Lecture 11

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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 $\{(x_1, y_1), \ldots, (x_n, y_n)\}$ 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.
- With a finite test set we get an *estimate* of the test error.
- A related quantity is the **expected** test error, in which we average the above over repeated samples of training data.
- Picture expected test error as repeating the following:
  1. Sample training and test data
  2. Train the model, and evaluate on test data.
- With just one training and test set we get an *estimate* of the expected 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

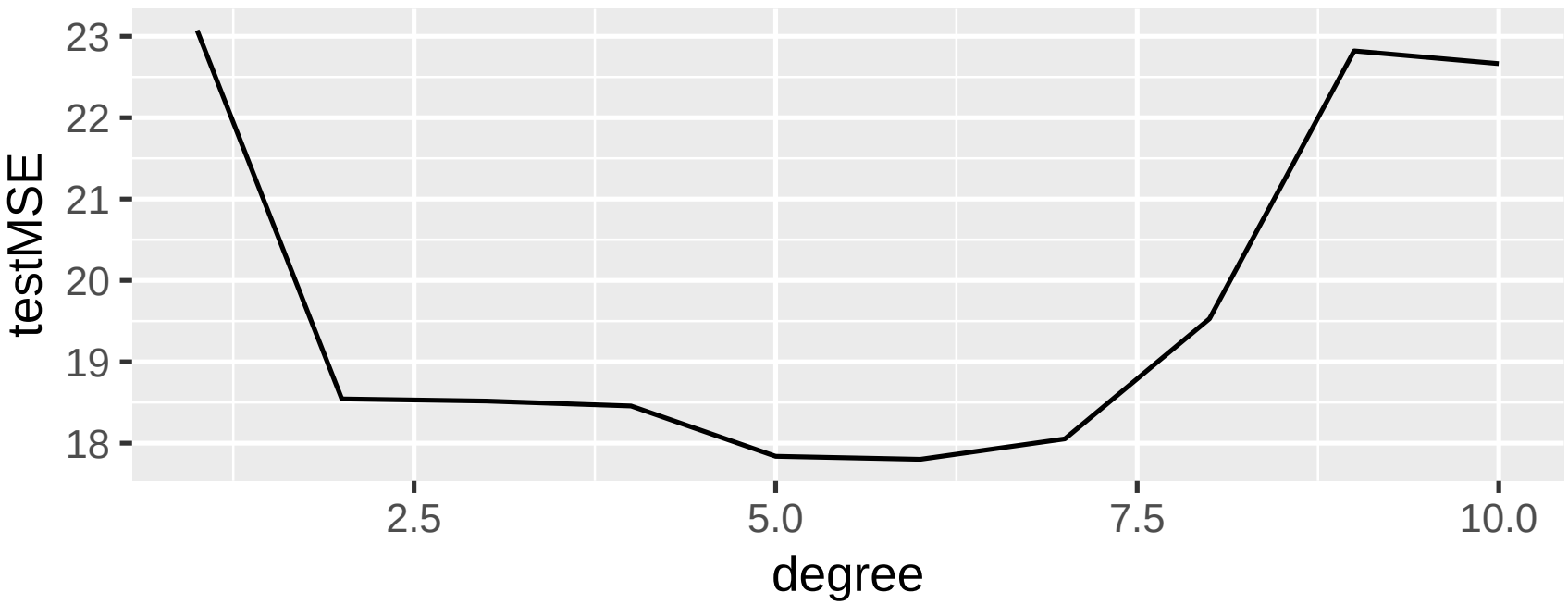
```
afit <- lm(mpg ~ poly(horsepower,2),data=Auto.train)
yhat.v <- predict(afit,newdata=Auto.validn)
tMSE <- with(Auto.validn,mean((mpg - yhat.v)^2))
tMSE
```

```
## [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

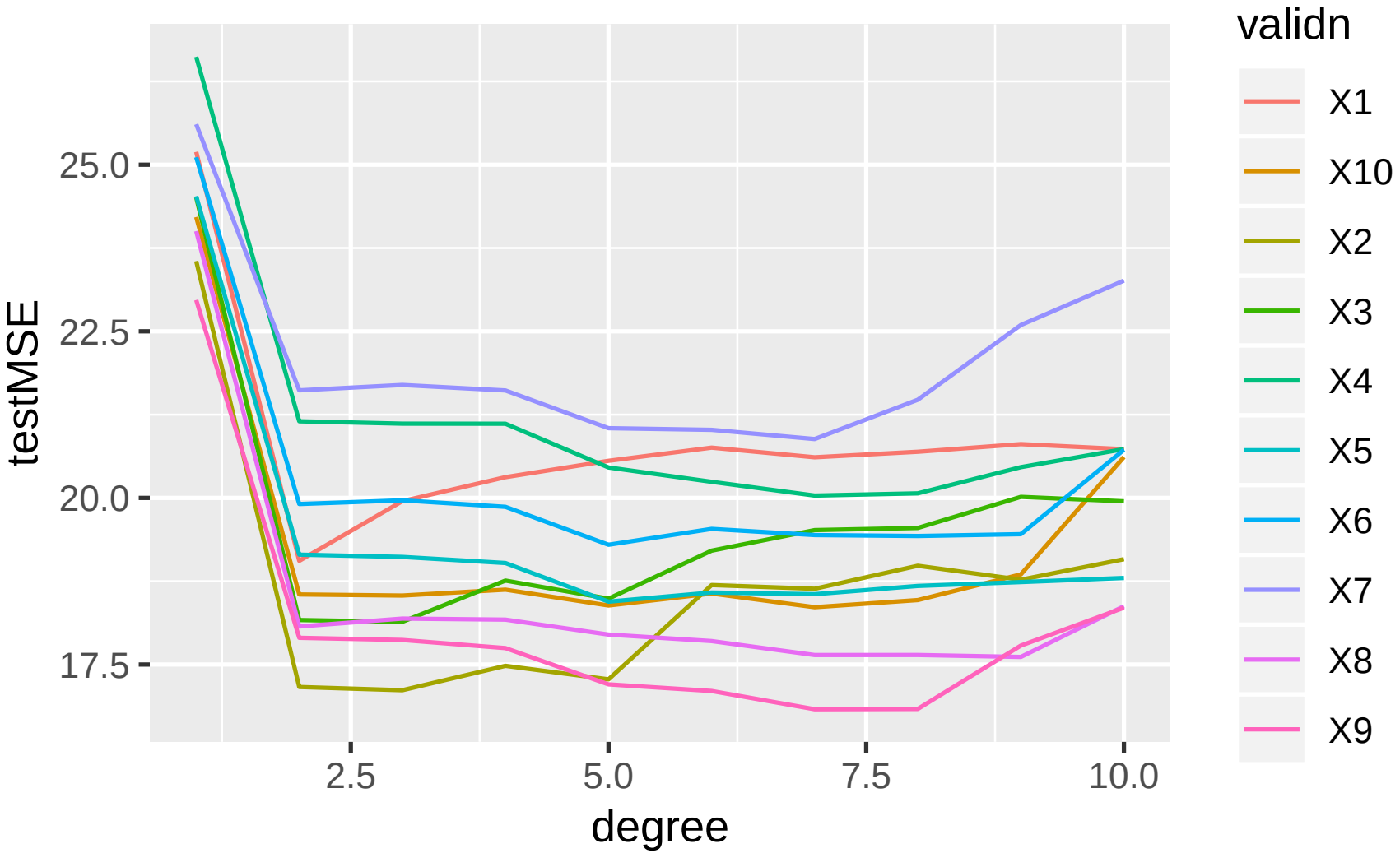
```
testMSE <- function(dd,train,validn) {
  afit <- lm(mpg ~ poly(horsepower,dd),data=train)
  yhat.v <- predict(afit,newdata=validn)
  return(with(validn,mean((mpg - yhat.v)^2)))
}
nd <- 10; dd <- (1:nd); tm <- rep(NA,nd)
for(i in dd) {
  tm[i] <- testMSE(i,Auto.train,Auto.validn)
}
dMSE <- data.frame(degree=dd,testMSE=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

- Estimates the expected test error.
- 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; $i = 1, \ldots, k$.
- 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:

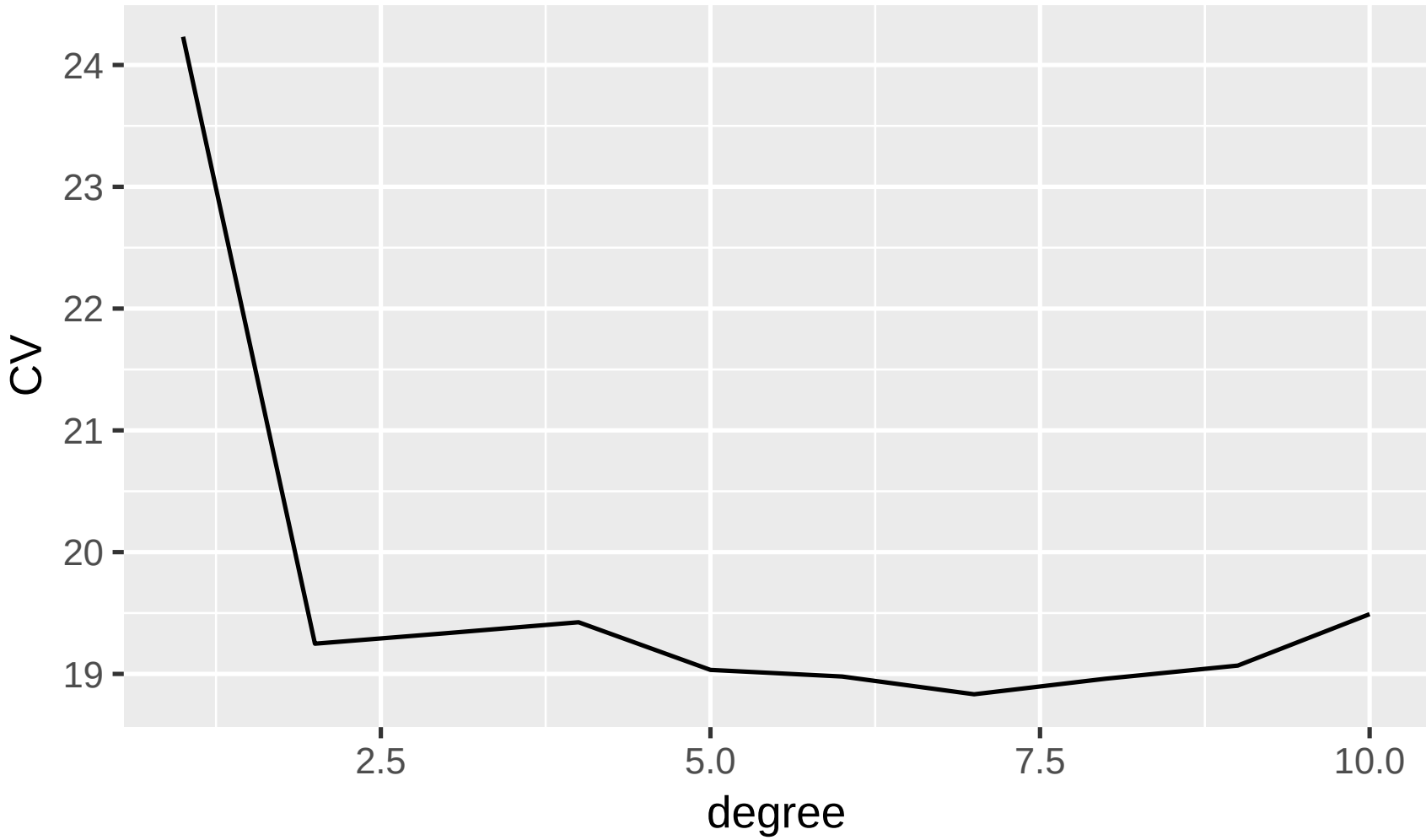
$$CV_{(n)} = \frac{1}{n} \sum_{i=1}^{n} \left(\frac{y_i - \hat{y}_i}{1 - h_i} \right)^2 ,$$

where $\hat{y}_i$ is the fitted value from the least squares fit and h_i is the leverage of the ith 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()
```

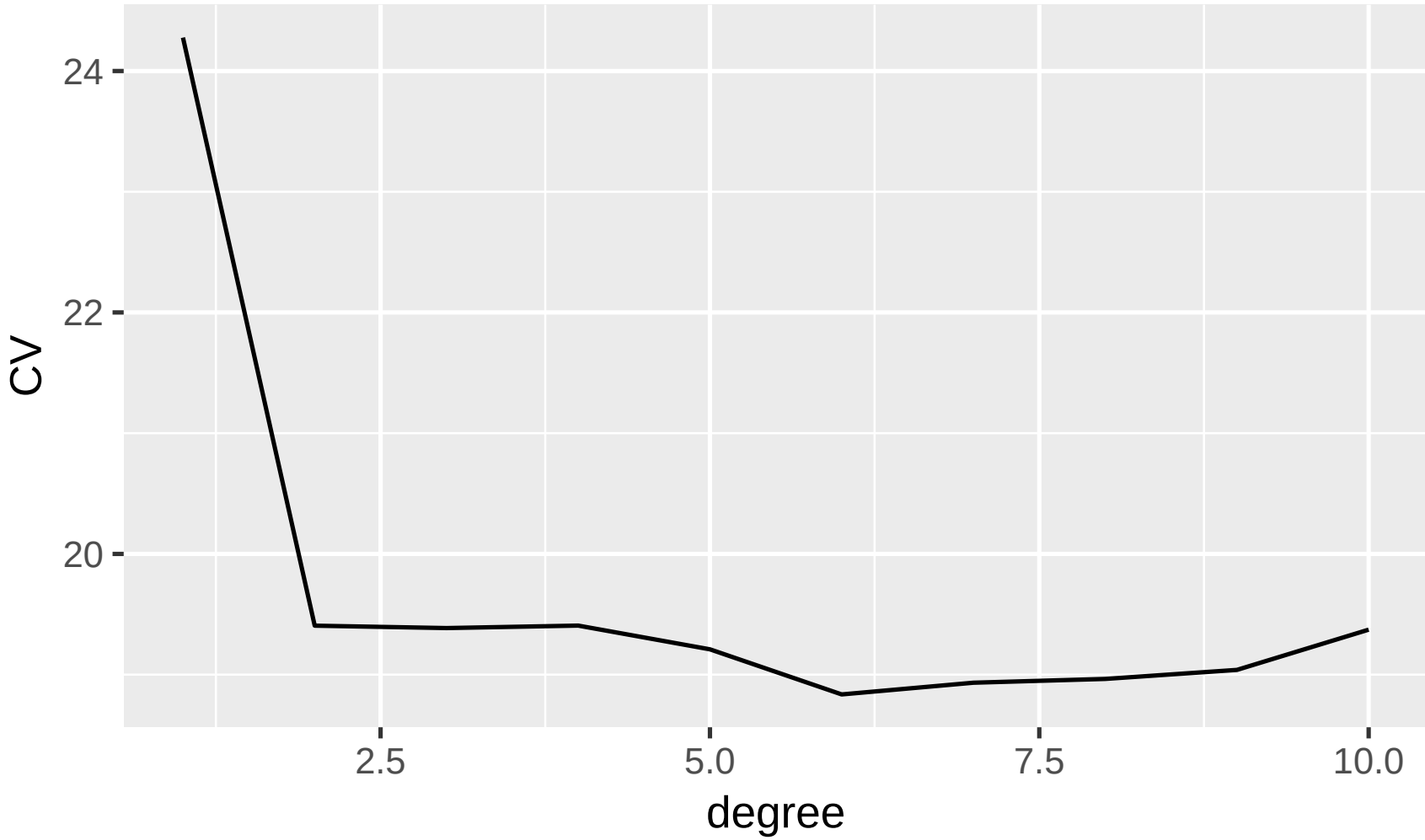


10-Fold CV on Auto Data

- 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 arrises 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,

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

- 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)
```

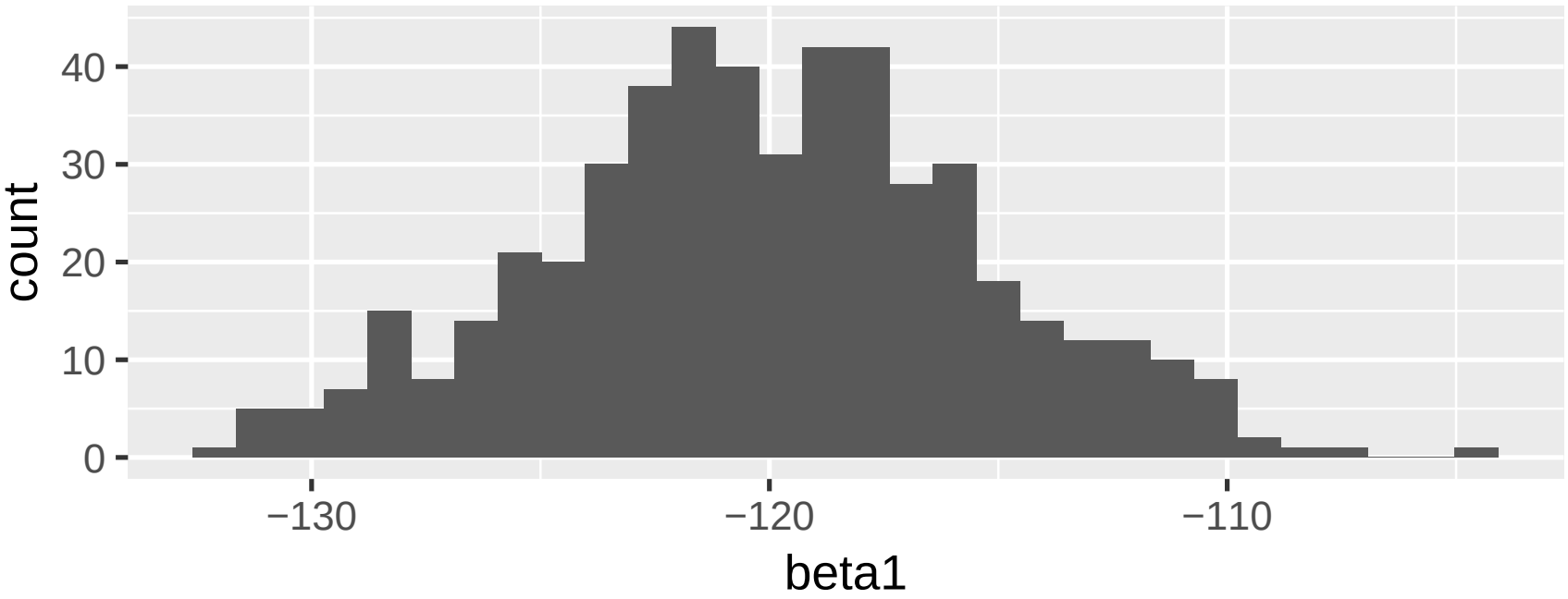
```
##      mpg horsepower
## 364 22.4        110
## 373 27.0         90
## 114 21.0        107
## 328 36.4         67
## 254 20.5         95
## 206 28.0         75
```

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
```