STOR 320 Modeling III

Lecture 18

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Introduction

- Instructions
  - Download Tutorial Zip
  - Unzip Folder
  - Required Packages
    - `library(modelr)`
    - `library(tidyverse)`
    - `library(purrr)`
    - `library(broom)`
  - Open .Rmd File and Knit

Discussion

- Problems With Current Approach
  - Same Model For All Locations
  - Not All Locations Used in Train
  - Not All Locations Used in Test
  - Residuals Indicate that Model Can Be Improved
  - Not Helpful for Forecasting
  - Ambiguous Results: No Clear Winner

Part 1: Cross Validation by Location

- Previously
  - Split Data in Train and Test
    - Train (28 Rivers)
    - Test (3 Rivers)
  - Purpose
    - Estimate Out-of-Sample Error
    - Pick Best Model Based on This Estimate
    - Combat Overfitting
    - Robustification
  - Goal: Find the Simplest Model that Adequately Predicts

Part 1: Cross Validation by Location

- Current Issues
  - Decision on Final Model Heavily Influenced by the Test Data
  - Loss of Data in Model Fitting
  - Not Appropriate in Small Datasets
- Cross Validation Idea
  - Split Data Into Many Groups
  - Each Group Acts as a Test Set
  - All Data is Used in Both Model Fitting and Model Testing
  - Help: Chapter 5 (ISLR)

Part 1: Cross Validation by Location

- Tidyverse Concepts
  - Chapter 20 (R4DS)
  - List-Columns
    - Columns in Data Frames or Tibbles Can Be Lists
    - What this Means
      - Column of Tables
      - Column of Models
      - Column of Functions
  - Functions
    - nest(): Converts Rows of a Data Frame into a List
    - unnest(): What do You Think It Does?

Part 1: Cross Validation by Location

- Run Chunk 1

  - Observe the Output
  - Column of Tibbles

- Run Chunk 2

  - Imagine We Wanted to Split
    - Test: Data For Location 103
    - Train: All Remaining Data
  - Use of filter() and unnest()
  - First Glimpse -> 365 x 8
  - Second Glimpse -> 10,972 x 8

Part 1: Cross Validation by Location

- Chunk 3

  - Run Each Line
  - What is Happening?
  - Use View() on DATA2 and Scan Through the Data
  - What do You Notice?

- Chunk 4

  - Create a Loop that Repeats this Process for Each Location
  - Each Location Is a Test Set
  - Predictions Saved are All Out-of-Sample
  - Run Chunk 4 to Test Your Code

Part 1: Cross Validation by Location

- Chunk 4 (Continued)

```
DATA2=DATA
DATA2$linpred=NA

for(k in unique(DATA2$L)){
  TEST = NEST.DATA %>% filter(L==k) %>%
unnest()
  TRAIN  = NEST.DATA %>% filter(L!=k) %>%
unnest()

  linmod=lm(W~A, data=TRAIN)
  linmodpred=predict(linmod,newdata=TEST)

  DATA2$linpred[which(DATA2$L==k)]=linmodpred
}
```

Part 1: Cross Validation by Location

- Chunk 5

  - In Our Data, We Have:
    - Actual Water Temperatures
    - Out-of-Sample Predicted Water Temperatures
  - Create RMSE.func() With Two Arguments
    - actual= vector of actual water temperatures
    - predict=vector of predicted water temperatures
  - Use This Function on the Two Columns in DATA2 for RMSE
    - actual=W
    - predict=linpred

Part 1: Cross Validation by Location

- Chunk 5 (Continued)

```
RMSE.func = function(actual,predict){
  mse=mean((actual-predict)^2,na.rm=T)
  rmse=sqrt(mse)
  return(rmse)
}

RMSE.func(actual=DATA2$W,
                    predict=DATA2$linpred)
```

```
RMSE.func(actual=DATA2$W,predict=DATA2$linpred)
1] 3.147084
```

Intermission

- Current

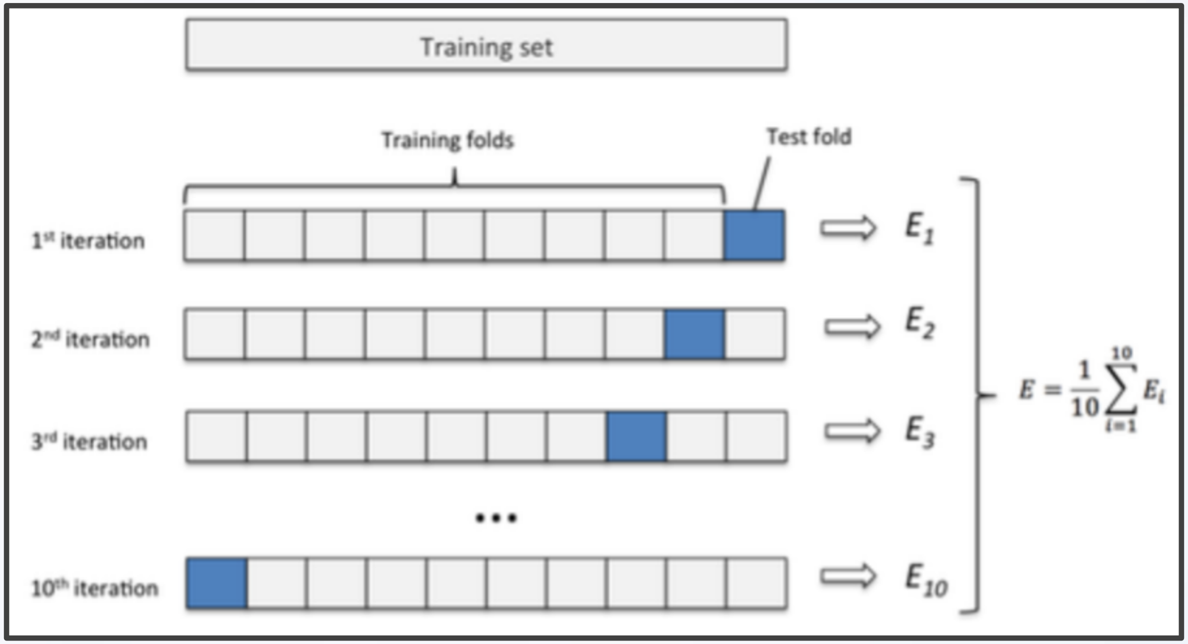
  - Using the Natural Grouping of Data for 31-Fold Cross Validation
  - Only Fit One Linear Model
  - Should Use Cross-Validation for Multiple Different Models and Compare Cross-Validated RMSE

- Next

  - Randomly Assign Observations to *K*-Folds
  - CV Function: crossv_kfold(*K*)

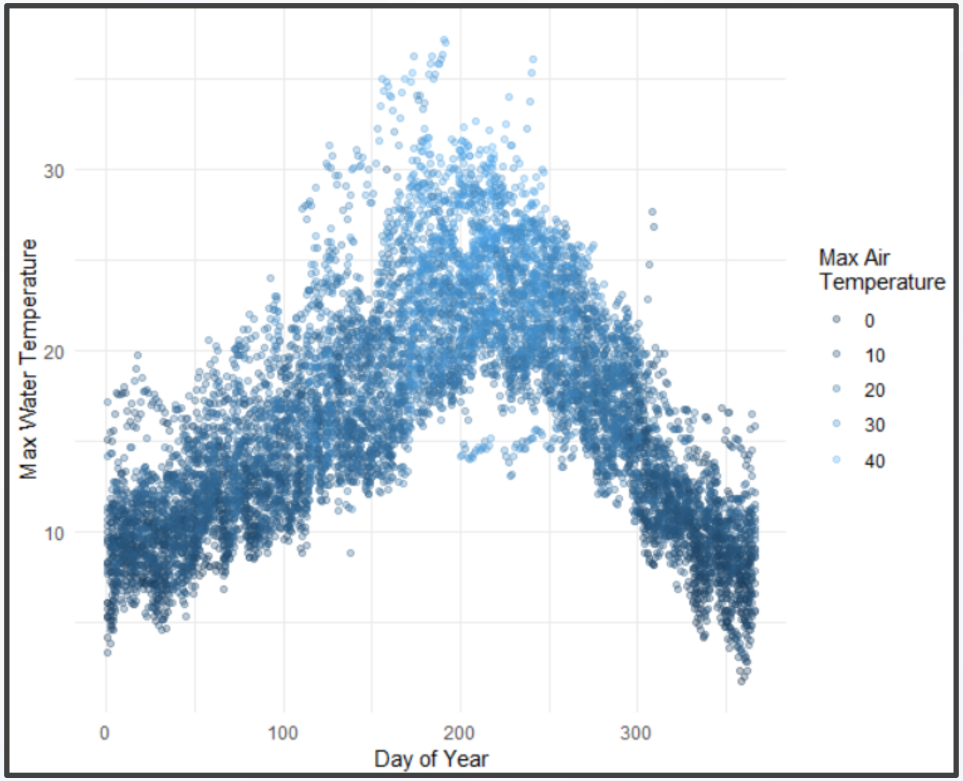
Part 2: K-Fold CV

- Overview (*K*=10)
  - Randomly Split Observations Into *K* Groups
  - Each Fold Acts as a Test Set
  - If Each Fold Contains Approximately the Same # of Observations,



Part 2: K-Fold CV

- Run Chunk 1
  - Variables (Julian Day)
  - Clear Non-Linear Relationship



Part 2: K-Fold CV

- General Polynomial Model

$$W = a + \sum_{i=1}^{I} b_i A^i + \sum_{j=1}^{J} c_j D^j + \varepsilon$$

  - Perform K-Fold CV to Estimate Out-of-Sample RMSE for Choices of *I=4* and *J=3*
  - Ultimate Goal is To Select Best *I* and *J*

Part 2: K-Fold CV

- Run Chunk 2
  - Fit Model with *I=4* and *J=3*
  - Functions from broom Package
    - tidy()
    - glance()
  - Used to Preview Models

```
tidy(polymodel)
A tibble: 8 x 5
term                    estimate std.error statistic  p.value
<chr>                      <dbl>     <dbl>     <dbl>    <dbl>
(Intercept)                 16.2    0.0273     595.   0.
poly(A, 4)1                328.     4.36        75.3  0.
poly(A, 4)2                 49.0    2.80        17.5  1.62e-67
poly(A, 4)3                  2.85   2.78         1.02 3.06e- 1
poly(A, 4)4                 -3.62   2.72        -1.33 1.84e- 1
poly(JULIAN_DAY, 3)1        46.0    2.78        16.6  8.85e-61
poly(JULIAN_DAY, 3)2      -226.     4.31       -52.5  0.
poly(JULIAN_DAY, 3)3       -59.3    2.89       -20.5  8.66e-92
```

```
glance(polymodel)
A tibble: 1 x 11
r.squared adj.r.squared sigma statistic p.value    df  logLik    AIC    BIC
    <dbl>         <dbl> <dbl>     <dbl>   <dbl> <int>   <dbl>  <dbl>  <dbl>
    0.797         0.797  2.71     5525.       0     8 -23804. 47626. 47691.
```

Part 2: K-Fold CV

- Run Chunk 3
  - Divide Data into 10 Folds
    - Use crossv_kfold() Function
    - Variables are Lists of Train and Test Sets
  - For Each Row, We Want to Fit on Train and Predict on Test

```
head(DATA3)
A tibble: 6 x 3
train           test            .id
<list>          <list>          <chr>
<S3: resample> <S3: resample> 01
<S3: resample> <S3: resample> 02
<S3: resample> <S3: resample> 03
<S3: resample> <S3: resample> 04
<S3: resample> <S3: resample> 05
<S3: resample> <S3: resample> 06
```

Part 2: K-Fold CV

- Run Chunk 4
  - Create Function to Fit Models
  - Apply Function to All Train Sets Using purrr::map() Function

```
DATA4=DATA3 %>%
       mutate(tr.model=map(train,train.model.func,i=i,j=j))
head(DATA4)
A tibble: 6 x 4
train          test           .id   tr.model
<list>         <list>         <chr> <list>
<S3: resample> <S3: resample> 01    <S3: lm>
<S3: resample> <S3: resample> 02    <S3: lm>
<S3: resample> <S3: resample> 03    <S3: lm>
<S3: resample> <S3: resample> 04    <S3: lm>
<S3: resample> <S3: resample> 05    <S3: lm>
<S3: resample> <S3: resample> 06    <S3: lm>
```

  - Functions from purrr Package
    - map() – Loop Over Train
    - map2() – Loop Over Fitted Models and Test

Part 2: K-Fold CV

- Run Chunk 5
  - purrr::map2() Iterates Function Over Two Arguments
  - For Every Test Set and Trained Model, We Use augment() to Get Predictions

```
DATA4.PREDICT = DATA4 %>%
          mutate(predict=map2(test,tr.model,~augment(.y,newdata=.x))) %>%
          select(predict) %>%
          unnest()
head(DATA4.PREDICT)
A tibble: 6 x 10
JULIAN_DAY  YEAR     L      W      A  TIME MONTH   DAY .fitted  .se.fit
     <int> <int> <int>  <dbl>  <dbl> <int> <int> <int>   <dbl>    <dbl>
         9  2003   103    9.8    5.1     9     1     9    7.27   0.138
        12  2003   103    9.9    6.2    12     1    12    7.67   0.119
        25  2003   103    9.8   14      25     1    25   10.4    0.0744
        30  2003   103    9.5    9      30     1    30    9.14   0.0803
        47  2003   103   12.5   11.4    47     2    16   10.5    0.0621
        50  2003   103   10.7   14      50     2    19   11.5    0.0548
```

  - Next, Compare Actual With Fitted Using RMSE.func()

```
RMSE.func(actual=DATA4.PREDICT$W,predict=DATA4.PREDICT$.fitted)
1] 2.709727
```

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Look Ahead

- What We Have Done
  - Specify *I* and *J*
  - Use 10-Fold Cross Validation to Estimate Out-of-Sample RMSE

- How We Should Use This
  - Choose Max *I* and Max *J*
    (Example: 10)
  - Initiate 10 x 10 Matrix of *NA*
  - Loop Through All *i* and *j* to Capture Out-of-Sample RMSE
  - Create a Tile Plot that Visualizes the RMSE for Each Combination of *i* and *j*
  - Choose Best *i* and *j*