4 PQHS 471 Notes Week 4

4.1 Week 4 Day 1

ISLR Chapter 5 covers two computational techniques — cross-validation and bootstrap — for model evaluation.

4.1.1 ISLR 5.1

Cross-validation (CV) can be used for two purposes: model assessment and model selection. In model assessment, we evaluate the generalizability of a model (e.g., prediction performance). In model selection, we select hyperparameters for the final model.

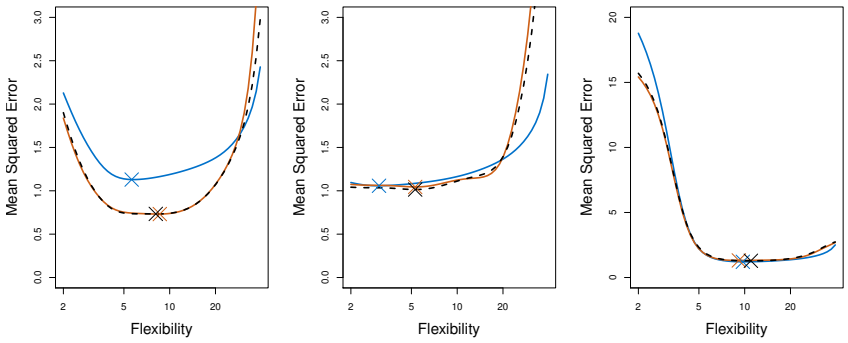
Some issues have been covered in my notes for week 1 (ISLR 2, HOML 1), week 2 (an R example), week 3 (ISLR 4).

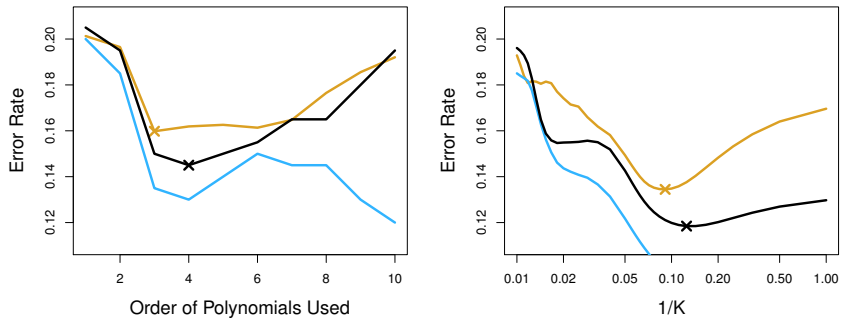
Bias: Validation and CV can overestimate test error rate when n is not large. (Reason: We effectively evaluate the prediction performance for a model that is *built on a dataset of sample size* n_{train}. What we are really interested in is the prediction performance for the final model that is *built on all available data*, which has size n. In general, the smaller sample size the more variability in a fitted model. Since $n_{train} < n$, there is always a tendency to overestimate the test error rate. When $n = 1000$ and $n_{train} = 800$, the amount of overestimation is probably ignorable. When $n = 100$ and $n_{train} = 80$ or even less, the amount of overestimation can be non-trivial. This bias may not have a large impact on model selection as long as the bias is similar across all models evaluated.

- 5.1.1: Validation set approach:
  - Results can vary due to random splitting, especially when n is not large. (Figure 5.2)
- 5.1.2: Leave-one-out (LOO) is n-fold CV. It is also called the jackknife.
  - n models are fit. Can be computationally expensive; except for least squares linear regression, for which fitting one model is sufficient. (5.2)
  - Bias is minimal because $n_{train} = n - 1$.
  - Variance may be high because the n models are very similar.
- 5.1.3: k-fold CV
  - Every observation has a chance to serve as a test point.
  - An improvement over 5.1.1. Useful for datasets that are not very large.
  - Less computational than 5.1.2. Similar performance on model selection as LOO (Figure 5.6)
- 5.1.4: Bias–variance trade-off in choice of k
  - As k decreases, bias increases (because overestimation of test error rate due to smaller sample size) but variance decreases (because the k models are less similar to each other).
  - When n is large (say, $n \geq 10000$), 5-fold CV is often enough.
  - When n is not very large, 10-fold CV (to avoid bias).
  - When n is small (say, $n \leq 200$), may repeat 10-fold CV several times to reduce the noise introduced by random partitioning. An example is in my week 2 notes.

5.1.5 contains an example of using CV on classification.

Figures 5.6 and 5.8 show that CV curves are good approximations of test error curves.





4.1.2 Simulation for the scenarios in ISLR 4.5

I wrote a function to generate a partition of the indices $\{1, 2, \cdots, n\}$ into K subsets.

```
cv.part = function(n, K) {
    s1 = n %/% K; s2 = n %% K
    pos2 = ifelse(rep(s2==0,K), (1:K)*s1, (1:K)*s1 + c(rep(0,K-s2), 1:s2))
    pos1 = c(1, pos2[-K]+1)
    part = sample(n,n)
    out=list()
    for(k in 1:K) out[[k]] = part[pos1[k]:pos2[k]]
    out
}
```

In `cv.part()`, if n can be divided by K, the subsets have equal size; if not, some of the subsets have an extra index. In `cv.glm()` in the R `boot` package, `sample(rep(1:K, ceiling(n/K)), n)` is used to generate a partition, which can lead to an uneven distribution. For example, when $n = 7$, $K = 3$, it can give a partition with subset sizes (1,3,3), while (2,2,3) is more desirable; when $n = 9$, $K = 4$, it can give a partition with subset sizes (0,3,3,3), while (2,2,2,3) is more desirable. The above function `cv.part()` always give the most desirable subset size distribution.

We need one more function:

```
cv.knn = function(train, class, krange, K) {
  ## train: X data frame
  ## class: Y vector
  ## krange: a vector of k values to be evaluated for k-NN
  ## K: K-fold CV to be used

  ## The values are:
  ## Nmiss: number of misclassification for k in krange
  ## k: the k in krange that has the smallest Nmiss. If there is a tie, the largest k.
  require(class)  ## for knn()
  n = length(class)
  part = cv.part(n, K)

  Nmiss = NULL
  for(k in krange) {
    nmiss = 0
    for(ii in 1:K) {
      idxtest = part[[ii]]
      nmiss = nmiss + sum(class[idxtest] !=
                          knn(train[-idxtest, ], train[idxtest, ], class[-idxtest], k))
    }
  Nmiss[k] = nmiss
```

```
  }
  names(Nmiss) = krange

  kminmiss = max(krange[which(Nmiss == min(Nmiss))])
  list(Nmiss=Nmiss, k=kminmiss)
}
```

We simulate Scenario 4 (ISLR 4.5). You can experiment other values and other scenarios.

```
library(MASS)  ## for mvrnorm() and LDA/QDA
library(class)  ## for knn()

ntrain=50; ntest=1000
mu1=c(0,0);  Sigma1=matrix(c(1,.5,.5,1),2)
mu2=c(2,-1); Sigma2=matrix(c(1,-.5,-.5,1),2)
## testing data of size ntest
t1 = mvrnorm(ntest, mu=mu1, Sigma=Sigma1)
t2 = mvrnorm(ntest, mu=mu2, Sigma=Sigma2)
ttx = data.frame(rbind(t1,t2))
tty = rep(c(0,1), each=ntest)

## simulate 100 datasets each of size ntrain, apply the 5 methods
ntally = matrix(,100,5)  ## 5 methods to be evaluated
for(ii in 1:100) {
  d1 = mvrnorm(ntrain, mu=mu1, Sigma=Sigma1)
  d2 = mvrnorm(ntrain, mu=mu2, Sigma=Sigma2)
  dd = data.frame(y=rep(c(0,1), each=ntrain), rbind(d1,d2))
  ntally[ii, ] = c(
    sum(tty != knn(dd[,2:3], ttx, dd$y, k=1)),  ## 1-NN
    sum(tty != knn(dd[,2:3], ttx, dd$y, k=cv.knn(dd[,2:3], dd$y, k=1:20, 10)$k)),  ## kNN-CV
    sum(tty != predict(lda(y ~ X1+X2, data = dd), ttx)$class),  ## LDA
    sum(tty != (predict(glm(y ~ X1+X2, data=dd, family=binomial), ttx, type='response') > 0.5)),
    sum(tty != predict(qda(y ~ X1+X2, data = dd), ttx)$class))  ## QDA
}

methodnames = c('1nn','knn-CV','LDA','Logistic','QDA')
plot(factor(rep(factor(methodnames, levels=methodnames), each=100)), as.numeric(ntally))
```

4.1.3 Assignment

1. Reading for next lecture: ISLR 5.2

4.2 Week 4 Day 2

4.2.1 ISLR 5.2 Bootstrap

Motivation: If we knew the true underlying distribution for our data, we would be able to evaluate various measures of interest, e.g., the variance of a complicated statistic calculated from a dataset of size n. We could do it by repeatedly sampling datasets of size n from the underlying distribution, and calculating the statistic of interest for each simulated dataset. Then the variance of the statistic could be calculated.

We can mimic this by treating the empirical distribution obtained from data as if it were the underlying distribution. Assuming no ties, the empirical distribution is multinomial with n categories each having $1/n$ probability. To sample a dataset of size n from this multinomial distribution is effectively to **sample with replacement** n data points from the original dataset. This is also true when there are ties.

0.632: The probability for an observation to be sampled into a bootstrap sample. (The correct value is $1-(1-\frac{1}{n})^n$, which is approximately $1-e^{-1}=0.632$.)

For example, we have data from an unknown distribution and we can estimate the 75th percentile of the distribution. We want to know the accuracy of this estimate. The `boot` package has a function `boot()` for this. It requires a function with two arguments: `data`, `index`.

```
library(boot)  ## for boot() and cv.glm()

## generate data from a mixture distribution
x = c(rnorm(40,0,2), runif(30,0,5), rgamma(30, 2, .3))
hist(x)

myvar = function(data, index)
    var(data[index])
myvar(x)

aa = boot(x, myvar, R=100)
aa
aa$t0; mean(aa$t)-aa$t0; sd(aa$t)
hist(aa$t)

my75th = function(data, index)
    quantile(data[index], .75)
my75th(x)

aa = boot(x, my75th, R=100)
aa
aa$t0; mean(aa$t)-aa$t0; sd(aa$t)
hist(aa$t)
```

4.2.2 Assignment

1. **Homework**: ISLR Chapter 5 Exercises 9 (`Boston` dataset in MASS)
2. Reading for next lecture: ISLR 6, HOML 4
3. ISLR Chapter 6 R Labs