

ETC3250: Resampling

Semester 1, 2020

Professor Di Cook

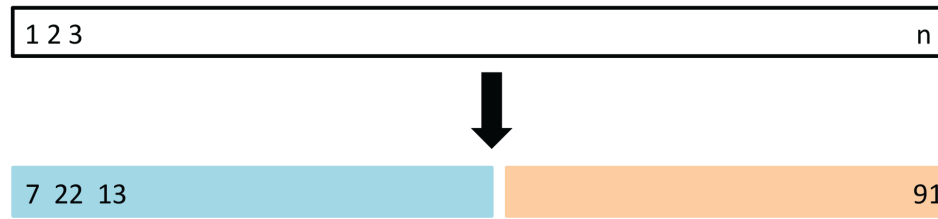
Econometrics and Business Statistics
Monash University

Week 3 (b)

Model assessment



Validating models



A set of n observations are randomly split into a training set (blue, containing observations 7, 22, 13, ...) and a validation set (yellow, all other observations not in training set).

Drawback: Only one split of data made, may not adequately estimate test error.

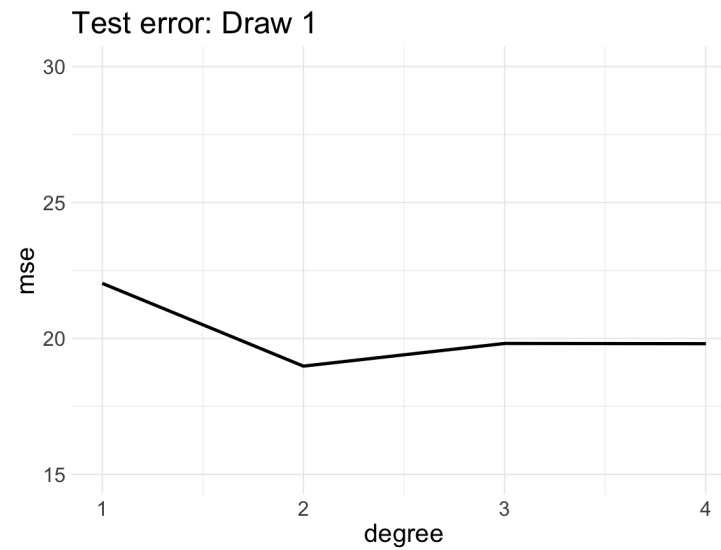
Validating models

Want to choose best degree of polynomial, for
 $\text{mpg} = \beta_0 + \beta_1 f(\text{horsepower}) + \varepsilon$

```
## [1] 2 4 7 9 10 11 12 14 15 16 18 21 23
```

Remember:

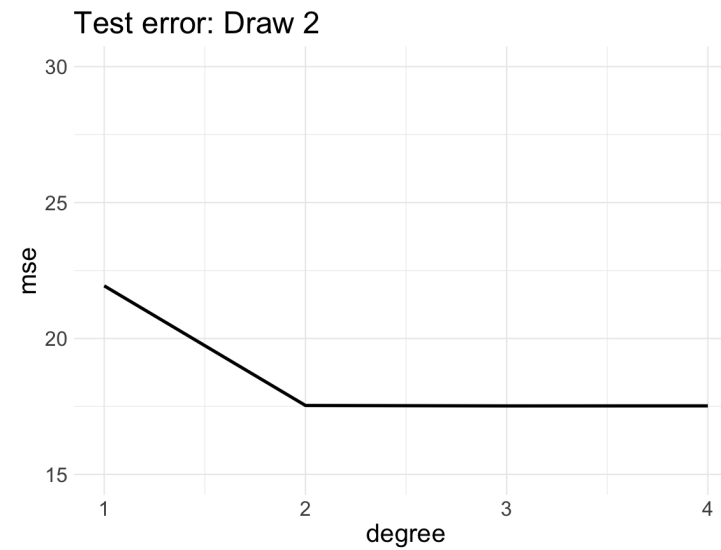
$$MSE = \frac{1}{n} \sum_{i=1}^n (y_i - \hat{y}_i)^2$$



Validating models

Want to choose best degree of polynomial, for
 $\text{mpg} = \beta_0 + \beta_1 f(\text{horsepower}) + \epsilon$

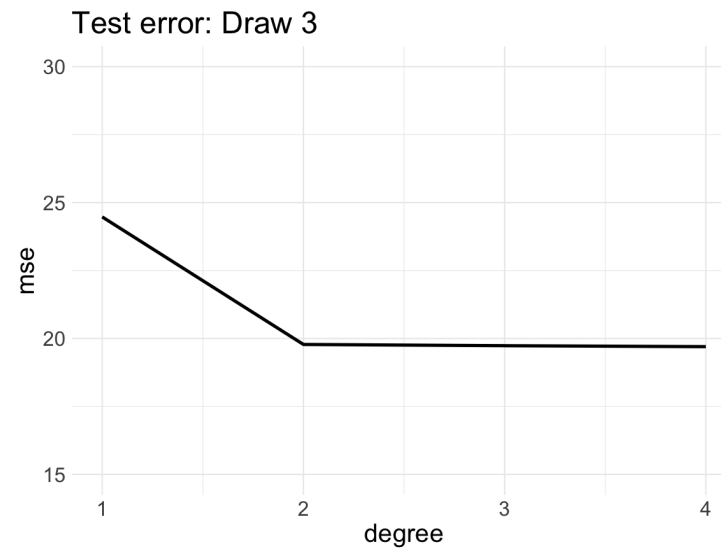
```
## [1] 3 4 5 6 9 10 13 14 17 20 23 24 25
```



Validating models

Want to choose best degree of polynomial, for
$$\text{mpg} = \beta_0 + \beta_1 f(\text{horsepower}) + \varepsilon$$

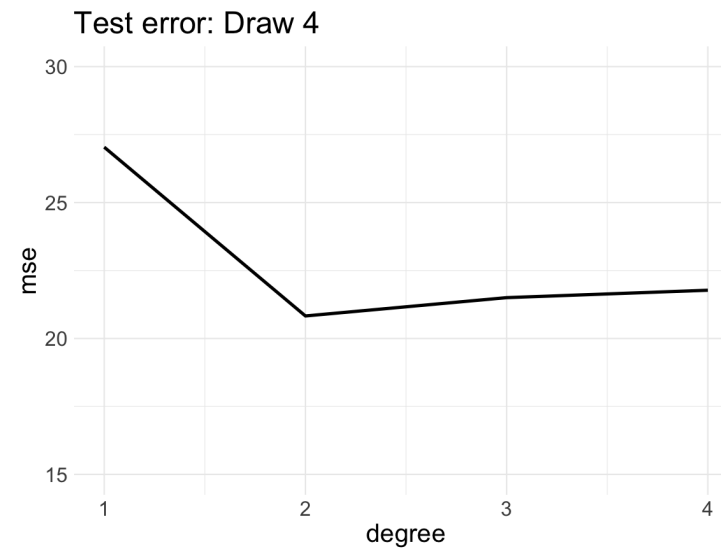
```
## [1] 1 3 4 5 8 9 10 12 13 14 15 16 20
```



Validating models

Want to choose best degree of polynomial, for
$$\text{mpg} = \beta_0 + \beta_1 f(\text{horsepower}) + \epsilon$$

```
## [1] 1 2 3 4 5 11 13 15 18 19 21 23 24
```

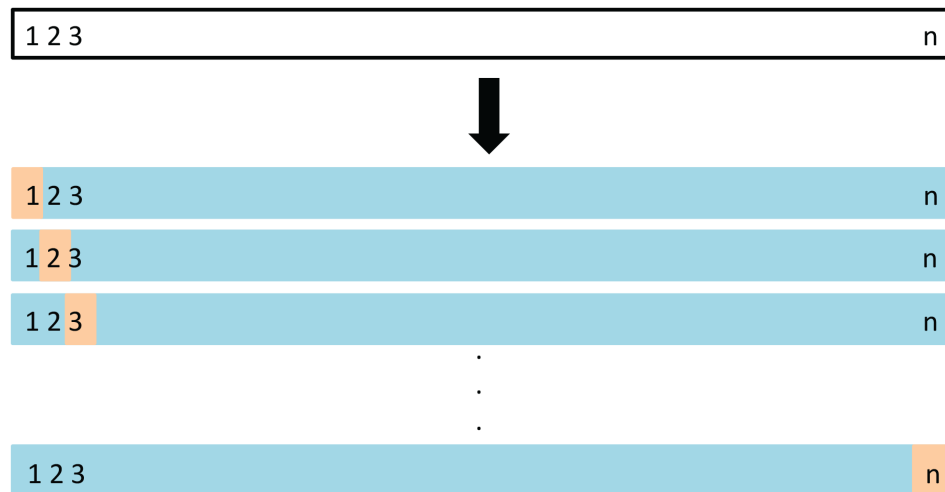




The **variability** between different draws of test sets can be **large**. This can provide poor choice of model, or misleading estimate of error.

LOOCV

Leave-one-out (LOOCV) cross-validation: n validation sets, each with **ONE** observation left out.



LOOCV

Leave-one-out (LOOCV) cross-validation: n validation sets, each with **ONE** observation left out. For each set, $i = 1, \dots, n$, compute the MSE_i .

The LOOCV estimate for the test MSE is the average of these n test error estimates:

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

LOOCV

There is a computational shortcut, for linear or polynomial models, where not all n models need to be fitted.

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

where $h_i = \frac{1}{n} + \frac{(x_i - \bar{x})^2}{\sum_{i'}^n (x_{i'} - \bar{x})^2}$ (known as *leverage* from regression diagnostics).

Let's take a look at how this works

```
# This has the cv.glm function
library(boot)
glm.fit <- glm(mpg ~ horsepower,
               data=Auto)
# MSE on all observations
mse(glm.fit, Auto)
```

```
## [1] 23.94366
```

```
# LOOCV by default
cv.glm(Auto, glm.fit)$delta[1]
```

```
## [1] 24.23151
```

Compare with manual calculation

```
# Drop one observation out for fitting
m <- NULL
for (i in 1:nrow(Auto)) {
  fit <- glm(mpg ~ horsepower,
             data=Auto[-i,])
  m <- c(m,
        (Auto[i,]$mpg -
         predict(fit, Auto[i,]))^2)
}
head(m, 3)
```

```
##      1      2      3
## 2.020010 1.250924 3.068052
```

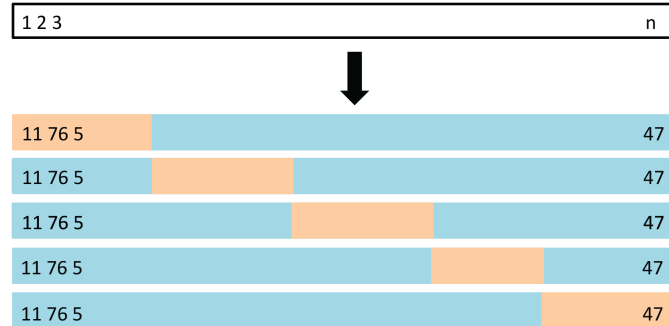
```
mean(m)
```

```
## [1] 24.23151
```



k-fold cross validation

1. Divide the data set into k different parts.
2. Remove one part, fit the model on the remaining $k - 1$ parts, and compute the MSE on the omitted part.
3. Repeat k times taking out a different part each time



k-fold cross validation

1. Divide the data set into k different parts.
2. Remove one part, fit the model on the remaining $k - 1$ parts, and compute the MSE on the omitted part.
3. Repeat k times taking out a different part each time

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

 LOOCV is a special case of k -fold cross-validation.

 Bias-variance trade-off:

- ⌚ one validation set overestimates test error, LOOCV approximately unbiased estimates, k -fold CV intermediate
- ⌚ LOOCV has higher variance than does k -fold CV
- ⌚ choice of $k = 5$ or 10 is a compromise

```
glm.fit <- glm(mpg ~ horsepower,  
              data=Auto)  
# MSE on all observations  
mse(glm.fit, Auto)
```

```
## [1] 23.94366
```

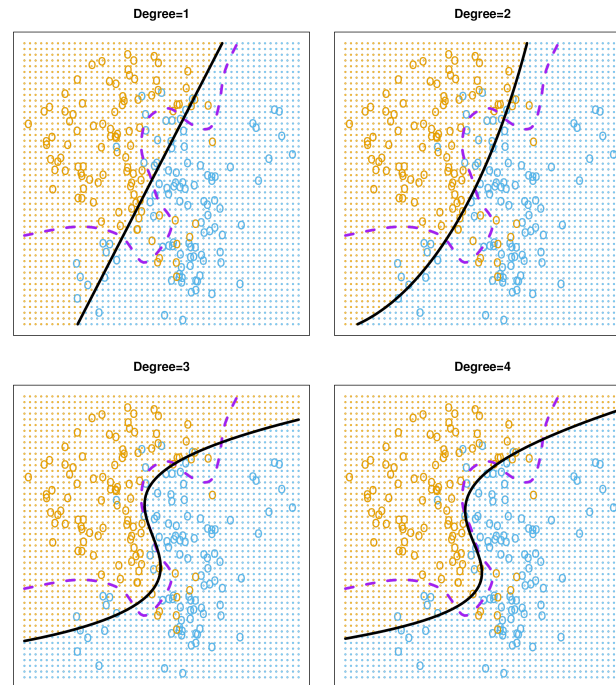
```
# LOOCV by default  
cv.glm(Auto, glm.fit)$delta[1]
```

```
## [1] 24.23151
```

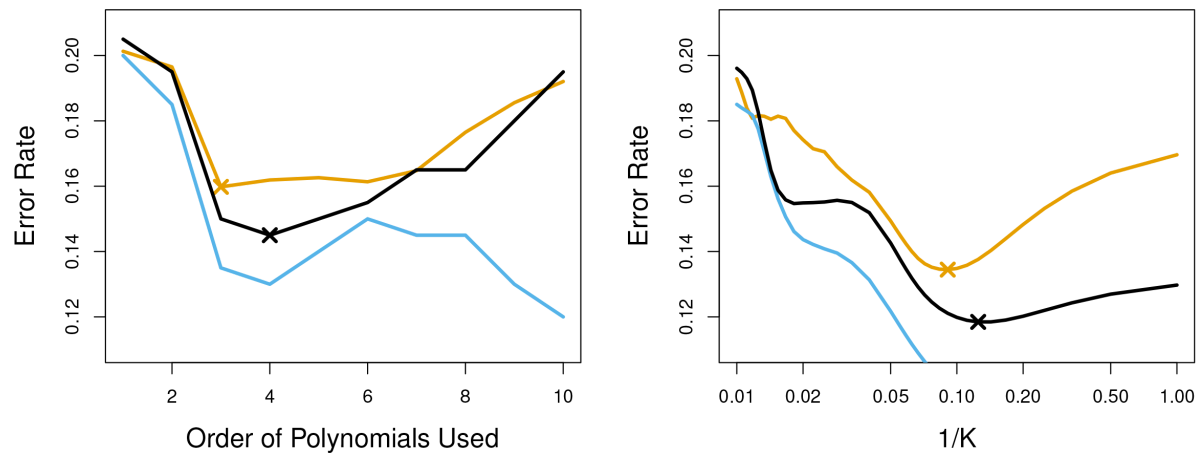
```
# 5-fold CV  
cv.glm(Auto, glm.fit, K=5)$delta[1]
```

```
## [1] 24.3191
```

Classification



Classification



Black line is 10-fold CV; training and TRUE test error for different choices of polynomial (left) and KNN classifier (right).

Bootstrap procedure

 Draw B independent bootstrap samples $X^{*(1)}, \dots, X^{*(B)}$ from \hat{P} :

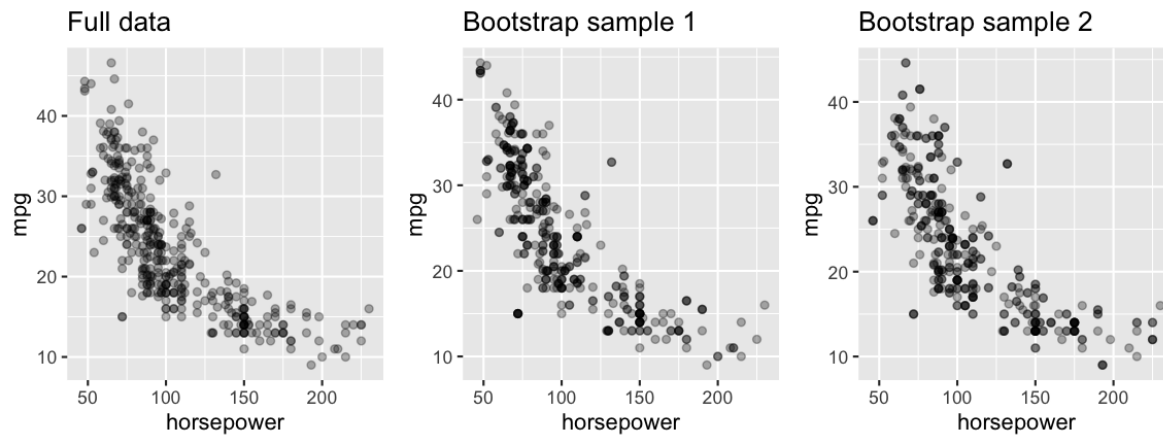
$$X_1^{*(b)}, \dots, X_n^{*(b)} \sim \hat{P} \quad b = 1, \dots, B.$$

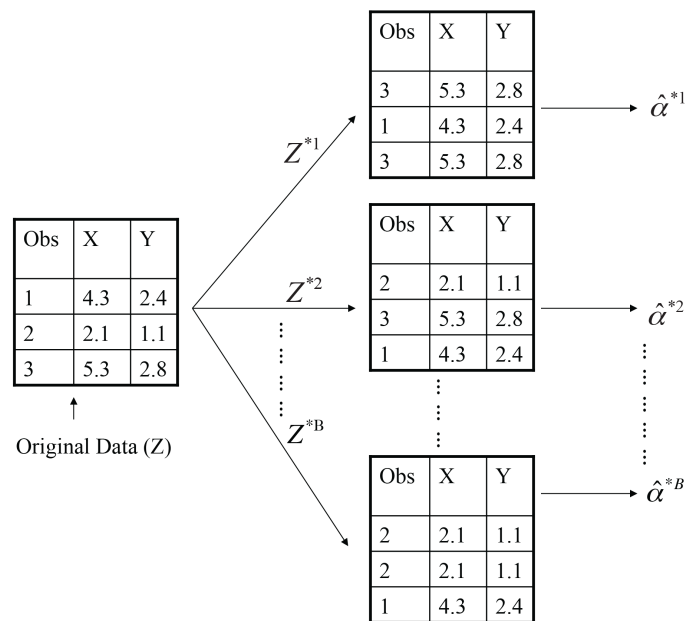
 Evaluate the bootstrap replications:

$$\hat{\theta}^{*(b)} = s(X^{*(b)}) \quad b = 1, \dots, B.$$

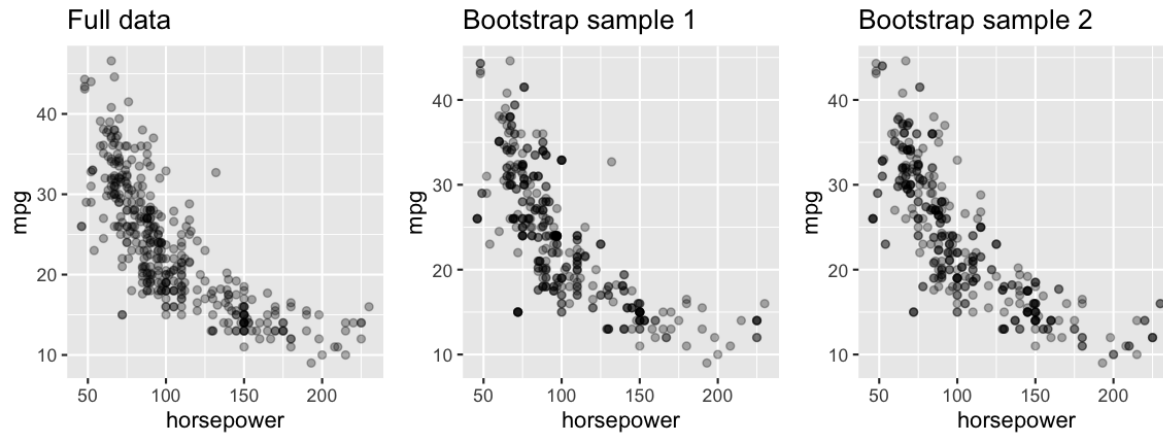
 Estimate the quantity of interest from the distribution of the $\hat{\theta}^{*(b)}$

Bootstrap samples






Bootstrap samples



Example - bootstrap model

 Fit the model on a set of bootstrap samples, and keep track of how well it predicts the original dataset

$$\text{Err}_{\text{boot}} = \frac{1}{B} \frac{1}{n} \sum_{b=1}^B \sum_{i=1}^n L(y_i, \hat{f}^{*b}(x_i))$$

 Each of these bootstrap data sets is created by sampling with replacement, and is the same size as our original dataset. As a result some observations may appear more than once in a given bootstrap data set and some not at all.

```
glm.fit <- glm(mpg ~ horsepower,  
              data=Auto)  
# MSE on all observations  
mse(glm.fit, Auto)
```

```
## [1] 23.94366
```

```
# LOOCV by default  
cv.glm(Auto, glm.fit)$delta[1]
```

```
## [1] 24.23151
```

```
# 5-fold CV  
cv.glm(Auto, glm.fit, K=5)$delta[1]
```

```
## [1] 24.07127
```

```
mse.fn <- function(d, index) {  
  glm.fit <- glm(mpg ~ horsepower,  
                 data=d[index,])  
  # MSE on all observations  
  return(m = mse(glm.fit,  
                 d[-unique(index),]) )  
}  
m <- NULL  
for (i in 1:1000) {  
  idx <- sample(nrow(Auto),  
                replace = TRUE)  
  m <- c(m, mse.fn(Auto, idx))  
}  
mean(m)
```

```
## [1] 24.33553
```

Bootstrap for error on a statistic

Overall median is 22.75

```
# Bootstrap median, and standard error
med.fn <- function(d, index) {
  med <- median(d$mpg[index])
  med
}
bmed <- boot(Auto, med.fn, R=1000)
```

bmed

```
##
## ORDINARY NONPARAMETRIC BOOTSTRAP
##
##
## Call:
## boot(data = Auto, statistic = med.fn, R = 1
##
##
## Bootstrap Statistics :
##      original    bias    std. error
## t1*      22.75 -0.10595    0.7653743
```


Uses and variants of the bootstrap

Common uses:

- Computing standard errors for complex statistics
- Prediction error estimation
- Bagging (Bootstrap aggregating) ML models

Types of bootstrap based on different assumptions:

- block bootstrap
- sieve bootstrap
- smooth bootstrap
- residual bootstrap
- wild bootstrap

Made by a human with a computer

Slides at <https://iml.numbat.space>.

Code and data at <https://github.com/numbats/iml>.

Created using R Markdown with flair by [xaringan](#), and [kunoichi](#) (female ninja) style.



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