

Statistics 452: Statistical Learning and Prediction

Chapter 5: Resampling Methods

Brad McNeney

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, bootstrap is used to estimate the variance of estimators.

Test Error

- ▶ Illustrate with squared error for quantitative Y .
- ▶ Training observations $\{(x_1, y_1), \dots, (x_n, y_n)\}$ are used to produce \hat{f} .
- ▶ If we had a large number of test observations (x_0, y_0) , the test MSE

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

reflects how well \hat{f} predicts new observations.

- ▶ With just a finite test set we get an *estimate* of the test error.

Validation

- ▶ This is what we have already been doing.
- ▶ We 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

- 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 4 5 6
```

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

```
## [1] 7 8 9 10 11 15
```

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

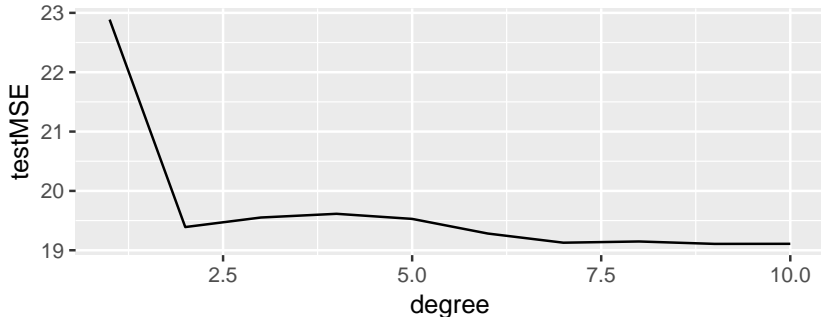
- ▶ Use the train half to train a polynomial model in horsepower and then estimate the test MSE on the validn half.
 - ▶ Software note: `poly()` returns polynomials and is useful in a model formula to save typing

```
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] 19.39095
```

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()
```

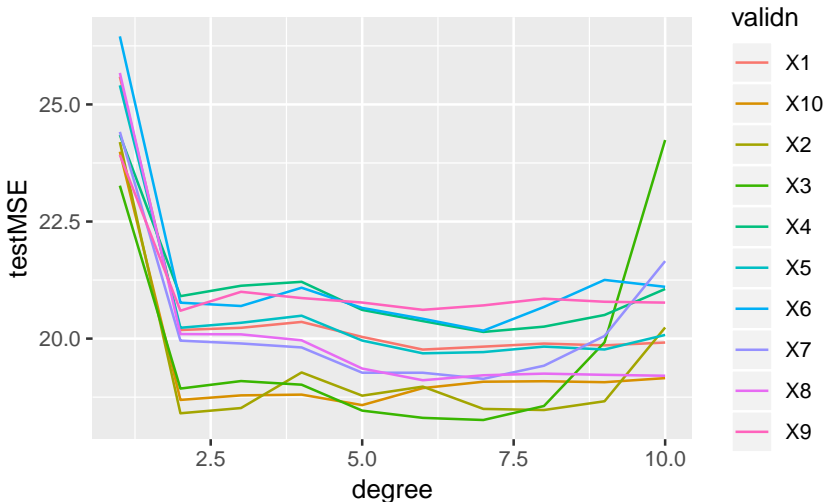


Validation with Different Validation Sets

```
nValid <- 10
valid <- function() {
  n <- nrow(Auto)
  train <- sample(1:n,size=n/2)
  Auto.train <- Auto[train,]
  Auto.validn <- Auto[-train,]
  tm <- rep(NA,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:

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

Test Error vs Expected Test Error

- ▶ A quantity related to test error is the expected test error, obtained by averaging the test error over repeated training sets,

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

where the outer *Ave* is over the training sets that give us \hat{f} .

- ▶ Cross validation estimates the expected test error.
 - ▶ A procedure with good expected test error tends to have good test error.

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:

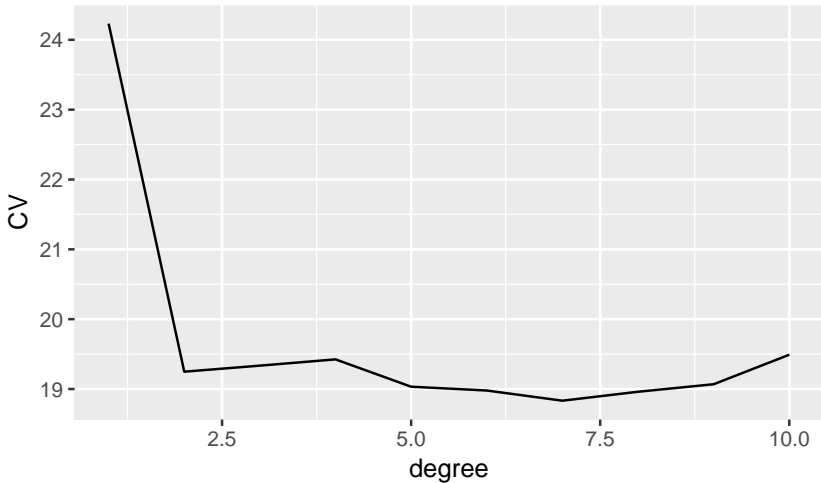
$$CV_{(n)} = \frac{1}{n} \sum_{i=1}^n \left(\frac{y_i - \hat{y}_i}{1 - h_i} \right)^2,$$

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()
```

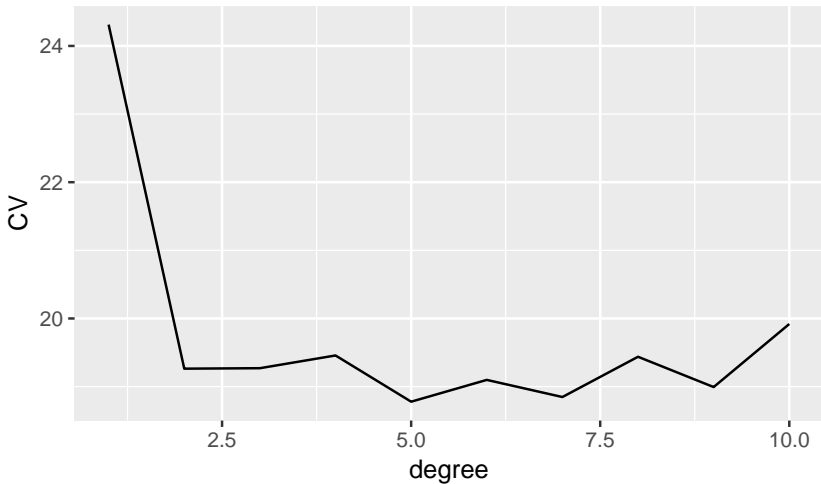


10-Fold CV on Auto Data

- ▶ 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.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”? Values $k = 5$ or 10 have been shown to work well empirically and are recommended.

Simulation Example

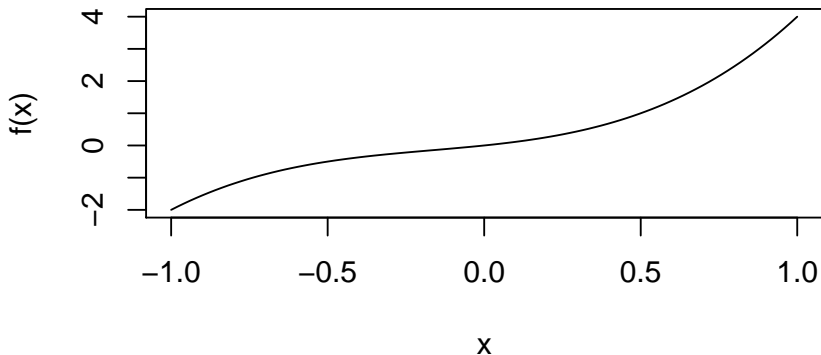
- ▶ We can illustrate the bias and variance of the CV estimator of the test error with one simulation model.
- ▶ Simulate from the model

$$Y = X + X^2 + 2X^3 + \epsilon$$

for $\epsilon \sim N(0, 1)$ and a fixed grid of X -values.

- ▶ Fit a linear regression.
- ▶ View the contributions to $CV_{(n)}$ and $CV_{(10)}$ and the variance of these two estimators.

```
n <- 100  
x <- seq(-1,1,length=n)  
plot(x,x+x^2+2*x^3,ylab="f(x)",type="l")
```



```
simdat <- function() {  
  y<-rnorm(n,mean=x+x^2+2*x^3,sd=1)  
  data.frame(y=y,x=x)  
}
```

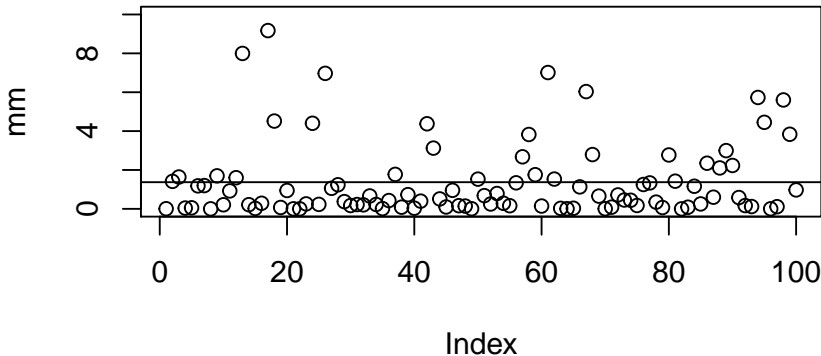
```

# LOOCV contributions for data set of size n.
# LOOCV estimate of test error is their average.
loocv.contrib <- function() {
  MSE <- rep(NA,n)
  dat <- simdat()
  for(i in 1:n) {
    fit <- lm(y~x,data=dat,subset=(-i))
    newdat <- data.frame(x=dat$x[i])
    pp <- predict(fit,newdata=newdat)
    MSE[i] <- (dat$y[i] - pp)^2
  }
  MSE
}

```

- Repeat the following a few times

```
mm <- loocv.contrib()  
plot(mm,ylim=c(0,10))  
abline(h=mean(mm)) # LOOCV estimate of test error
```



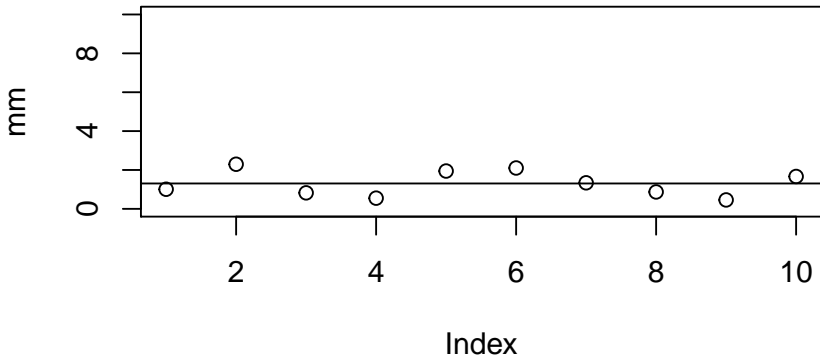
```

# 10-fold CV contributions for data set of size n
cv.contrib <- function(n=100,k=10) {
  MSE <- rep(NA,k)
  dat <- simdat()
  inds <- sample(1:n)
  for(i in 1:(n/k)) {
    ss <- inds[(i-1)*k + (1:(n/k))]
    fit <- lm(y~x,data=dat,subset=(-ss))
    newdat <- data.frame(x=dat$x[ss])
    pp <- predict(fit,newdata=newdat)
    MSE[i] <- mean((dat$y[ss] - pp)^2)
  }
  MSE
}

```


- Repeat the following a few times

```
mm <- cv.contrib()  
plot(mm,ylim=c(0,10))  
abline(h=mean(mm)) # Estimate of test error
```



- ▶ Hard to see how the CV estimates (horizontal lines) vary over samples, so record them over many simulations.

```
set.seed(123)
NREPS <- 1000
LOOCVres <- CVres <- rep(NA, NREPS)
for(i in 1:NREPS) {
  LOOCVres[i] <- mean(loocv.contrib())
  CVres[i] <- mean(cv.contrib())
}
mean(LOOCVres); var(LOOCVres); mean(CVres); var(CVres)
```

```
## [1] 1.218233
```

```
## [1] 0.02905049
```

```
## [1] 1.219598
```

```
## [1] 0.02943189
```

- ▶ Can see suggestion of lower bias from LOOCV, but not lower variance of 10-fold CV for this scenario.

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 text 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 used to obtain the estimates to include variable selection and/or other smoothing (more on this later).

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
## 1 23.0          86
## 2 46.6          65
## 3 15.0          72
## 4 13.0         140
## 5 16.0         180
## 6 24.0          75
```

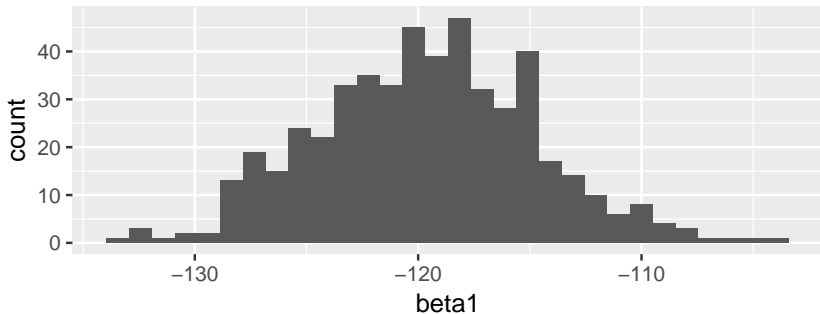
Bootstrap Standard Errors

- ▶ 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] 4.911742
```

```
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

Boostrapping with the boot Package

- The boot package can be used for bootstrap sampling

```
library(boot)
# Write a function to take the dataset and indices
# of a resample as input and return our statistic
regCoef <- function(dat,inds) {
  fit <- lm(mpg~poly(horsepower,2),data=dat[inds,])
  coefficients(fit)[2]
}
beta1Boot <- boot(Auto,regCoef,B)
with(beta1Boot,sd(t))
```

```
## [1] 4.686192
```

Bootstrap Confidence Intervals

- ▶ The percentiles of the bootstrap distribution can also be used as a confidence interval.
- ▶ E.G., the interval between the 2.5th and 97.5th percentiles of the bootstrap distribution are an approximate 95% CI.

```
boot.ci(beta1Boot,type="perc")
```

```
## BOOTSTRAP CONFIDENCE INTERVAL CALCULATIONS
## Based on 500 bootstrap replicates
##
## CALL :
## boot.ci(boot.out = beta1Boot, type = "perc")
##
## Intervals :
## Level      Percentile
## 95%      (-128.8, -110.2 )
## Calculations and Intervals on Original Scale
```