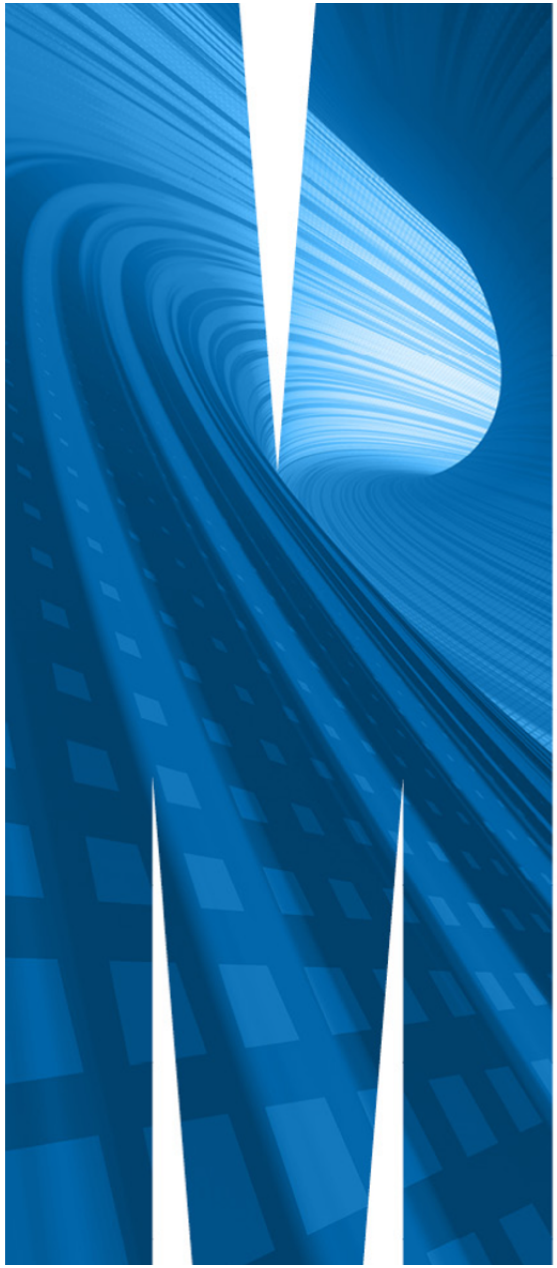
MONASH University

ETC3250/5250: Introduction to Machine Learning

Resampling for model development and choice



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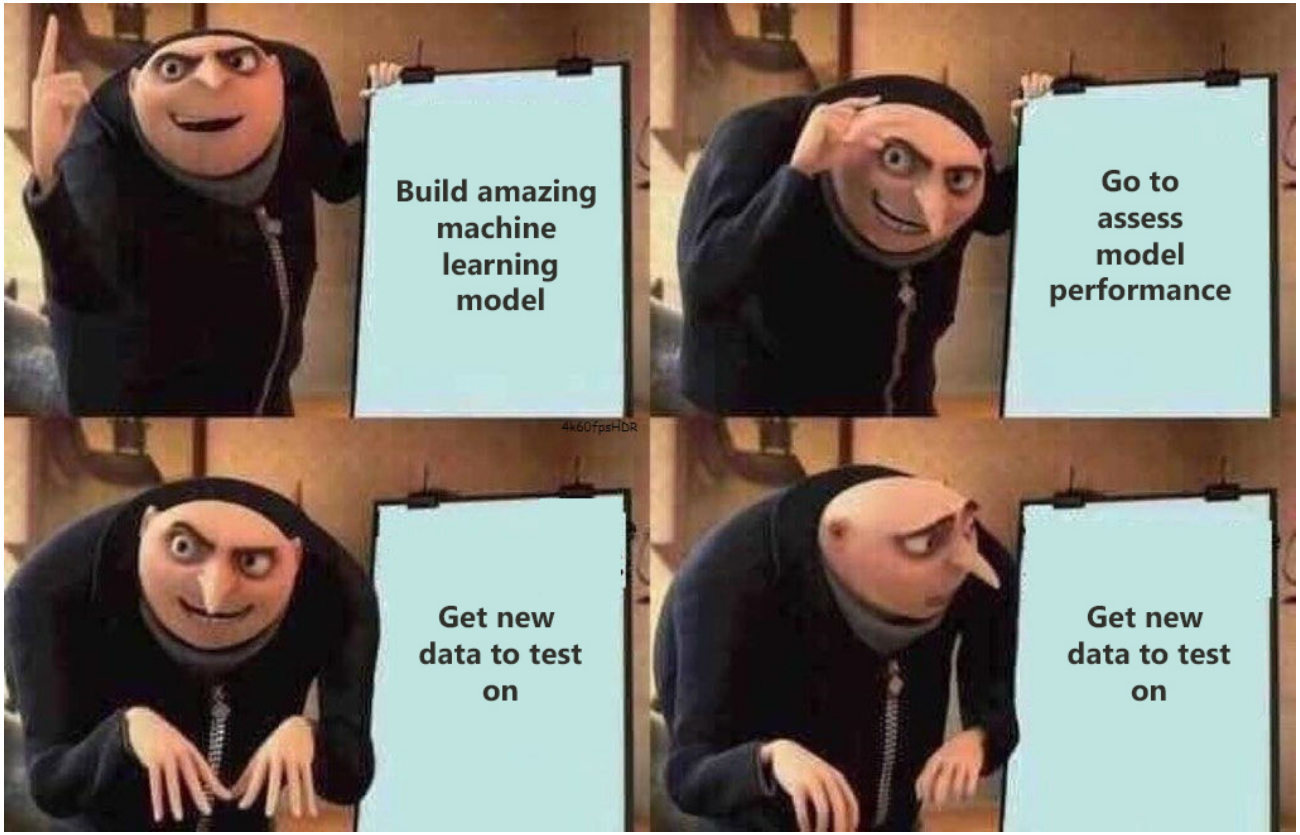
Week 3b

Model development and choice

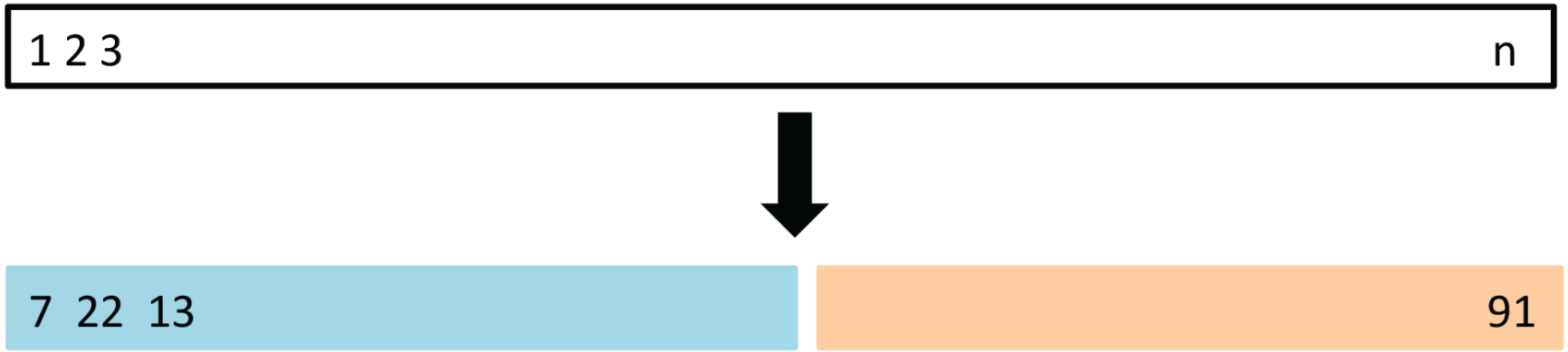


How do you get new data?

Resampling

- Training/test split: make one split of your data, keeping one purely for assessing future performance.
- Leave-one-out: make n splits, fitting multiple models and using left-out observation for assessing variability.
- k-fold: break data into k subsets, fitting multiple models with one group left out each time.
- Bootstrap: make many samples, with replacement, using out-of-bag observations for testing.

Training and test sets



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

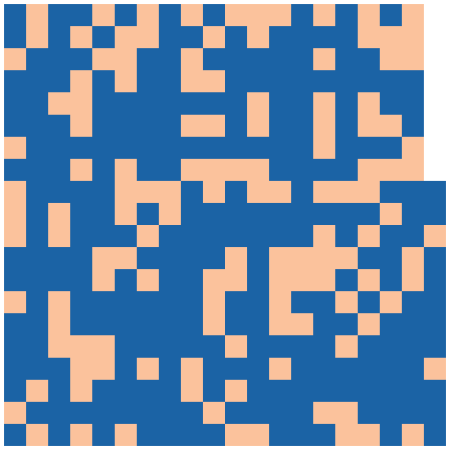
Drawback: Only one split of data made, may have a lucky or unlucky split, accurately estimating test error relies on the one sample.

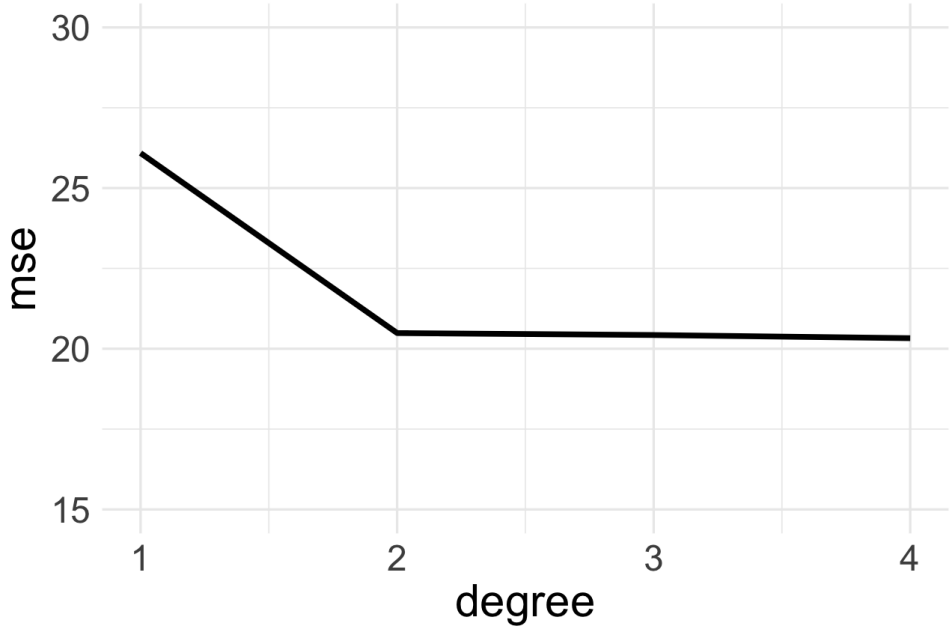
(Chapter5/5.1.pdf)

Training/test set split and choosing polynomial degree (1/4)

$$\text{mpg} = \beta_0 + \beta_1 f(\text{horsepower}) + \varepsilon$$

Split into 2/3 training and 1/3 test sets.

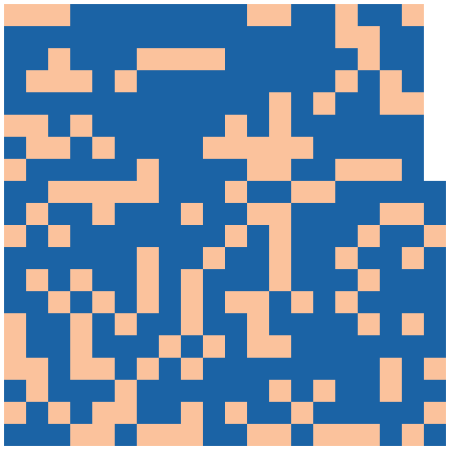


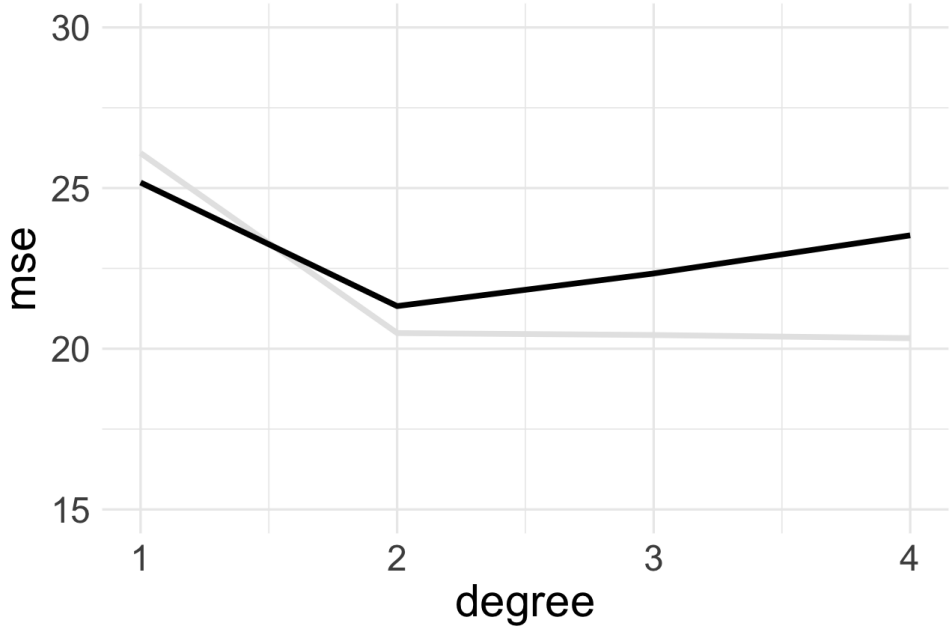


Training/test set split and choosing polynomial degree (2/4)

$$\text{mpg} = \beta_0 + \beta_1 f(\text{horsepower}) + \varepsilon$$

Split into 2/3 training and 1/3 test sets.

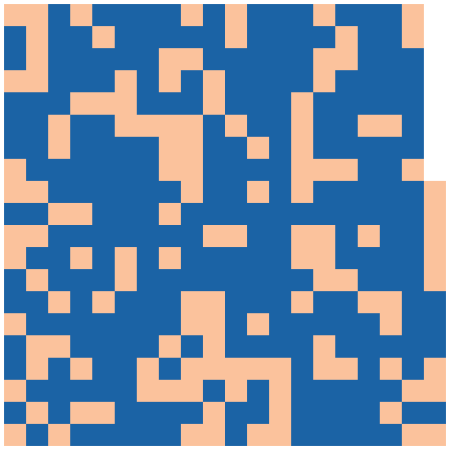


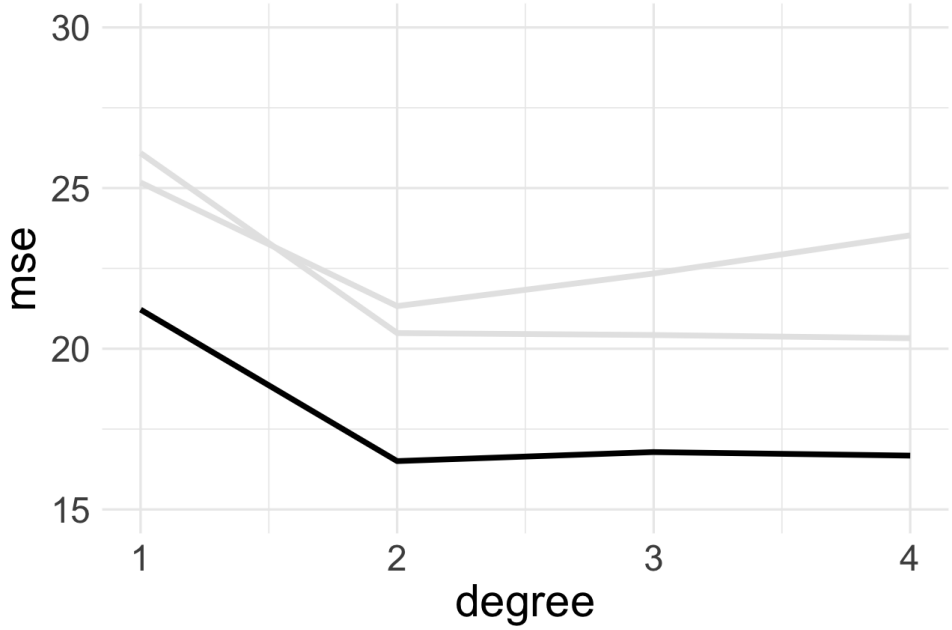


Training/test set split and choosing polynomial degree (3/4)

$$\text{mpg} = \beta_0 + \beta_1 f(\text{horsepower}) + \varepsilon$$

Split into 2/3 training and 1/3 test sets.

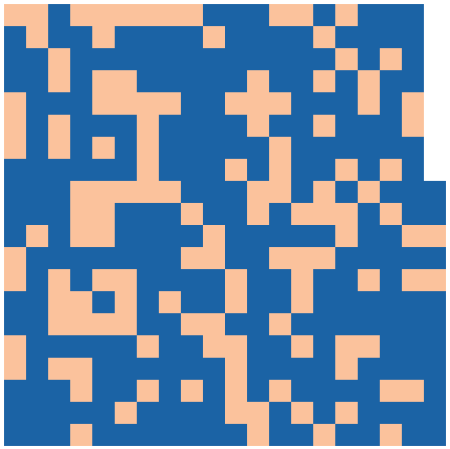


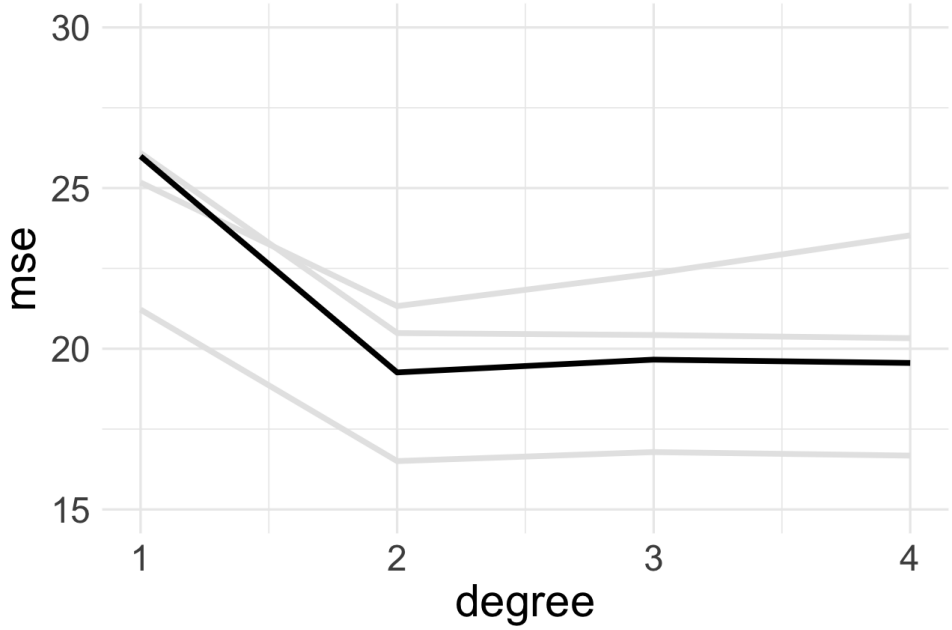


Training/test set split and choosing polynomial degree (4/4)

$$\text{mpg} = \beta_0 + \beta_1 f(\text{horsepower}) + \varepsilon$$

Split into 2/3 training and 1/3 test sets.





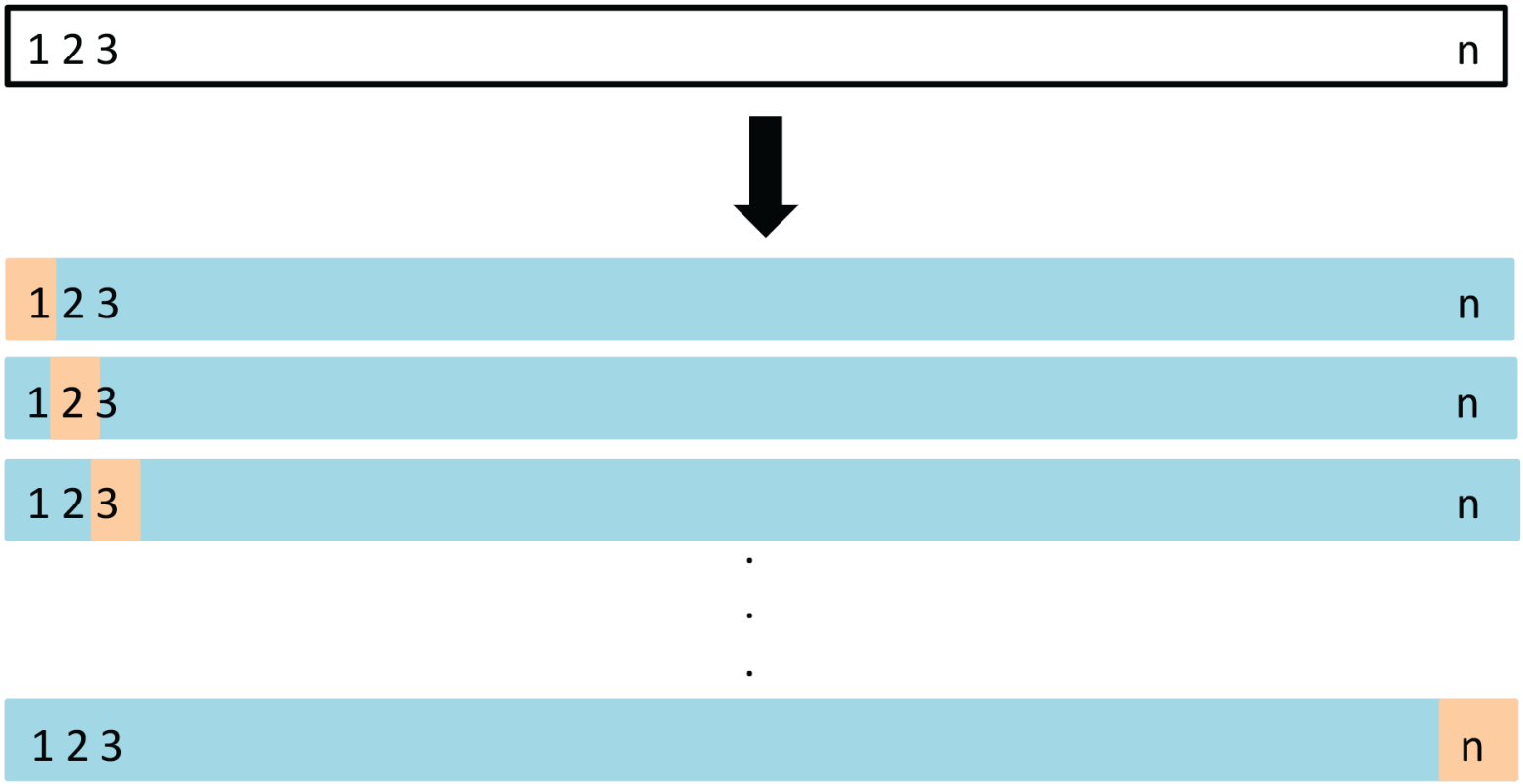
One split may not be enough

Test MSE changes if a different split is made. For this example, though the choice would be degree = 2, regardless of the split.

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

LOOCV

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



LOOCV

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

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

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

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

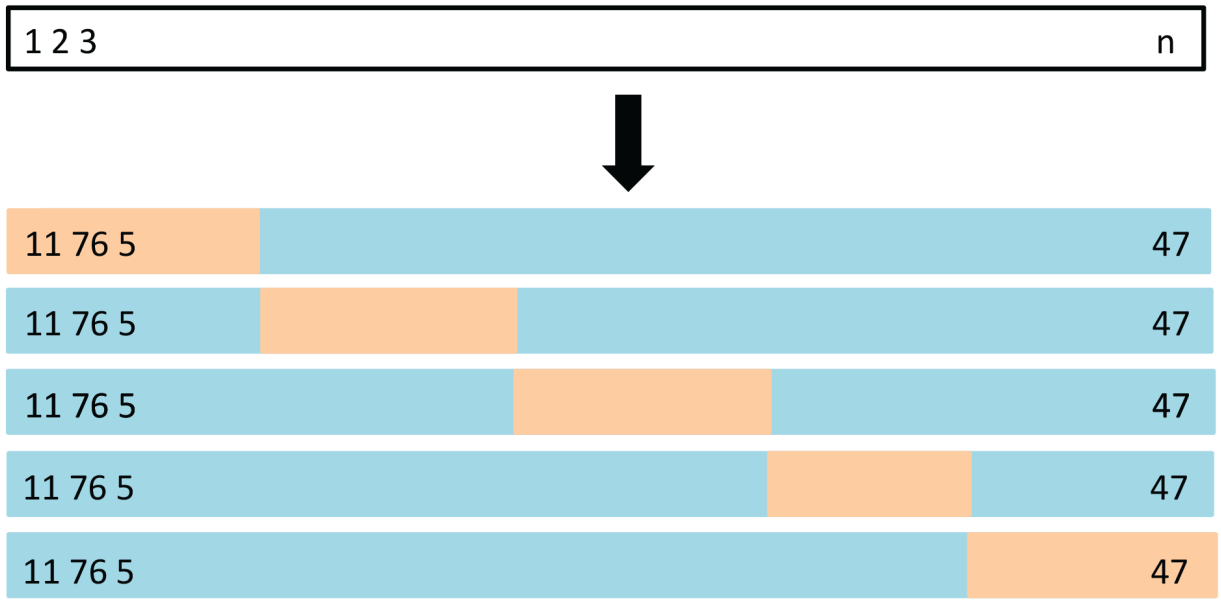
$$CV_{(n)} = \frac{1}{n} \sum_{i=1}^{n} \frac{(y_i - \hat{y})^2}{1 - h_i}$$

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).

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

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



(Chapter 5/ 5.5)

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

Cross-validation MSE is:

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

No shortcut for calculation.

Choice of k=5-10 is typically reasonable

Try it

```
set.seed(2021)
auto_folds <- vfold_cv(data = Auto)
auto_folds
```

```
## #  10-fold cross-validation
## # A tibble: 10 x 2
##    splits           id
##    <list>           <chr>
##  1 <split [352/40]> Fold01
##  2 <split [352/40]> Fold02
##  3 <split [353/39]> Fold03
##  4 <split [353/39]> Fold04
##  5 <split [353/39]> Fold05
##  6 <split [353/39]> Fold06
##  7 <split [353/39]> Fold07
##  8 <split [353/39]> Fold08
##  9 <split [353/39]> Fold09
```

Data is split into 10 subsets

Next, write a function for the four polynomial models:

1. Fit the model to `training(split) -> analysis(split)`
2. Assess the model fit with `testing(split) -> assessment(split)`
3. Report the MSE

Recommended reading: Alison Hill's Take a Sad Script & Make it Better: Tidymodels Edition

```r
# Model specification
lm_mod <-
  linear_reg() %>%
  set_engine("lm")

# We want to fit the four polynomial models
compute_fold_mse <- function(split){
  # Set up polynomials
  auto_prep <-
    recipe(mpg ~ horsepower,
           data = analysis(split)) %>%
    step_poly(horsepower, degree = 4) %>%
    prep()
  train_baked <- bake(auto_prep, new_data = NULL)
  test_baked <- bake(auto_prep, new_data = assessment(split))

  # Fit four models
  fit1 <-
```

Check the calculation for one fold

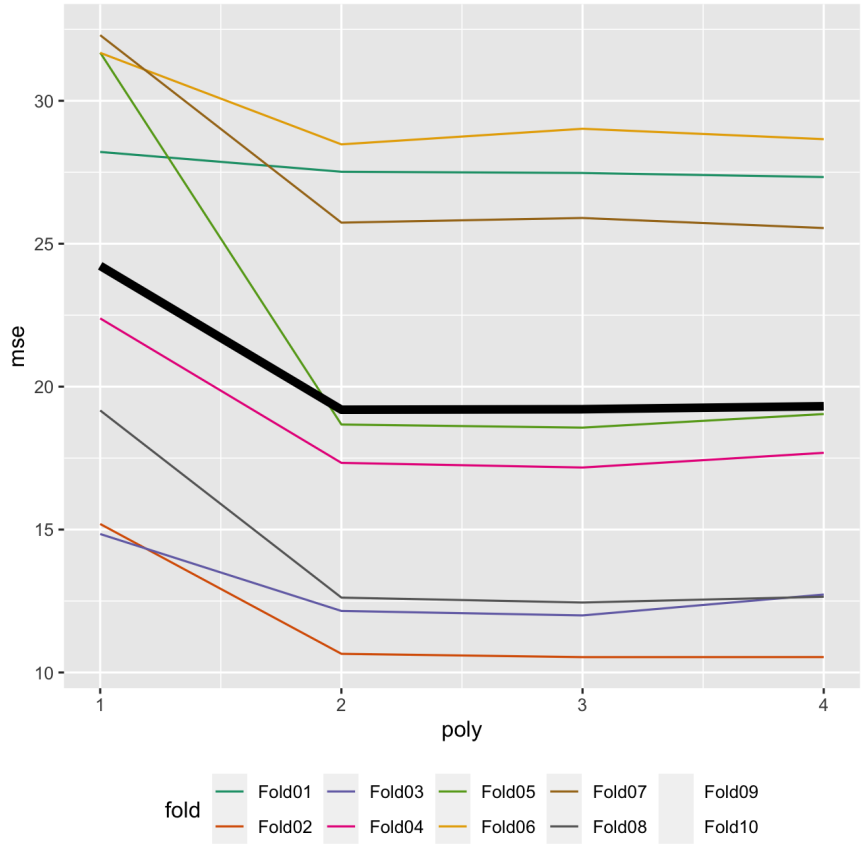
```
compute_fold_mse(auto_folds$splits[[1]])
```

```
##   poly      mse     id
## 1    1 28.21266 Fold01
## 2    2 27.51733 Fold01
## 3    3 27.47538 Fold01
## 4    4 27.33215 Fold01
```

Compute across all folds

```
kfold_results <-
  map_df(
    auto_folds$splits,
    ~compute_fold_mse(.x))
kfold_results
```

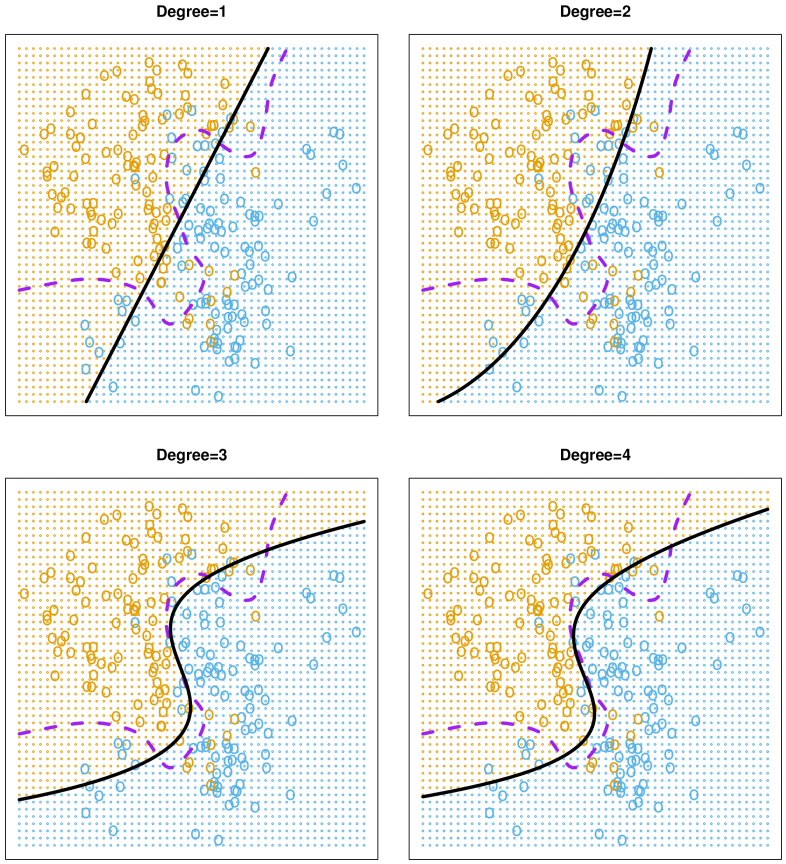
```
##    poly      mse     id
## 1     1 28.21266 Fold01
## 2     2 27.51733 Fold01
## 3     3 27.47538 Fold01
## 4     4 27.33215 Fold01
## 5     1 15.19469 Fold02
## 6     2 10.65360 Fold02
## 7     3 10.53691 Fold02
## 8     4 10.53989 Fold02
## 9     1 14.84492 Fold03
## 10    2 12.15279 Fold03
```



Black is the average MSE across folds.

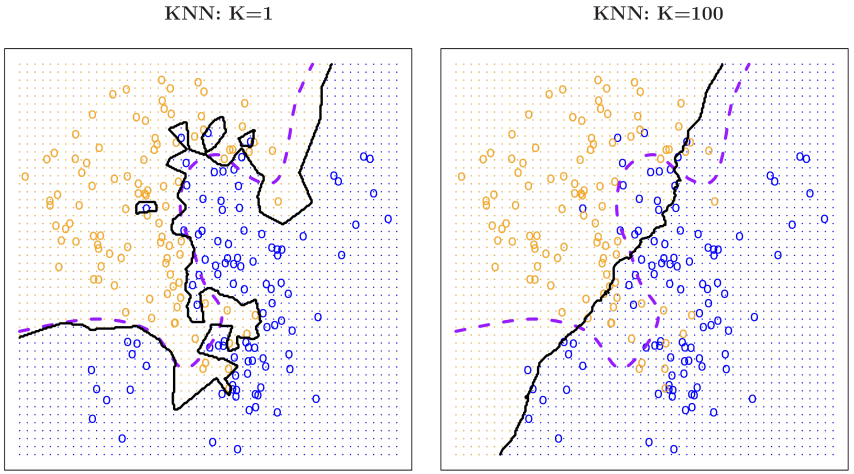
Classification

Polynomial



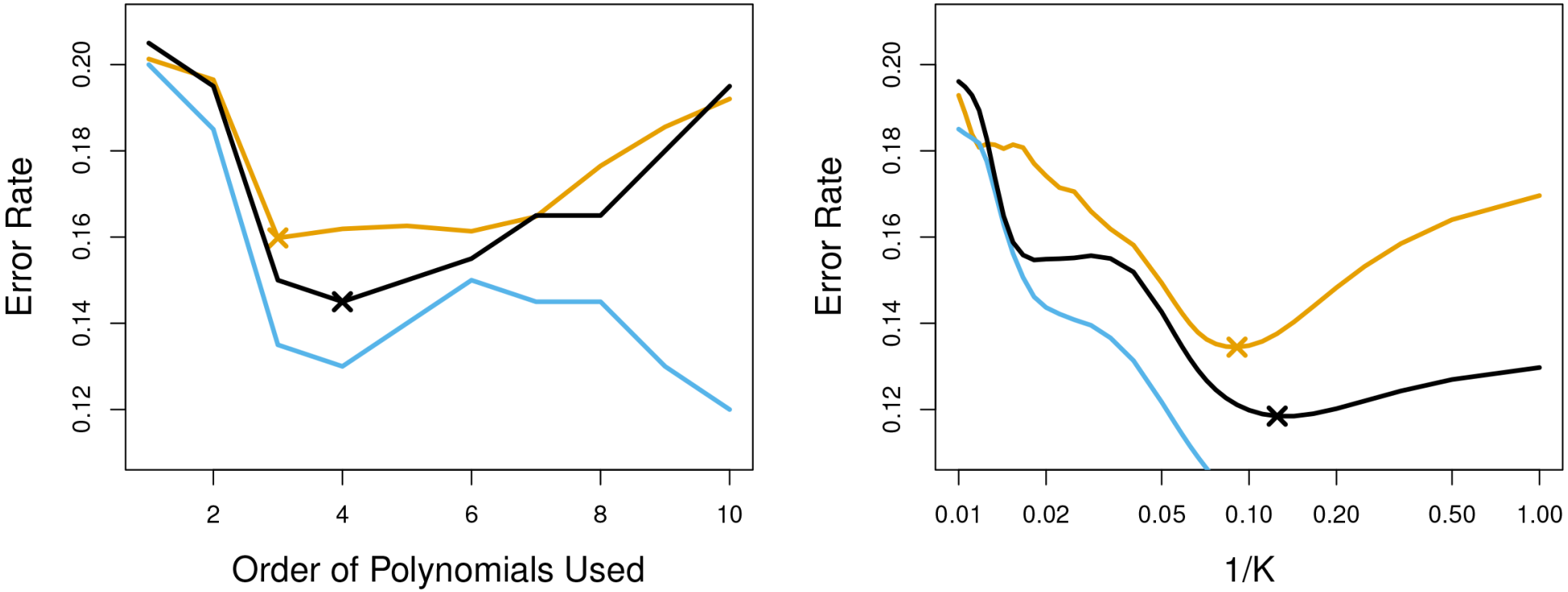
(Chapter 5/ 5.7)

kNN



(Chapter2/2.16.pdf)

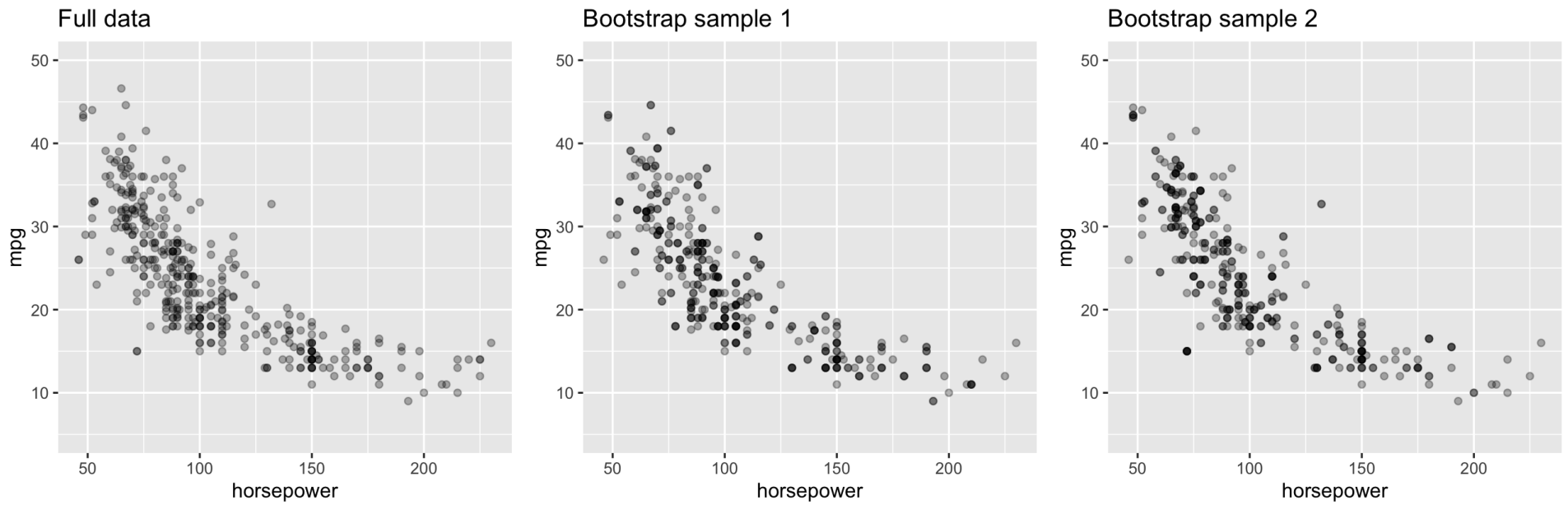
Classification



Black line is 10-fold CV; training and test error (based on knowing the true boundary) for different choices of polynomial (left) and KNN classifier (right).

(Chapter 5/ 5.8)

Bootstrap samples



Can you see the differences between the data in each plot?

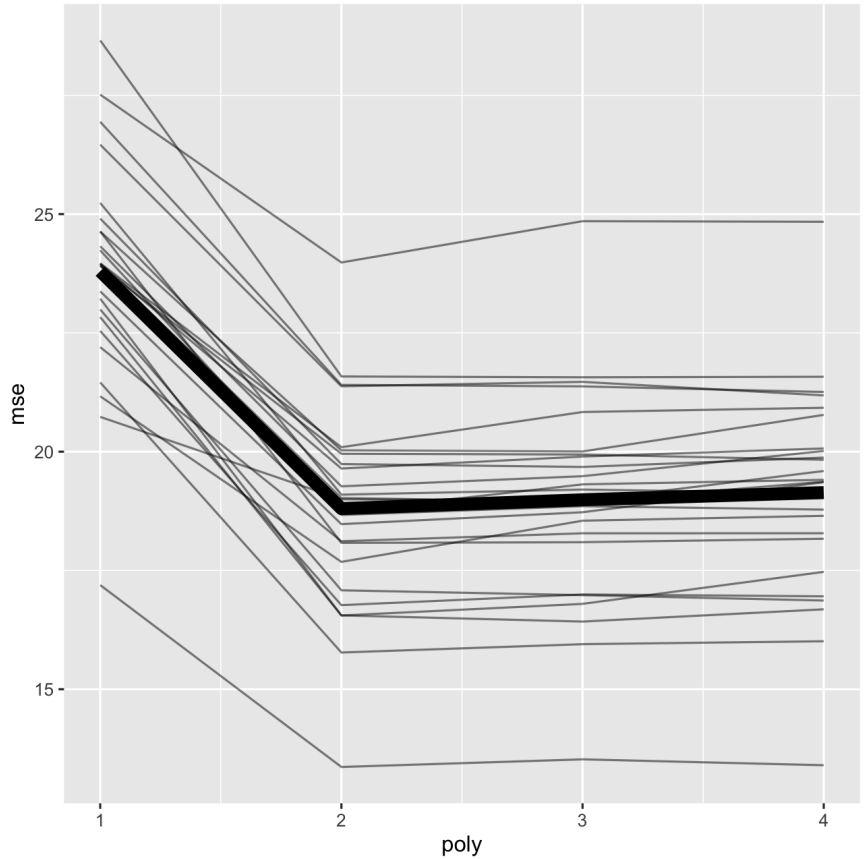
Bootstrap MSE

- 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.
- Fit the model on each set of bootstrap samples, and calculate MSE for the observations left out of each sample (out-of-bag), call this $MSE_{(b)}$

$$MSE_{boot} = \frac{1}{B}\sum_{b=1}^{B} MSE_{(b)}$$

```
auto_boots <- bootstraps(Auto)
boot_results <-
  map_df(
    auto_boots$splits,
    ~compute_fold_mse(.x))
boot_results
```

```
##      poly      mse          id
## 1       1 23.21917 Bootstrap01
## 2       2 16.55211 Bootstrap01
## 3       3 16.79716 Bootstrap01
## 4       4 17.47072 Bootstrap01
## 5       1 22.19960 Bootstrap02
## 6       2 18.11473 Bootstrap02
## 7       3 18.28226 Bootstrap02
## 8       4 18.28313 Bootstrap02
## 9       1 23.92274 Bootstrap03
## 10      2 18.66828 Bootstrap03
## 11      3 18.85320 Bootstrap03
```

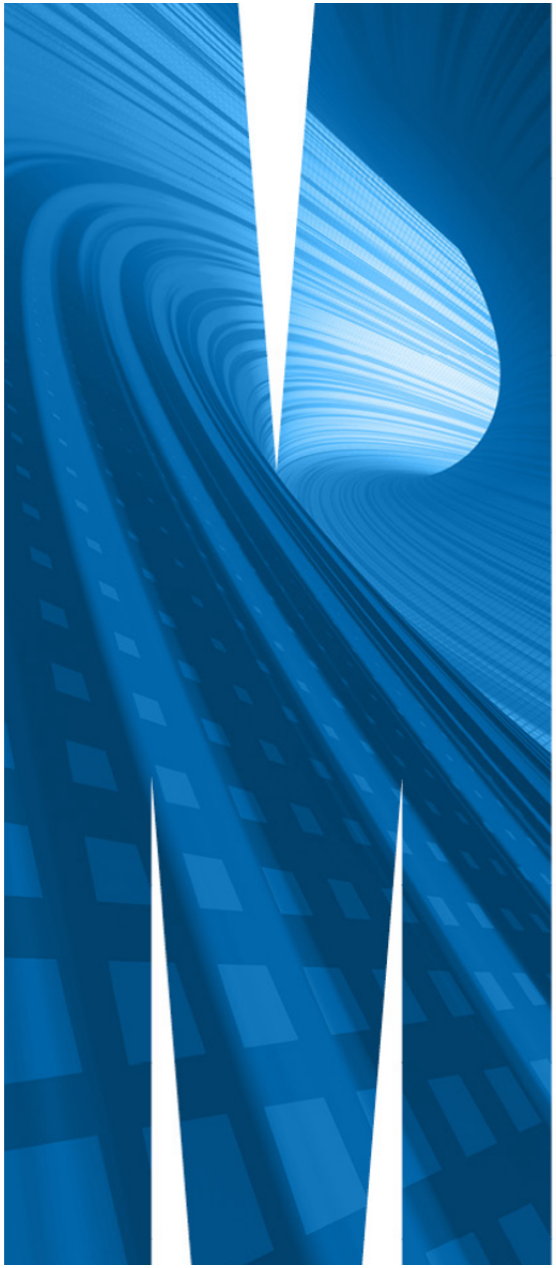


Best model is quadratic polynomial

All the resampling suggest the same decision

Summary

Re-sampling provides robust estimate of future error, and the variation you are likely to see, in the statistic being calculated, in future samples.



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Week 3b