

# Resampling and Cross-Validation

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Math 243: Stat Learning

September 27th, 2021

## Outline

In today's class, we will...

- Define and discuss resampling and cross-validation
- Investigate methods of cross-validation (LOOCV and k-fold cv)
- Implement CV in R

## Section 1

### Cross Validation

## Poll: Training Error

Which of the following methods are likely to have the smallest training error rate for regression problems?

- a. Multiple linear regression
- b. Simple linear regression
- c. Non-linear regression with polynomials
- d. KNN with  $K = 1$
- e. KNN with  $K = p$

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One fix is to partition data into training and test sets.

- Build the model using only the training data
- Assess accuracy using only test data.

# Fuel Economy

The FuelEconomy data set from the AppliedPredictiveModeling package contains fuel efficiency and other variables for 1107 cars and trucks from 2010, with data taken from the <http://fueleconomy.gov> website

```
library(AppliedPredictiveModeling)
data(FuelEconomy)
head(cars2010)
```

```
##      EngDispl NumCyl Transmission      FE AirAspirationMethod NumGears
## 1088       4.7     8          AM6 28.0198 NaturallyAspirated       6
## 1089       4.7     8          M6 25.6094 NaturallyAspirated       6
## 1090       4.2     8          M6 26.8000 NaturallyAspirated       6
## 1091       4.2     8          AM6 25.0451 NaturallyAspirated       6
## 1092       5.2    10          AM6 24.8000 NaturallyAspirated       6
## 1093       5.2    10          M6 23.9000 NaturallyAspirated       6
##      TransLockup TransCreeperGear DriveDesc IntakeValvePerCyl
## 1088            1                0 TwoWheelDriveRear           2
## 1089            1                0 TwoWheelDriveRear           2
## 1090            1                0 AllWheelDrive             2
## 1091            1                0 AllWheelDrive             2
## 1092            0                0 AllWheelDrive             2
## 1093            0                0 AllWheelDrive             2
##      ExhaustValvesPerCyl CarlineClassDesc VarValveTiming VarValveLift
## 1088            2        2Seaters           1              0
## 1089            2        2Seaters           1              0
## 1090            2        2Seaters           1              0
## 1091            2        2Seaters           1              0
## 1092            2        2Seaters           1              0
## 1093            2        2Seaters           1              0
```

## Important Predictors

Let's consider just numeric variable first:

```
cars2010 %>%
  select_if(is.numeric) %>%
  cor(cars2010$FE)

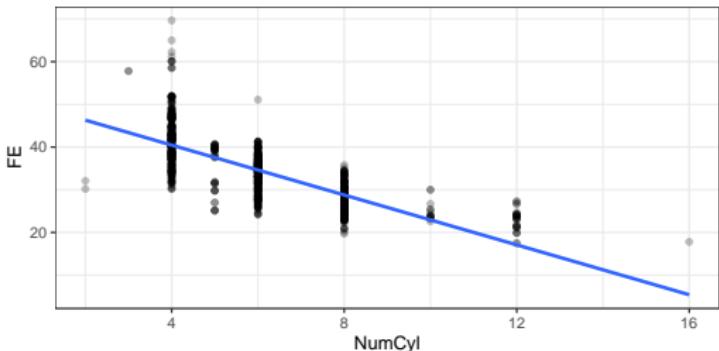
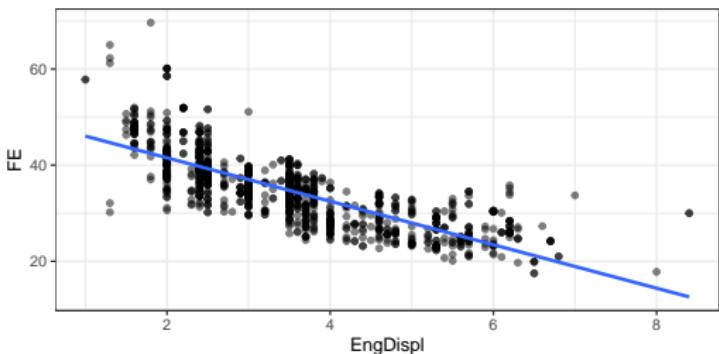
##                                     [,1]
## EngDispl           -0.78739383
## NumCyl            -0.74021798
## FE                 1.00000000
## NumGears           -0.21128488
## TransLockup        -0.27193887
## TransCreeperGear   -0.06962168
## IntakeValvePerCyl  0.28034403
## ExhaustValvesPerCyl 0.33565285
## VarValveTiming     0.12495278
## VarValveLift        0.09621127
```

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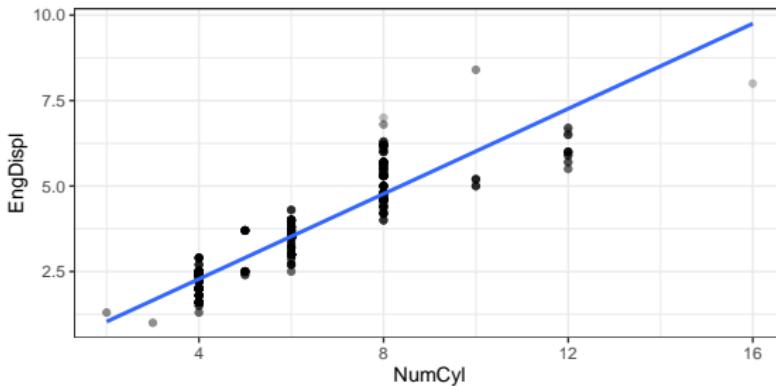


## Collinearity

- We may want to include both EngDispl and NumCyl in our model for FE.
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```
cor(cars2010$EngDispl, cars2010$NumCyl)
```

```
## [1] 0.90626
```

## Validation Set

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library(rsample)
set.seed(999)
cars_initial <- initial_split(cars2010)
cars_train <- training(cars_initial)
cars_val <- testing(cars_initial)
```

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set.seed(999)
cars_initial <- initial_split(cars2010)
cars_train <- training(cars_initial)
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```

- The `dim` function in `rsample` returns the number of observations and variables present in a split:

```
cars_train %>% dim()
```

```
## [1] 831 14
```

```
cars_val %>% dim()
```

```
## [1] 276 14
```

## Two Models

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summary(mod1)

##
## Call:
## lm(formula = FE ~ EngDispl, data = cars_train)
##
## Residuals:
##      Min       1Q   Median       3Q      Max 
## -12.6152  -3.2808  -0.4195   2.6322  27.1747 
## 
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)    
## (Intercept) 50.5639    0.4667 108.34 <2e-16 ***
## EngDispl    -4.4990    0.1252 -35.92 <2e-16 ***
## ---        
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
## 
## Residual standard error: 4.648 on 829 degrees of freedom
## Multiple R-squared:  0.6088, Adjusted R-squared:  0.6084 
## F-statistic: 1290 on 1 and 829 DF,  p-value: < 2.2e-16
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```
mod2 <- lm(FE ~ EngDispl + NumCyl, data = cars_train)
summary(mod2)

##
## Call:
## lm(formula = FE ~ EngDispl + NumCyl, data = cars_train)
##
## Residuals:
##      Min       1Q   Median       3Q      Max 
## -13.4549  -3.1297  -0.3406  2.5093 27.3736 
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)    
## (Intercept) 51.6430    0.5480 94.246 < 2e-16 ***
## EngDispl    -3.5000    0.2982 -11.738 < 2e-16 ***
## NumCyl     -0.7691    0.2086 -3.686 0.000242 *** 
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 4.613 on 828 degrees of freedom
## Multiple R-squared:  0.6151, Adjusted R-squared:  0.6142 
## F-statistic: 661.7 on 2 and 828 DF, p-value: < 2.2e-16
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- And we'll create another model that also includes NumCyl.

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- The MLR model has lower RSE, higher  $R^2$ , and all predictors are significant. But is it really the better model?

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```
mod1_preds <- predict(mod1, cars_val)
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mod1_mse

## [1] 115.4423
```

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```
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```
mod2_preds <- predict(mod2, cars_val)
mod2_mse <- mean( (cars2011$FE - mod2_preds)^2)
mod2_mse
```

```
## [1] 117.9783
```

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```

```
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```

- The MLR model (mod2) now has slightly higher MSE than the SLR model (mod1)
  - But could this be a fluke of a random validation set?

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**Cross-Validation** is using resampling techniques to assess model accuracy.

## Section 2

### Cross-Validation

## $k$ -fold Cross Validation

- $k$ -fold CV randomly partitions data into  $k$  sets of size  $n/k$ .
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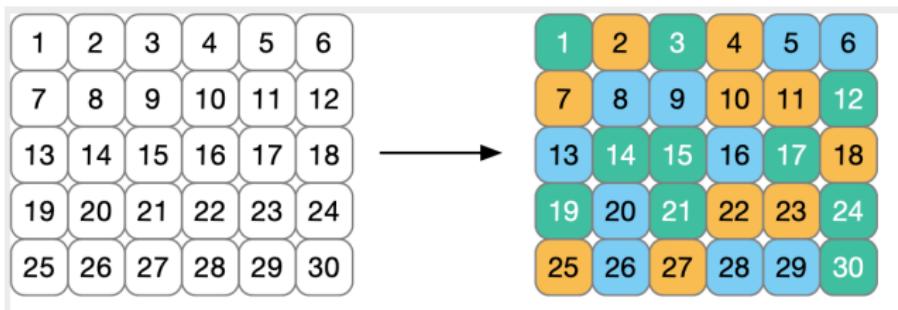
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- Since the partition into folds is random,  $CV_{(k)}$  still has some variability. But less than just using a single validation set.
  - To reduce variability further,  $k$ -fold CV can be performed multiple times, and the results of  $CV_{(k)}$  themselves averaged.

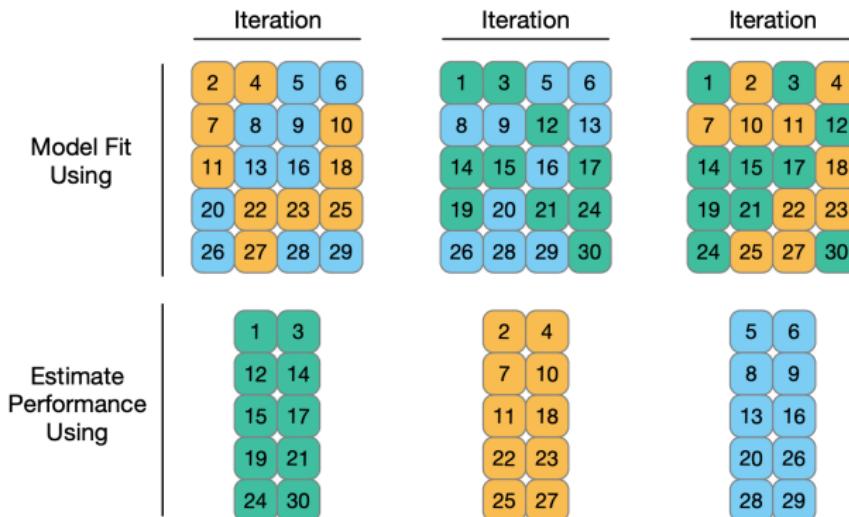
## 3-fold CV

- Consider 30 training observations below. Colors indicate a random fold allocation.



## 3-fold CV

- Each iteration uses 2 of the folds to build a model, and the remaining fold to assess performance.



- Overall performance is obtained by averaging across iterations.

## CV in R

We'll use the `vfold_cv` function in `rsample` to perform cross-validation.

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- The above code breaks the data into 10 (nearly) equal folds and stores results as a `resample` object with 2 parts:
  - `id`, a vector with fold identifiers (i.e "Fold01", "Fold02", ... )
  - `Splits`, a list whose elements correspond to each split of the data into  $k - 1$  training and 1 validation sets

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- **Goal:** Write function to do each of the following
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  - ② Fit linear model
  - ③ Predict on assessment data
  - ④ Assess accuracy

## Create Functions

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    - Let's practice coding!
  - Goal:** Write function to do each of the following
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  - Fit linear model
  - Predict on assessment data
  - Assess accuracy

```
cv_model1 <- function(split){  
  mod <- lm(FE ~ EngDispl, data = analysis(split))  
  val <- assessment(split)  
  preds <- predict(mod, val)  
  mse <- mean( (val$FE - preds)^2 )  
  mse  
}
```

## Get Results!

- Now, we'll apply this function to each split in `folds_cars` using the `map_dbl` function from the `purrr` package

```
library(purrr)
folds_cars$mod1_results <- map_dbl(folds_cars$splits, cv_model1)
folds_cars %>% head()

## # A tibble: 6 x 3
##   splits           id    mod1_results
##   <list>        <chr>     <dbl>
## 1 <split [996/111]> Fold01      18.0
## 2 <split [996/111]> Fold02      17.1
## 3 <split [996/111]> Fold03      25.0
## 4 <split [996/111]> Fold04      25.9
## 5 <split [996/111]> Fold05      21.2
## 6 <split [996/111]> Fold06      16.4
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- And to find the average CV MSE, we take the mean of the `results` column:

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```

- And to find the average CV MSE, we take the mean of the results column:

```
CV_MSE_mod1 <- mean(folds_cars$mod1_results)
CV_MSE_mod1
```

```
## [1] 21.44501
```

## Repeat

And now we repeat, but for `mod2`:

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```
cv_model2 <- function(split){  
  mod <- lm(FE ~ EngDispl + NumCyl, data = analysis(split))  
  val <- assessment(split)  
  preds <- predict(mod, val)  
  mse <- mean( (val$FE - preds)^2 )  
  mse  
}  
  
folds_cars$mod2_results <- map_dbl(folds_cars$splits, cv_model2)  
  
CV_MSE_mod2 <- mean(folds_cars$mod2_results)
```

## Repeat

And now we repeat, but for mod2:

```
cv_model2 <- function(split){  
  mod <- lm(FE ~ EngDispl + NumCyl, data = analysis(split))  
  val <- assessment(split)  
  preds <- predict(mod, val)  
  mse <- mean( (val$FE - preds)^2 )  
  mse  
}  
  
folds_cars$mod2_results <- map_dbl(folds_cars$splits, cv_model2)  
  
CV_MSE_mod2 <- mean(folds_cars$mod2_results)  
  
data.frame(model = c("1", "2"), cv_mse = c(CV_MSE_mod1, CV_MSE_mod2))  
  
##   model   cv_mse  
## 1      1 21.44501  
## 2      2 21.26763
```

## Repeat

And now we repeat, but for mod2:

```
cv_model2 <- function(split){  
  mod <- lm(FE ~ EngDispl + NumCyl, data = analysis(split))  
  val <- assessment(split)  
  preds <- predict(mod, val)  
  mse <- mean( (val$FE - preds)^2 )  
  mse  
}  
  
folds_cars$mod2_results <- map_dbl(folds_cars$splits, cv_model2)  
  
CV_MSE_mod2 <- mean(folds_cars$mod2_results)  
  
data.frame(model = c("1", "2"), cv_mse = c(CV_MSE_mod1, CV_MSE_mod2))  
  
##   model   cv_mse  
## 1      1 21.44501  
## 2      2 21.26763
```

- It looks like after performing 10-fold CV, model 2 is better afterall!