Resampling Methods: Cross Validation

Section 5.1

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Recall The Goal

- Let Y be the response (dependent variable).
- Let $X = (X_1, X_2, \ldots, X_p)$ be p different predictors (independent) variables.
- We assume there is some sort of relationship between X and Y, which can be written in the general form

$$Y = f(X) + \epsilon$$

- Our goal is to apply a statistical leaning method to estimate f, which is $\hat{f}$.

Measuring the Quality of Fit

- We need some way to measure how well is predictions actually match the observed data.

- For regression problems, use what is called the **mean squared error** MSE.

$$MSE = \frac{1}{n}\sum_{i}^{n}\left(y_i - \hat{f}(x_i)\right)^2,$$

  Where $\hat{f}(x_i)$ is the prediction that $\hat{f}$ gives for the ith observation.

- For classification problems, we use the error rate.

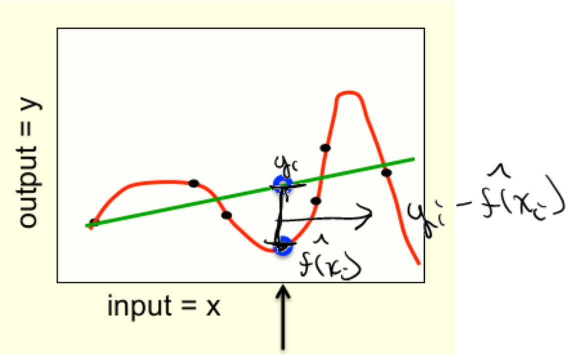
$$Err = \frac{\text{count of miss-classified observations}}{n}$$

- **Problem**: We are more interested in seeing the accuracy of these *trained* models with unseen data.

- **Solution**: We can split the data into training and testing.

Training error, Overfitting

- Training error may not be a good metric of model performance
- Sometimes good training test performance is more indicative of **overfitting**
- This results in fitting the **noise** instead of **true signal**

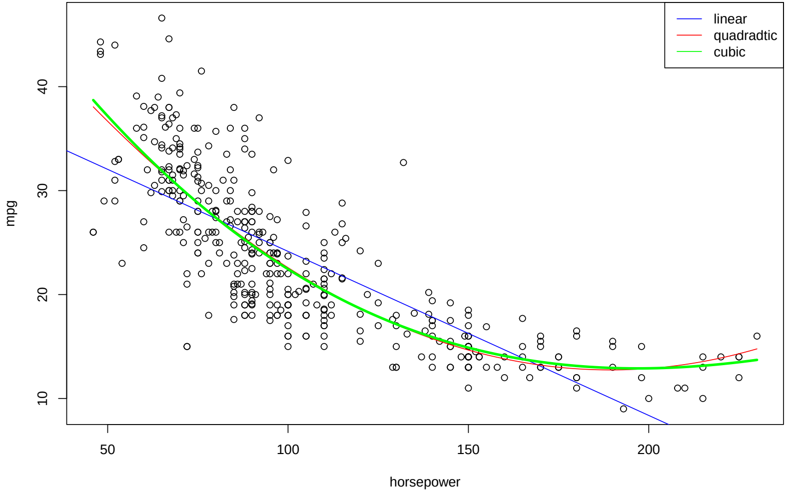


Example

Recall studying the relationship between *mpg* and *horsepower* in *Auto* data set. It appeared to be non-linear, but unclear whether a quadratic or cubic regression would provide best model.

Let's try comparing

- **linear** regression, $mpg = \beta_0 + \beta_1 hp + \varepsilon$
- **quadratic** regression & $mpg = \beta_0 + \beta_1 hp + \beta_2 hp^2 + \varepsilon$
- **cubic** regression $mpg = \beta_0 + \beta_1 hp + \beta_2 hp^2 + \beta_3 hp^3 + \varepsilon$


linear
quadradtic
cubic
mpg
10
20
30
40
horsepower
50
100
150
200

Equations of the Models

We split 392 total observations for 90% into training and 10% into testing. We train the following models (*hpwr* for *horsepower*)

$$\begin{aligned}
\text{linear}: mpg &= \beta_0 + \beta_1 hpwr + \epsilon \\
\text{quadratic}: mpg &= \beta_0 + \beta_1 hpwr + \beta_2 hpwr^2 + \epsilon \\
\text{cubic}: mpg &= \beta_0 + \beta_1 hpwr + \beta_2 hpwr^2 + \beta_3 hpwr^3 + \epsilon
\end{aligned}$$

R-Code to Split Data into Training/Testing

```
library(ISLR)
library(leaps)
set.seed(100)
sample1 = sample(1:nrow(Auto),floor(nrow(Auto)*.9))
train1.auto = Auto[sample1,]
test1.auto = Auto[-sample1,]

auto.reg = regsubsets(mpg ~ poly(horsepower,3),
                      data = train1.auto)
auto.res = summary(auto.reg)
auto.stat = cbind(auto.res$adjr2,auto.res$cp,auto.res$bic)
colnames(auto.stat) = c("Adj.R2","Cp","BIC")
rownames(auto.stat) = c("Degree 1","Degree 2","Degree 3")
```

What is the Best Statistical Learning Model?

	Adj.R2	Cp	BIC
Degree 1	0.5882040	68.543035	-301.5810
Degree 2	0.6549004	2.080382	-358.9212
Degree 3	0.6539887	4.000000	-353.1388

What about the testing data? Can we find these values for all statistical learning problems?

Best model:

$$mpg = \beta_0 + \beta_1 hp + \beta_2 hp^2 + \varepsilon$$

MSE of Auto Data

```
          Taining     Test
Degree 1 23.65730 26.54721
Degree 2 19.76901 12.37769
Degree 3 19.76444 12.19651
```

This is by random sample. If we reproduce this do we get the same results?

R Code to Get the Training/Testing MSE

```r
#Creating the models
auto1.lm = lm(mpg ~ horsepower, data = train1.auto)
auto1.lm2 = lm(mpg ~ poly(horsepower,2),data = train1.auto)
auto1.lm3 = lm(mpg ~ poly(horsepower,3),data = train1.auto)

#MSE on Training data
mse.lm1 = mean(auto1.lm$residuals^2)
mse.lm2 = mean(auto1.lm2$residuals^2)
mse.lm3 = mean(auto1.lm3$residuals^2)


#MSE on Test data
```

test obs newdata

```r
mse.test1 = sum((test1.auto$mpg - predict(auto1.lm,test1.auto))^2)/nrow(test1.auto)
mse.test2 = sum((test1.auto$mpg - predict(auto1.lm2,test1.auto))^2)/nrow(test1.auto)
mse.test3 = sum((test1.auto$mpg - predict(auto1.lm3,test1.auto))^2)/nrow(test1.auto)

mse1 = cbind(c(mse.lm1,mse.lm2,mse.lm3),c(mse.test1,mse.test2,mse.test3))
colnames(mse1) = c("Taining","Test")
rownames(mse1) = c("Degree 1","Degree 2","Degree 3")
mse1
```

```
mse1
          Taining     Test
Degree 1 23.30938 30.01736
Degree 2 18.83155 20.67362
Degree 3 18.82720 20.49544
```

Lab Questions

1. In R repeat the code with set.seed(10). Do you get the same results?

   as with set.seed(100)

   a) Yes
   b) No
2. Is your different from others in the class?
   a) Yes
   b) No

Resampling Methods

- **Resampling methods** involve repeatedly drawing samples from a training set and refitting a model of interest on each sample in order to obtain additional information about the fitted model.
- Could potentially be computationally expensive, because they involve fitting the same statistical method multiple times using different subsets of the training data.
- Two most commonly used resampling methods:
  - Cross-validation - can be used to estimate the test error associated with a given statistical learning method in order to evaluate its performance.
  - Bootstrap - can be used to provide a measure of accuracy of a parameter estimate or of a given statistical learning method.

Validataion Set Approach

- We may not always be able to get a random *test* set thus a **validation set** (or **hold-out set**) is used.

  1. Randomly divide data set into two parts:

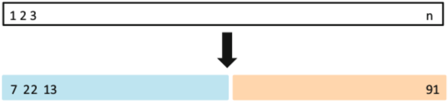
     - Training set
     - Validation set

  2. Fit the model on the training data, and use the fitted model to predict responses for validation data.

  3. Note: The validation set error rate ≈ test error rate.

Validation Set Approach: *Auto* Data Set

1. We will randomly subdivide the data evenly into training and tesing subsets. We split 392 total observations evenly - 196 for training, 196 for testing.



Validation set *Auto* dataset

2. We train the following models (*hpwr* for *horsepower*)

$$\begin{aligned} \text{linear}: mpg &= \beta_0 + \beta_1 hpwr + \epsilon \\ \text{quadratic}: mpg &= \beta_0 + \beta_1 hpwr + \beta_2 hpwr^2 + \epsilon \\ \text{cubic}: mpg &= \beta_0 + \beta_1 hpwr + \beta_2 hpwr^2 + \beta_3 hpwr^3 + \epsilon \end{aligned}$$

3. For each model, we calculate the Mean Squared Error (MSE)

$$MSE = \frac{1}{196}\sum_{i=1}^{196}(mpg_i - \widehat{mpg}_i)^2$$

   on the validation set.

After running those steps 1, 2 & 3 in *R* with *set.seed*(10):

```
       Linear Quadratic    Cubic
MSE 26.43531  19.87043 20.26584
```

R Code

```
#Setting the test/training data
set.seed(10)
sample = sample(1:nrow(Auto),nrow(Auto)/2)
train = Auto[sample,]
test = Auto[-sample,]

#Creating the models
auto.lm = lm(mpg ~ horsepower, data = train)
auto.lm2 = lm(mpg ~ poly(horsepower,2),data = train)
auto.lm3 = lm(mpg ~ poly(horsepower,3),data = train)

#Getting the predicted values hat(mpg) from test data
auto.pred = predict(auto.lm,newdata = test,se.fit = TRUE)
auto.pred2 = predict(auto.lm2,newdata = test,se.fit = TRUE)
auto.pred3 = predict(auto.lm3,newdata = test,se.fit = TRUE)

#Getting the MSE for each model
mse1 = mean((Auto$mpg - predict(auto.lm,Auto))[-sample]^2)
mse2 = mean((Auto$mpg - predict(auto.lm2,Auto))[-sample]^2)
mse3 = mean((Auto$mpg - predict(auto.lm3,Auto))[-sample]^2)
mse = cbind(mse1,mse2,mse3)
colnames(mse) = c("Linear","Quadratic","Cubic")
rownames(mse) = c("MSE")
mse
```

Split evenly

Test

Validation Set Approach Drawbacks

Validation set approach has two big drawbacks:

1. **Inconsistency** (or split-to-split variability) of error estimates. Below are the results of running validation set approach for 10 different subdivisions of data into training and validation set.

2. If we use less data for the training data, this results in a worse performance which will overestimate the MSE.

```
       Linear Quadratic    Cubic
 [1,] 25.10785  18.92612 18.86757
 [2,] 23.70434  19.39133 19.42871
 [3,] 23.79941  17.80241 17.75963
 [4,] 26.57825  21.92669 23.00028
 [5,] 25.31348  18.26249 18.25828
 [6,] 24.34163  19.68245 20.05409
 [7,] 22.39375  17.93359 17.88024
 [8,] 24.88608  18.18242 18.71694
 [9,] 25.20107  18.28719 18.37039
[10,] 26.41646  21.67991 21.71969
```

Leave-One-Out Cross-Validation (LOOCV)

In LOOCV, for **each data point** i, $i = 1, \ldots, n$, we

1. Split data into two subsets:
   - Training set: $(x_1, y_1), \ldots, (x_{i-1}, y_{i-1}), (x_{i+1}, y_{i+1}), \ldots, (x_n, y_n)$
   - Test "set" of just one observation: (x_i, y_i).
2. Use training set to fit the model and produce prediction $\hat{y}_i$.
3. Calculate $MSE_i = (y_i - \hat{y}_i)^2$

The **LOOCV estimate** for test (squared) error is

$$CV_{(n)} = \frac{1}{n} \sum_{i=1}^{n} MSE_i$$

Leave-One-Out Cross-Validation (LOOCV)

Illustration of data subdivision for LOOCV as opposed to validation set approach (where training and test set were of comparable sizes).

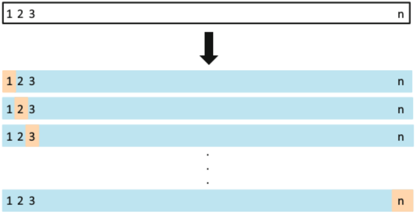


FIGURE 5.3. *A schematic display of LOOCV. A set of n data points is repeatedly split into a training set (shown in blue) containing all but one observation, and a validation set that contains only that observation (shown in beige). The test error is then estimated by averaging the n resulting MSE's. The first training set contains all but observation 1, the second training set contains all but observation 2, and so forth.*

Leave-One-Out Cross Vaidation In R

```
mse.loocv = matrix(nrow = nrow(Auto), ncol = 3)
for (i in 1:nrow(Auto)) {
  sample = i
  #Creating the models
  auto.lm = lm(mpg ~ horsepower, data = Auto[-sample,])
  auto.lm2 = lm(mpg ~ poly(horsepower,2),data = Auto[-sample,])
  auto.lm3 = lm(mpg ~ poly(horsepower,3),data = Auto[-sample,])

  #Getting the MSE for each model
  mse.loocv[i,1] = (Auto$mpg[sample] - predict(auto.lm,Auto[sample,]))^2
  mse.loocv[i,2] = (Auto$mpg[sample] - predict(auto.lm2,Auto[sample,]))^2
  mse.loocv[i,3] = (Auto$mpg[sample] - predict(auto.lm3,Auto[sample,]))^2
}
colMeans(mse.loocv)
```

```
[1] 24.23151 19.24821 19.33498
```

Leave-One-Out Cross-Validation: Pros & Cons

Advantages

- Always yields the same result. E.g., for *Auto* **data example**, LOOCV test error estimates are below.
- Nearly the whole data set is used at each step (more data $\Longrightarrow$ less bias in test error estimate)

```
       Linear Quadratic    Cubic
[1,] 24.23151  19.24821 19.33498
```

Disadvantages

- computationally demanding
- bias-variance trade-off

Both **validation set** and **LOOCV** are very general methods, and can be used with any predictive model.

Function in R for LOOCV

- Since this method is very heavy computationally there is a function in R that can create the **MSE**, called cv.glm.
- Requires the package `boot`.
- Requires the models to be created using the function glm().

Information about `cv.glm`

- **Value**: The returned value is a list with the following components
- **call**: The original call to cv.glm.
- **K**: The value of K used for the K-fold cross validation. (In LOOCV $K = n$)
- **delta**: A vector of length two. The first component is the raw cross-validation estimate of prediction error. The second component is the adjusted cross-validation estimate. The adjustment is designed to compensate for the bias introduced by not using leave-one-out cross-validation.
- **seed**: The value of .Random.seed when cv.glm was called.

```
library(boot)
auto.glm = glm(mpg ~ horsepower,data = Auto)
cv.glm (Auto, auto.glm)$delta
```

$\leftarrow mpg = \beta_0 + \beta_1 * hp + \epsilon$

```
[1] 24.23151 24.23114
```

For Multiple Models

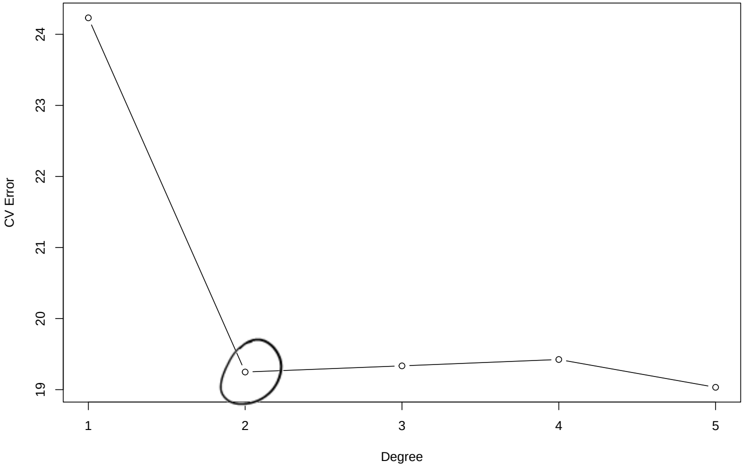
We can repeat this for multiple degrees for a polynomial regression.

```r
#Repeat Up to fifth degree
cv.error = rep(0,5)
for (i in 1:5) {
  glm.fit = glm(mpg ~ poly(horsepower,i),data = Auto)
  cv.error[i] = cv.glm(Auto,glm.fit)$delta[1]
}
cv.error = t(as.matrix(cv.error))
colnames(cv.error) = c("Degree 1", "Degree 2", "Degree 3", "Degree 4", "Degree 5")
cv.error
```

```
     Degree 1 Degree 2 Degree 3 Degree 4 Degree 5
[1,] 24.23151 19.24821 19.33498 19.42443 19.03321
```

$$mpg = \beta_0 + \beta_1 hp + \beta_2 hp^2 + \beta_3 hp^3 + \varepsilon$$

Plot



Lab Questions

3. You run the code for the Leave-One-Out Cross Validation. Do you get the same results as in the previous slide?
   a) Yes
   b) No
4. Where is the highest difference in the MSE?
   a) Between 1st degree and 2nd degree
   b) Between 2nd degree and 3rd degree
   c) Between 3rd degree and 4th degree
   d) Between 4th degree and 5th degree

K-fold Cross-Validation

K-**fold Cross-Validation** is an alternative to LOOCV where

1. Data is randomly divided into K **subsets** or *folds* of approximately equal size, n_K.
2. The first **fold** is treated as a validation set.
3. The method is fit on the remaining $k-1$ folds.
4. The mean squared error, MSE_1 is then computed on the observations in the held-out fold.
5. This procedure is repeated k times; each time a different group of observations is treated as a validation set. Which results in k estimates of the test error, $\text{MSE}_1, \text{MSE}_2, \ldots, \text{MSE}_k$
6. The K-fold CV (squared) test error estimate is

$$CV_{(k)} = \frac{1}{K}\sum_{j=1}^{K} MSE_j$$

Lab Question

5. For what K does K-fold CV become a leave-one-out CV?

   a) 1

   b) 5

   c) 10

   d) Unlimited values (k = n, number of observations in the data).

K-fold Cross-Validation

Illustration of random data subdivision into training and testing subsets for 5-fold CV (as opposed to LOOCV and validation set approaches):

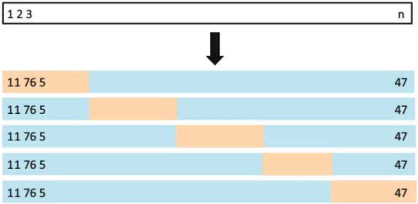


FIGURE 5.5. *A schematic display of 5-fold CV. A set of n observations is randomly split into five non-overlapping groups. Each of these fifths acts as a validation set (shown in beige), and the remainder as a training set (shown in blue). The test error is estimated by averaging the five resulting MSE estimates.*

R Code

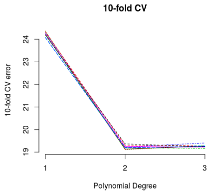
```
#use K = 10
cv.error.10 = rep(0,5)
set.seed(3)
for (i in 1:5) {
  glm.fit = glm(mpg ~ poly(horsepower,i),data = Auto)
  cv.error.10[i] = cv.glm(Auto,glm.fit,K = 10)$delta[1]
}
cv.error.10
```

```
[1] 24.11129 19.21875 19.18225 19.49981 18.94992
```

K-fold Cross-Validation: Pros & Cons

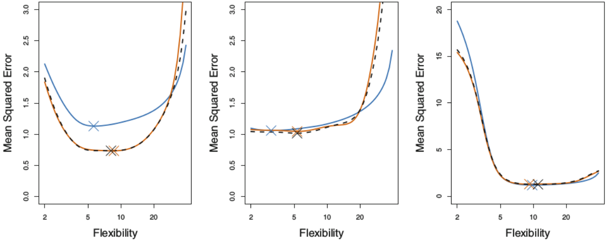
Advantages to K-fold CV over LOOCV:

- Computational: Doing *LOOCV* ($\equiv$ K-fold CV for $K = n$) is tough for computationally intensive models, as opposed to 5- or 10-fold CV, especially for large n.
- The model is fit only $K << n$ times.
- K-fold CV doesn't lose in estimation quality to *LOOCV*.
- The variability in K-fold error estimates is negligible. Below are the 10-fold CV results for polynomial fits to *Auto* data:



k-fold Cross-Validation: Pros & Cons

And it doesn't lose in estimate efficiency (show the plots of how close the LOOCV and *k*-fold estimates are for simulated data set).



Bias-Variance Tradeoff

K-fold CV also often gives more accurate estimates of the test error rate than LOOCV. This has to do with a **bias-variance trade-off**:

- *LOOCV* estimates model's test error with less bias, as it uses $\approx$ all observations ($n - 1$ out of n) to obtain the estimate at each run.
- Nonetheless, the sample-to-sample variation of *LOOCV* is higher than that for K-fold CV
- That is if we were to use a different sample from the population, then LOOCV test error estimate would (on average) change more drastically compared to K-fold CV.
- **Why?**

Bias-Variance Tradeoff

- In *LOOCV* we train n models on an almost identical set of observations $\implies$ error estimates are highly correlated and are very sample-dependent.
- In contrast, for K-fold CV we average the outputs of K models trained on less correlated subsets (overlap is smaller). $K = 5$ or 10 were shown empirically to yield optimal test error estimates.

Cross-Validation for Classification

CV can easily be used for classification when the response variable is categorical.

The biggest difference of CV for classification as opposed to regression: to estimate a test error, we use

$$\mathbf{Err} = \# \text{ of misclassified observations},$$

instead of squared error $\sum_i (y_i - \hat{y}_i)^2$

E.g. LOOCV error rate for classification

$$CV_{(n)} = \frac{1}{n} \sum_{i=1}^{n} Err_i, \quad \text{where } Err_i = \boldsymbol{I}(y_i \neq \hat{y}_i)$$

Same story for validation set approach and K-fold CV.