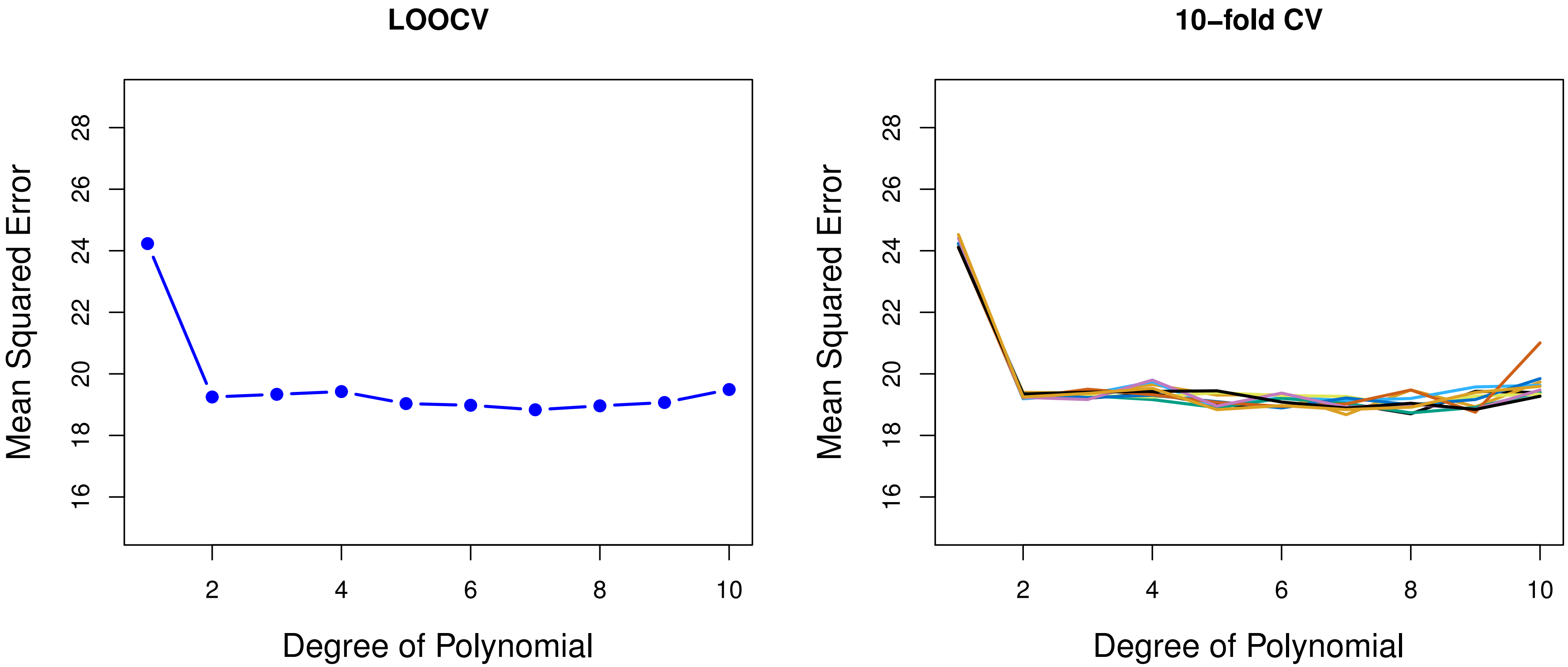
Projection Matrix

where $\hat{y}_i$ is the ith 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 ith 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.

Véase ecuación (3.37) para regresión lineal con un predictor para hi

Auto data revisited



Cross-validation was used on the Auto data set in order to estimate the test error that results from predicting mpg using polynomial functions of horsepower.
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.

Where does the name came from?

- The use of the term bootstrap derives from the phrase *to pull oneself up by one's bootstraps*, widely thought to be based on one of the eighteenth century "The Surprising Adventures of Baron Munchausen" by Rudolph Erich Raspe:

  The Baron had fallen to the bottom of a deep lake. Just when it looked like all was lost, he thought to pick himself up by his own bootstraps.

- It is not the same as the term "bootstrap" used in computer science meaning to "boot" a computer from a set of core instructions, though the derivation is similar.

** Bootstrapping methods were introduced in the late 1970s by statistician Bradley Efron.*

A simple example

Objetivo: estimar una cantidad.

- 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 $\mathrm{Var}(\alpha X + (1 - \alpha)Y)$.
- One can show that the value that minimizes the risk is given by

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

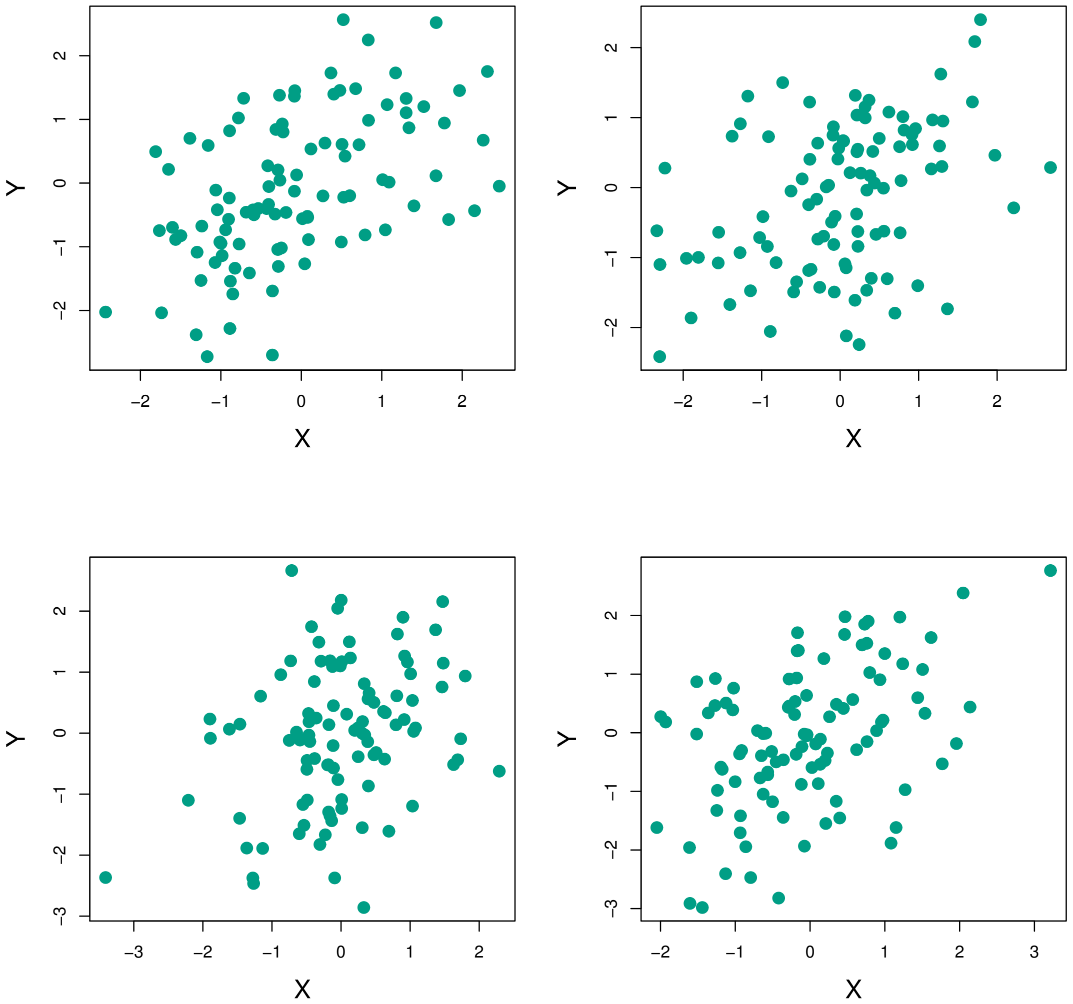
where $\sigma_X^2 = \mathrm{Var}(X), \sigma_Y^2 = \mathrm{Var}(Y)$, and $\sigma_{XY} = \mathrm{Cov}(X, Y)$.

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 $\hat{\alpha}_1, \hat{\alpha}_2, \ldots, \hat{\alpha}_{1000}$.
- The left-hand panel of the Figure on slide 29 displays a histogram of the resulting estimates.
- 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

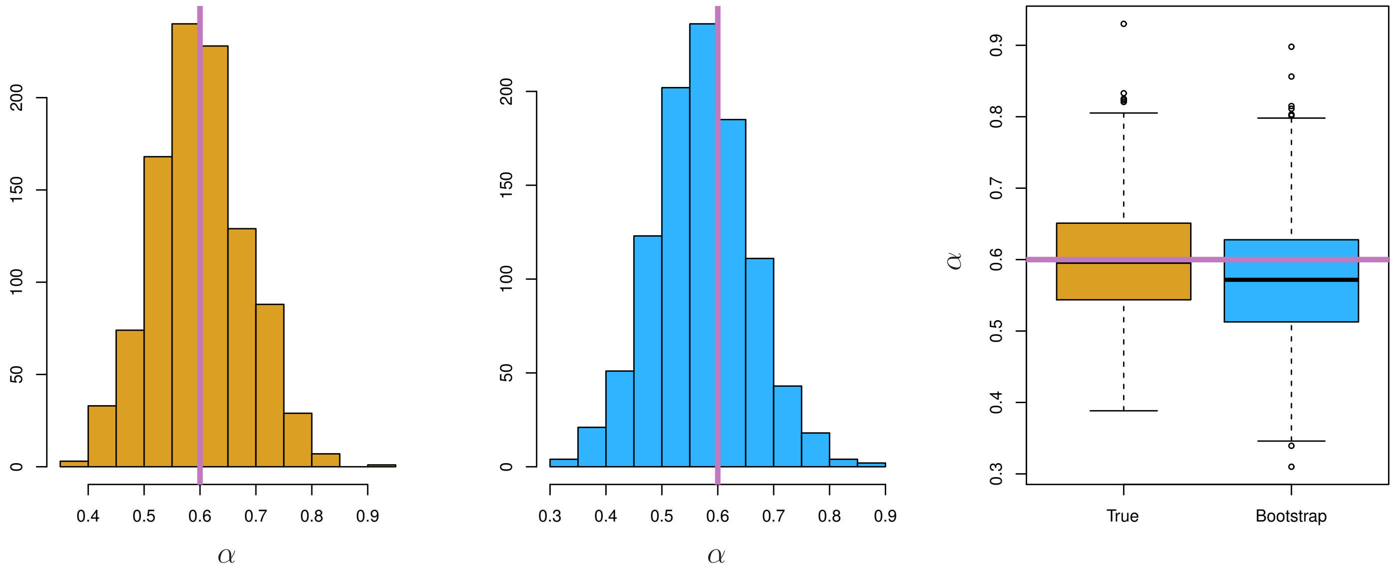
$$\bar{\alpha} = \frac{1}{1000} \sum_{r=1}^{1000} \hat{\alpha}_r = 0.5996,$$

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 $\hat{\alpha}$: $\mathrm{SE}(\hat{\alpha}) \approx 0.083$.
- 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.

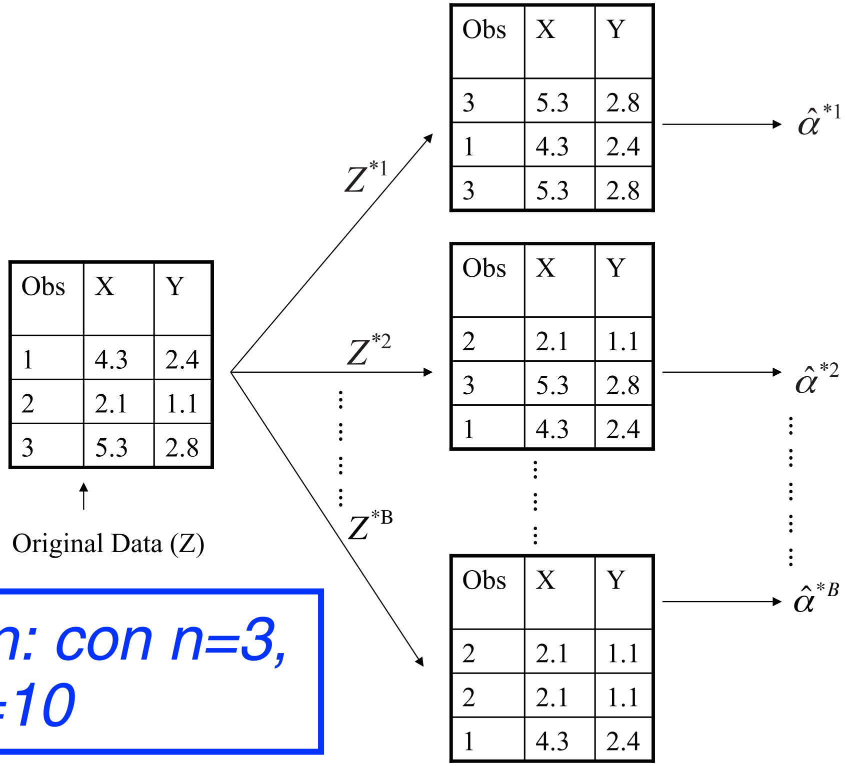
Bootstrapping: muestreo con repetición

Now back to the real world

- 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.

Combinaciones con repetición de n observaciones, tomadas de n en n

Example with just 3 observations



Observación: con n=3, B<=10

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, $Z^{*1}, Z^{*2}, \ldots, Z^{*B}$, and B corresponding α estimates, $\hat{\alpha}^{*1}, \hat{\alpha}^{*2}, \ldots, \hat{\alpha}^{*B}$.
- We estimate the standard error of these bootstrap estimates using the formula

$$\mathrm{SE}_B(\hat{\alpha}) = \sqrt{\frac{1}{B-1}\sum_{r=1}^{B}\left(\hat{\alpha}^{*r} - \bar{\hat{\alpha}}^{*}\right)^2}.$$

- This serves as an estimate of the standard error of $\hat{\alpha}$ estimated from the original data set. See center and right panels of Figure on slide 29. Bootstrap results are in blue. For this example $\mathrm{SE}_B(\hat{\alpha}) = 0.087$.

Can the bootstrap estimate prediction error?

- In cross-validation, each of the K validation folds is distinct from the other $K-1$ folds used for training: *there is no overlap*. This is crucial for its success. *Why?*
- To estimate prediction error using the bootstrap, we could think about using each bootstrap dataset as our training sample, and the original sample as our validation sample.
- But each bootstrap sample has significant overlap with the original data. About two-thirds of the original data points appear in each bootstrap sample. *Can you prove this?*
- This will cause the bootstrap to seriously underestimate the true prediction error. *Why?*