



# *Modeling IV*

# Introduction



- Instructions
  - Download Tutorial 13 Zip
  - Unzip Folder
  - Required Packages
    - `library(tidyverse)`
    - `library(modelr)`
    - `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



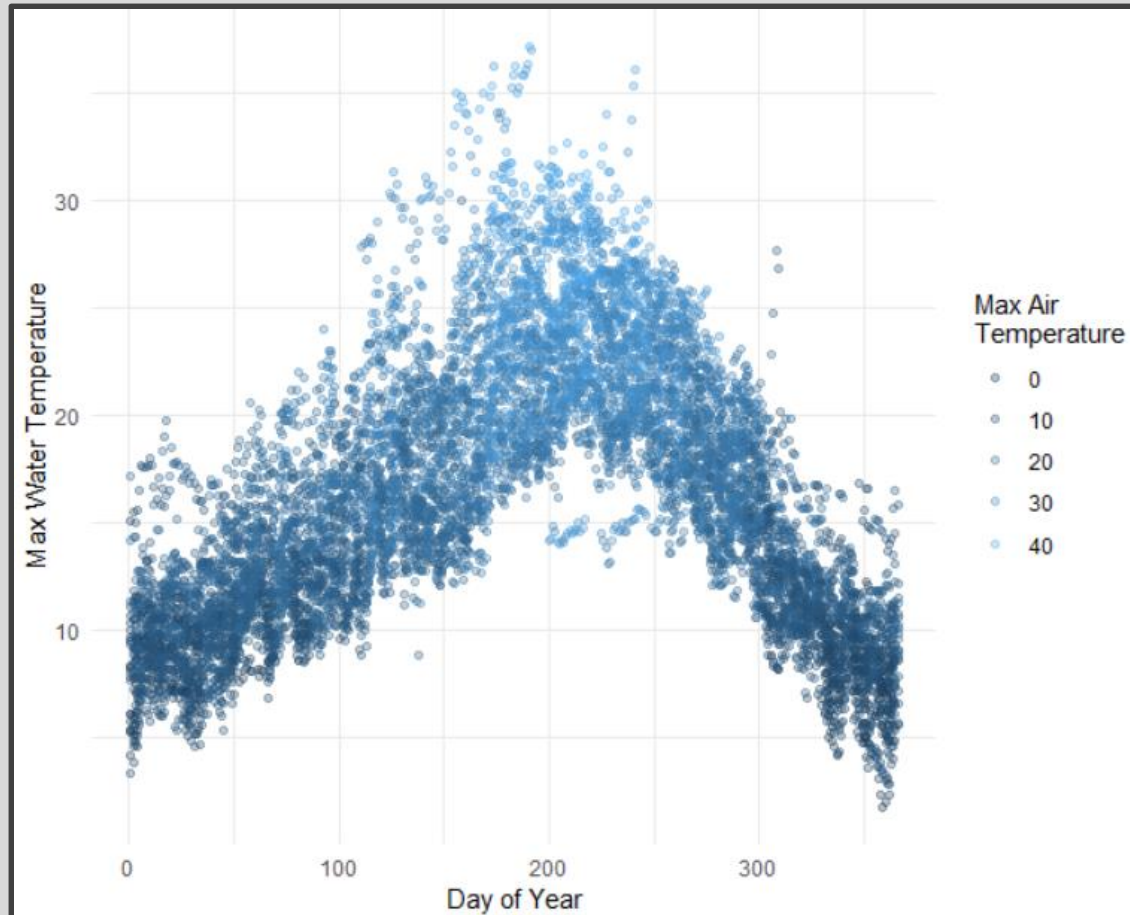
- Overview ( $K=10$ )
  - Randomly Split Observations Into  $K$  Groups
  - Each Fold Acts as a Test Set
  - If Each Fold Contains Approximately the Same # of Observations,



## 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 For Previewing Data

```
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>
1  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>
1 <S3: resample> <S3: resample> 01
2 <S3: resample> <S3: resample> 02
3 <S3: resample> <S3: resample> 03
4 <S3: resample> <S3: resample> 04
5 <S3: resample> <S3: resample> 05
6 <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>  
1 <S3: resample> <S3: resample> 01    <S3: 1m>  
2 <S3: resample> <S3: resample> 02    <S3: 1m>  
3 <S3: resample> <S3: resample> 03    <S3: 1m>  
4 <S3: resample> <S3: resample> 04    <S3: 1m>  
5 <S3: resample> <S3: resample> 05    <S3: 1m>  
6 <S3: resample> <S3: resample> 06    <S3: 1m>
```

- 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>  
1     9  2003  103  9.8  5.1     9     1     9  7.27  0.138  
2    12  2003  103  9.9  6.2    12     1    12  7.67  0.119  
3    25  2003  103  9.8  14     25     1    25 10.4  0.0744  
4    30  2003  103  9.5   9     30     1    30  9.14  0.0803  
5    47  2003  103 12.5 11.4    47     2    16 10.5  0.0621  
6    50  2003  103 10.7  14     50     2    19 11.5  0.0548
```

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

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

## 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  $j$

Closing



Disperse  
and Make  
Reasonable  
Decisions