

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)
```

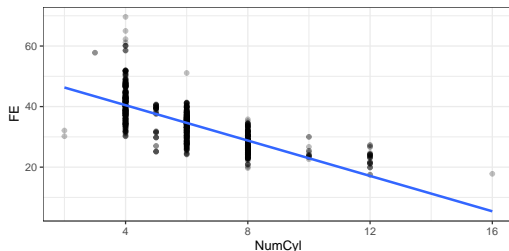
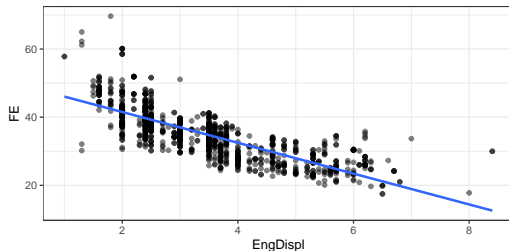
```
##           [,1]  
## EngDispl    -0.78739383  
## NumCyl      -0.74021798  
## FE           1.00000000  
## NumGears    -0.21128488  
## TransLockup -0.27193887  
## TransCreeperGear -0.06962168  
## IntakeValvePerCyl 0.28034403  
## ExhaustValvesPerCyl 0.33565285  
## VarValveTiming  0.12495278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

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## IntakeValvePerCyl           0.28034403  
## ExhaustValvesPerCyl         0.33565285  
## VarValveTiming              0.12495278  
## VarValveLift                0.09621127
```

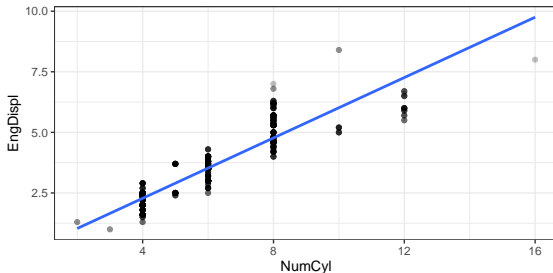


Collinearity

- We may want to include both `EngDispl` and `NumCyl` in our model for FE.
 - But if both are strongly correlated with FE, they may also be strongly correlated with each other. . .

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- But if both are strongly correlated with FE, they may also be strongly correlated with each other...



```
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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Let's create a validation set using `initial_split` in the `rsample` package

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

- 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

- Since `EngDispl` is most strongly correlated with `FE`, we will include it in our models.
- And we'll create another model that also includes `NumCyl`.

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```
mod1 <- lm(FE ~ EngDispl, data = cars_train)
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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mod2 <- lm(FE ~ EngDispl + NumCyl, data = cars_train)
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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?

Assess on Validation Set

Let's check MSE on the validation set.

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```
mod1_preds <- predict(mod1, cars_val)
mod1_mse <- mean( (cars2011$FE - mod1_preds)^2 )
mod1_mse
```

```
## [1] 115.4423
```

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```

```
## [1] 115.4423
```

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

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

Assess on Validation Set

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mod1_preds <- predict(mod1, cars_val)
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mod2_mse
```

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

- 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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What are some problems with the Training / Validation approach?

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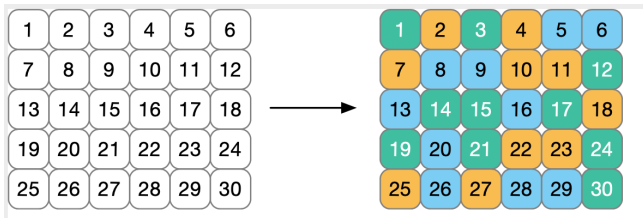
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- Since the partition into folds is random, $CV_{(k)}$ still has some variability. But less than just using a single validation set.
 - To reduce variability further, k -fold CV can be performed multiple times, and the results of $CV_{(k)}$ themselves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

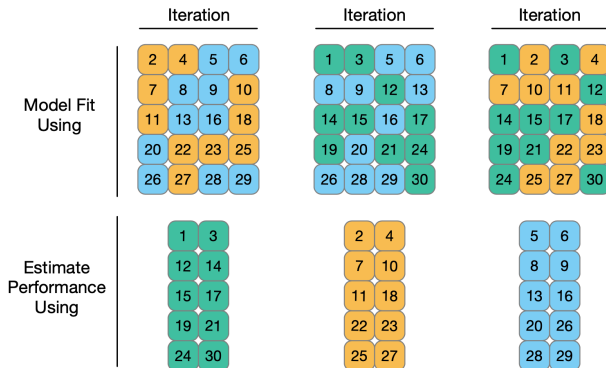
3-fold CV

- 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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set.seed(927)
folds_cars <- vfold_cv(cars2010, v = 10)
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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", ...)
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folds_cars$splits[[1]] %>% analysis()
```

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- And to get the corresponding validation set, we apply `assessment` to the same element

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 - ① Obtain analysis set
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 - 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
 - 1 Obtain analysis set
 - 2 Fit linear model
 - 3 Predict on assessment data
 - 4 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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## 5 <split [996/111]> Fold05      21.2
## 6 <split [996/111]> Fold06      16.4
```

- 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`:

Repeat

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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$mod2_results <- map_dbl(folds_cars$plits, 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$mod2_results <- map_dbl(folds_cars$plits, 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$mod2_results <- map_dbl(folds_cars$plits, 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!