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

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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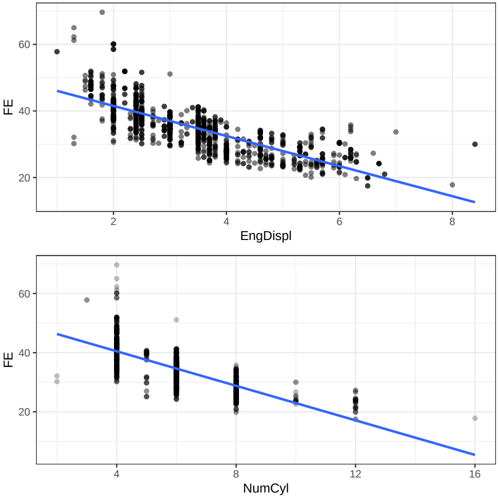

Collinearity

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

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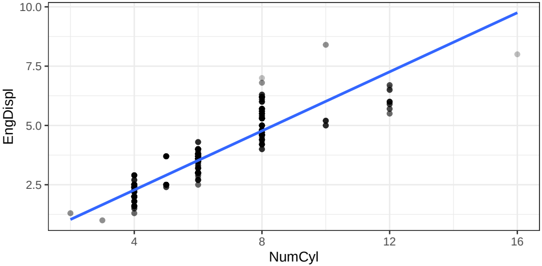


```
cor(cars2010$EngDispl, cars2010$NumCyl)
```

```
## [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)
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] 830  14
```

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

```
## [1] 277  14
```

Two Models

- Since `EngDispl` is most strongly correlated with `FE`, we will include it in our models.
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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
## -14.766  -3.196  -0.502   2.744  27.000
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept)  51.0108     0.4683  108.93   <2e-16 ***
## EngDispl     -4.6501     0.1256  -37.03   <2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 4.7 on 828 degrees of freedom
## Multiple R-squared:  0.6235, Adjusted R-squared:  0.6231
## F-statistic:  1371 on 1 and 828 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
## -15.2623  -3.0929  -0.3346   2.6825  27.1432
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept)  51.6371     0.5341  96.678   <2e-16 ***
## EngDispl     -4.0121     0.2924 -13.724   <2e-16 ***
## NumCyl       -0.4795     0.1986  -2.415    0.016 *
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 4.686 on 827 degrees of freedom
## Multiple R-squared:  0.6261, Adjusted R-squared:  0.6252
## F-statistic: 692.5 on 2 and 827 DF,  p-value: < 2.2e-16
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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] 115.3013
```

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mod1_mse
```

```
## [1] 115.3013
```

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

```
## [1] 115.7683
```

Assess on Validation Set

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

```
## [1] 115.7683
```

- 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

Resampling

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
    - Remaining $k-1$ subsets are used as training set to build the model.

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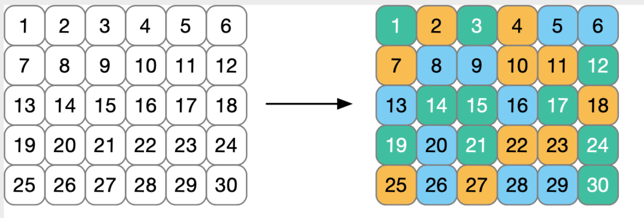
- Since the partition into folds is random, $CV_{(k)}$ still has some variability. But less than just using a single validation set.
  - To reduce variability further, k-fold CV can be performed multiple times, and the results of $CV_{(k)}$ themselves averaged.

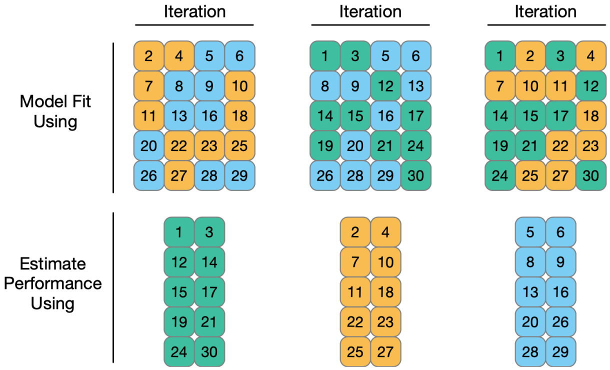
3-fold CV

- 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)
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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:
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folds_cars$splits[[1]] %>% analysis()
```

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  - Let's practice coding!
- **Goal:** Write function to do each of the following

1. Obtain analysis set
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```
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:

```
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)
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And now we repeat, but for mod2:

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

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  - While LOOCV does not consistently have higher variance or lower bias than k-fold CV, in almost all cases, it will produce estimates of MSE that are significantly less accurate than other resampling techniques.