

Lecture 11

Brad McNeney

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Resampling Methods

- ▶ Cross-validation and bootstrap.
- ▶ Grouped together because they involve random sampling of subsets of the data.
- ▶ But purpose is different: CV estimates the test error, which is useful for model selection; the bootstrap is used to estimate the variance of estimators.
- ▶ Reference: Chapter 5 of An Introduction to Statistical Learning with Applications in R, James et al. (electronic copy available through library)

Model Fitting

- ▶ A general data generating model is

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

where

- ▶ f is a fixed but unknown function that is the **systematic** component of the model
 - ▶ We usually take $f(X)$ to be the mean of Y given X .
- ▶ ϵ is an error component, assumed to be independent of X and to have mean zero.
 - ▶ Even if Y is, say, binary, the errors have mean zero.
- ▶ We may have models for f of different complexity and need to choose the degree of complexity.
 - ▶ One criterion for the “best” complexity is the one that minimizes the test error.

Test Error

- ▶ The test error is based on the average squared prediction error over test observations.
 - ▶ Think of having “training” observations $\{(x_1, y_1), \dots, (x_n, y_n)\}$ are used to produce an estimate \hat{f} of f , and a large number of test observations (x_0, y_0) .

- ▶ The test MSE is defined as

$$\text{Ave}(y_0 - \hat{f}(x_0))^2,$$

where the average is over future x_0 's.

- ▶ We then average this average over repeated samples of training data.
- ▶ Picture this as repeating the following:
 1. Sample training and test data
 2. Train the model, and use on the test data to obtain the average squared error

and averaging the average from step 2.

- ▶ With just one training and test set we can get an *estimate* of the test error.

Validation

- ▶ If we don't have a test set we can split our data into two parts, a training set and a validation, or hold-out set.
 - ▶ Use the training set for fitting and the validation set for estimating the test error.

Validation on the Auto Data

- ▶ Use a data set called Auto from the ISLR package.
- ▶ Split the Auto data in half.

```
library(tidyverse)
library(ISLR)
data(Auto)
Auto <- dplyr::select(Auto,mpg,horsepower)
n <- nrow(Auto)
set.seed(42)
# Split in half
train <- sort(sample(1:n,size=n/2)) # sorting not necessary
head(train)
```

```
## [1] 1 2 3 7 11 14
```

```
validn <- setdiff(1:n,train)
head(validn)
```

```
## [1] 4 5 6 8 9 10
```

```
Auto.train <- Auto[train,]
Auto.validn <- Auto[validn,] # same as Auto[-train,]
```

- ▶ Use the train half to train a polynomial model in horsepower and then estimate the test MSE on the validn half.
 - ▶ Software note: `poly()` returns polynomials and is useful in a model formula to save typing

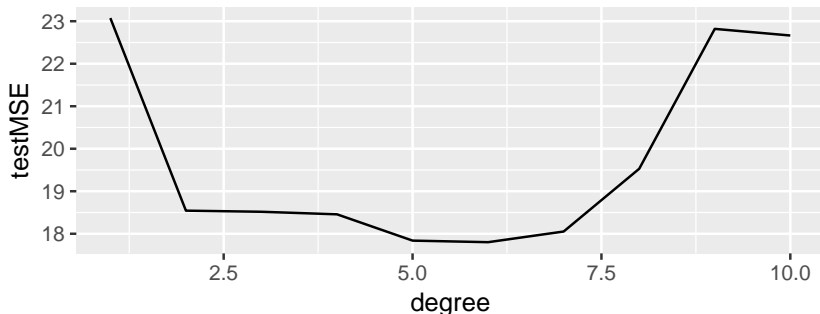
```
afit <- lm(mpg ~ poly(horsepower,2),data=Auto.train)
yhat.v <- predict(afit,newdata=Auto.validn)
tMSE <- with(Auto.validn,mean((mpg - yhat.v)^2))
tMSE
```

```
## [1] 18.54359
```

```
# afit <- lm(mpg ~ poly(horsepower,5),data=Auto.train)
# aa <- mutate(Auto.validn,pred=predict(afit,newdata=Auto.validn))
# ggplot(aa,aes(x=horsepower,y=mpg)) +
#   geom_point() + geom_line(aes(y=pred))
```

Validation to Select the Degree of Polynomial

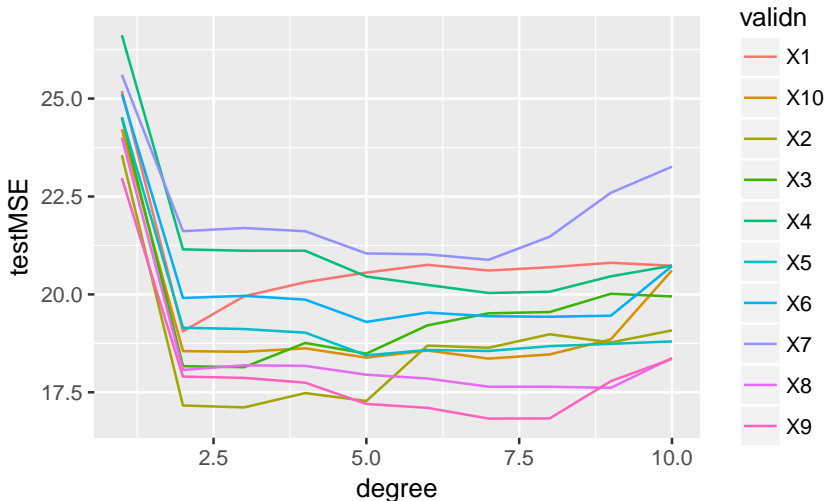
```
testMSE <- function(dd,train,validn) {  
  afit <- lm(mpg ~ poly(horsepower,dd),data=train)  
  yhat.v <- predict(afit,newdata=validn)  
  return(with(validn,mean((mpg - yhat.v)^2)))  
}  
nd <- 10; dd <- (1:nd); tm <- rep(NA,nd)  
for(i in dd) {  
  tm[i] <- testMSE(i,Auto.train,Auto.validn)  
}  
dMSE <- data.frame(degree=dd,testMSE= tm)  
ggplot(dMSE,aes(x=degree,y=testMSE)) + geom_line()
```



Validation with Different Validation Sets

```
nValid <- 10
valid <- function() {
  n <- nrow(Auto)
  train <- sample(1:n,size=n/2)
  Auto.train <- Auto[train,]
  Auto.validn <- Auto[-train,]
  tm <- vector(mode="numeric",length=nd)
  for(i in dd) {
    tm[i] <- testMSE(i,Auto.train,Auto.validn)
  }
  tm
}
tMSE <- replicate(nValid,valid())
tMSE <- data.frame(degree=dd,tMSE)
tMSE <- gather(tMSE,validn,testMSE,X1:X10,-degree)
```

```
ggplot(tMSE,aes(x=degree,y=testMSE,color=validn))+ geom_line()
```



► Note the variability in the estimated test MSE.

Cross-Validation (CV)

- ▶ Rather than a single data split, do multiple splits into “folds” of approximately equal size.
 - ▶ Common numbers of folds are $k = n$, 10 and 5.
- ▶ Train on all but one hold-out fold, and test on the hold-out to get MSE_i ; $i = 1, \dots, k$.
- ▶ Repeat for each fold and average the estimated test MSEs:

$$CV_{(k)} = \frac{1}{k} \sum_{i=1}^k \text{MSE}_i.$$

Leave-Out-One CV (LOOCV)

- ▶ Break the data into n folds, with one observation in each fold.
- ▶ Computational trick for a linear model fit by least squares:

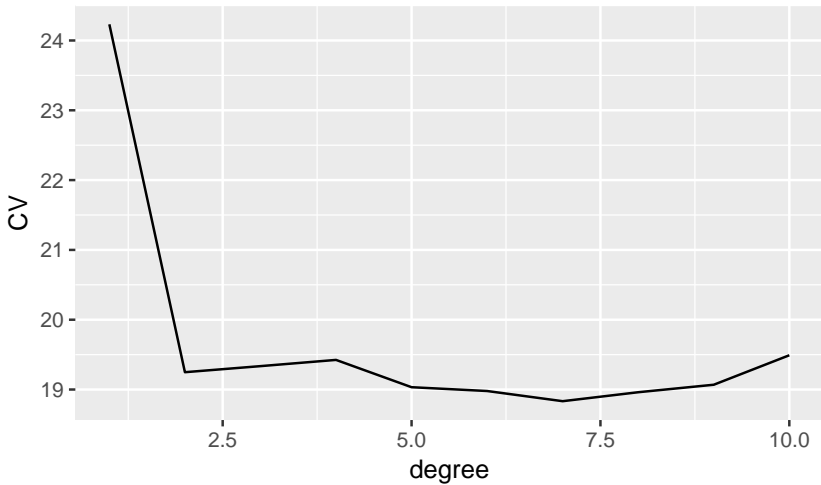
$$CV_{(n)} = \frac{1}{n} \sum_{i=1}^n \left(\frac{y_i - \hat{y}_i}{1 - h_i} \right)^2,$$

where \hat{y}_i is the fitted value from the least squares fit and h_i is the leverage of the i th observation.

LOOCV on Auto Data

```
loocv <- function(dd) {  
  CVn <- rep(NA,length(dd))  
  for(i in dd) {  
    fit <- lm(mpg ~ poly(horsepower,i),data=Auto)  
    hh <- hatvalues(fit)  
    ff <- fitted.values(fit)  
    CVn[i] <- with(Auto,mean(((mpg-ff)/(1-hh))^2))  
  }  
  CVn  
}  
cv.err <- loocv(dd)  
cv.err <- data.frame(degree=dd,CV=cv.err)
```

```
ggplot(cv.err,aes(x=degree,y=CV)) + geom_line()
```

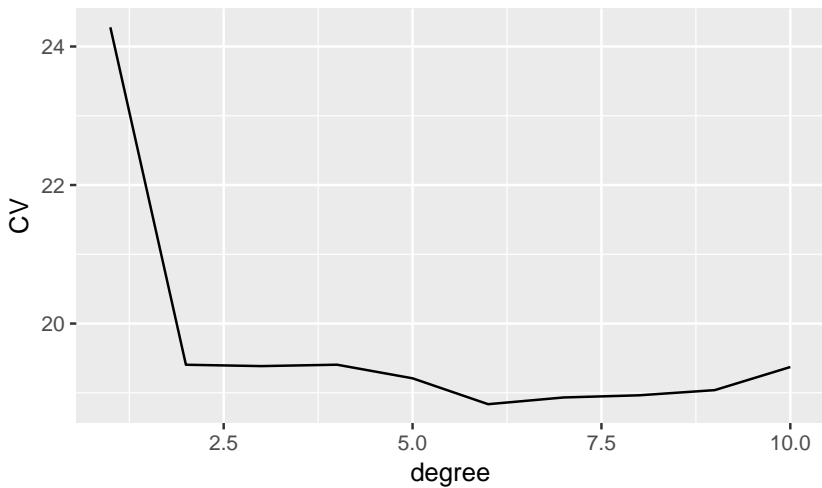


10-Fold CV on Auto Data

- ▶ Can use a function `cv.glm()` from the `boot` package.
 - ▶ Uses output from `glm()`.
 - ▶ `glm` default is normal errors; i.e., `lm()`.

```
library(boot)
cv.err <- rep(NA,nd)
set.seed(123)
for(i in dd) {
  fit <- glm(mpg ~ poly(horsepower,i),data=Auto)
  cc <- cv.glm(Auto,fit,K=10)
  cv.err[i] <- cc$delta[1] # CV estimate of prediction error
}
cv.err <- data.frame(degree=dd,CV=cv.err)
```

```
ggplot(cv.err,aes(x=degree,y=CV)) + geom_line()
```



Bias-Variance Trade-Off for k -Fold CV

- ▶ In general, computation of k -fold CV increases with k .
- ▶ But more important is the accuracy of the CV estimator as a function of k .
- ▶ There are two components to accuracy, bias and variance.
 - ▶ It can be shown that the bias of the CV estimator of the test error *decreases* as k increases.
 - ▶ It can be shown that the variance of the CV estimator *increases* with k .

Bias

- ▶ If data splitting results in a training set that is small, the error of the statistical learning method will be larger than if we fit to all data.
- ▶ Implies an upward bias in the estimate of the test error.
- ▶ On the other extreme, LOOCV uses almost all the data to train, and so will have almost no bias.

Variance

- ▶ This is harder to reason through.
- ▶ The LOOCV estimate is an average of many squared errors that are (i) highly variable, and (ii) positively correlated.
 - ▶ Averaging many things is good.
 - ▶ The positive correlation arises from using mostly the same data to fit the model each time.
- ▶ For k -fold CV with smaller k , we average fewer MSEs that are (i) less variable and (ii) less correlated.
- ▶ Which “wins”? Turns out that $k = 5$ or 10 have been shown to work well empirically.

CV on Classification Problems

- ▶ We have illustrated the idea behind CV when the response is quantitative.
- ▶ We then use the MSE (mean squared error) to quantify test error.
- ▶ For classification problems we measure the error of a procedure by the misclassification error.
- ▶ For example,

$$CV_{(n)} = \frac{1}{n} \sum_{i=1}^n I(y_i \neq \hat{y}_i)$$

- ▶ See the reference text (ISLR) for examples.

The Bootstrap

- ▶ The bootstrap uses resampling to quantify uncertainty in an estimator.

Assumptions and sampling distributions

- ▶ Under model assumptions, the sampling distribution of the statistics used for inference are known.
 - ▶ Sampling distribution: Distribution of a statistic over repeated samples of data **from the population**.
 - ▶ For regression coefficients, the sampling distribution leads to t-tests and CIs
- ▶ The bootstrap is a data-driven approach to approximating the sampling distribution of inferential statistics.
 - ▶ Find the distribution of a statistic over repeated samples of data **from the original sample**.
 - ▶ Reasonable if original sample is representative of the population.
 - ▶ Base inference on the bootstrap approximate distribution.

Advantages

- ▶ Bootstrap may give reasonable uncertainty estimates when assumptions for traditional inference don't hold.
- ▶ We can expand the definition of the “procedure” to include variable selection, rather than just model fitting for a given model complexity.

Resampling

- ▶ Resampling means drawing samples, with replacement, from the original sample.
 - ▶ E.G., drawing cars, with replacement.

```
set.seed(42)
n <- nrow(Auto)
Autos <- data.frame(index=1:n,Auto)
resamAuto <- sample_n(Auto,size=n,replace=TRUE)
head(resamAuto)
```

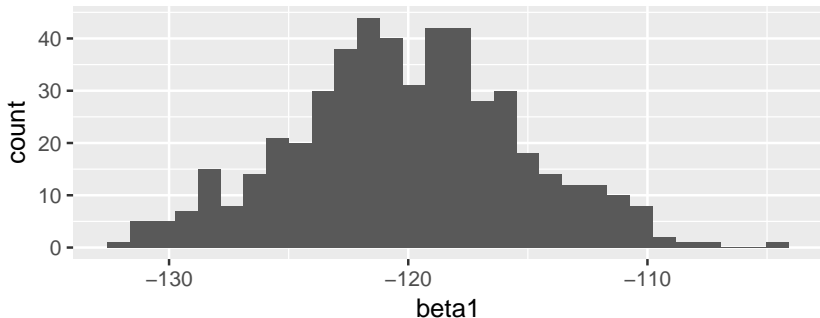
```
##      mpg horsepower
## 364 22.4          110
## 373 27.0           90
## 114 21.0          107
## 328 36.4           67
## 254 20.5           95
## 206 28.0           75
```


Bootstrap Standard Errors

- ▶ Resample some number B times.
- ▶ For each resample compute the estimates.
- ▶ Take the sample SD of the bootstrap estimates.

```
B <- 500; beta1Boot <- rep(NA,B)
for(i in 1:B) {
  rAuto <- sample_n(Auto,size=n,replace=TRUE)
  fit <- lm(mpg~poly(horsepower,2),data=rAuto)
  beta1Boot[i] <- coefficients(fit)[2]
}
beta1Boot <- data.frame(beta1=beta1Boot)
```

```
ggplot(beta1Boot,aes(x=beta1)) + geom_histogram()
```



```
with(beta1Boot,sd(beta1))
```

```
## [1] 4.72912
```

```
fit <- lm(mpg~poly(horsepower,2),data=Auto)  
round(summary(fit)$coefficients[2,],4)
```

```
## Estimate Std. Error t value Pr(>|t|)  
## -120.1377 4.3739 -27.4668 0.0000
```