BIOS 635: Cross-Validation

Kevin Donovan

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Review

- Homework 4 due on 2/26 at 11PM through GitHub Classroom
- Article Evaluation 1 assigned, due on 3/2 through GitHub Classroom
- Last lecture: nonlinear modeling using splines

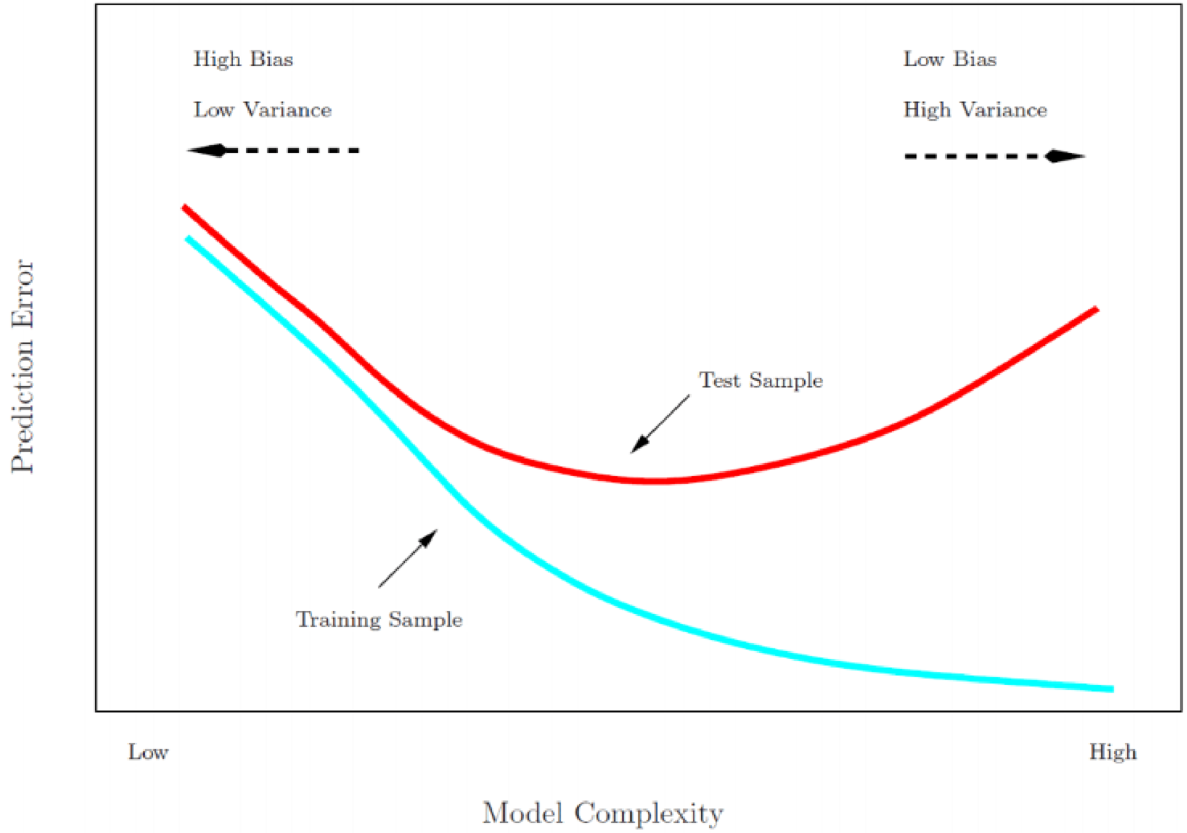
Prediction Error

- Recall prediction error can be calculated a variety of subsets of your data

  1. **training error**: average error when predicting outcome on data used to create algorithm
  2. **testing error**: average error when predicting outcome on data from that used in training

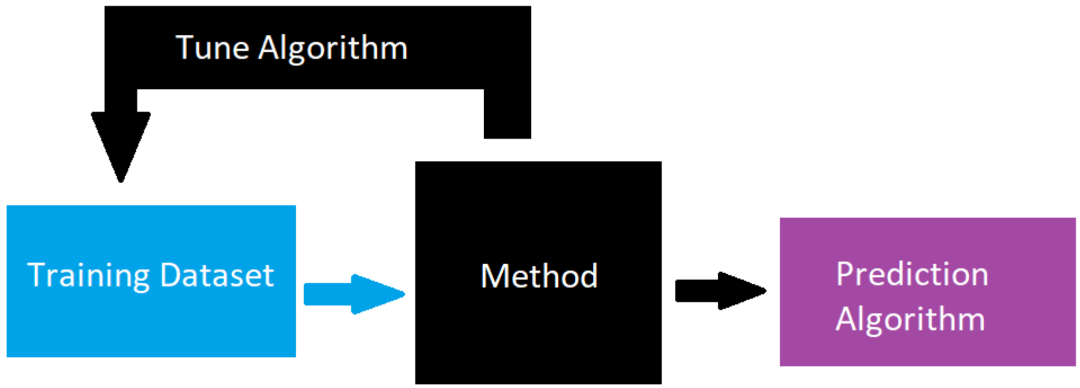
- Training error poor measure of algorithm's performance on general sample from population

  - ***Biased downward***
  - *Need separate and **independent** datasets for testing and training*

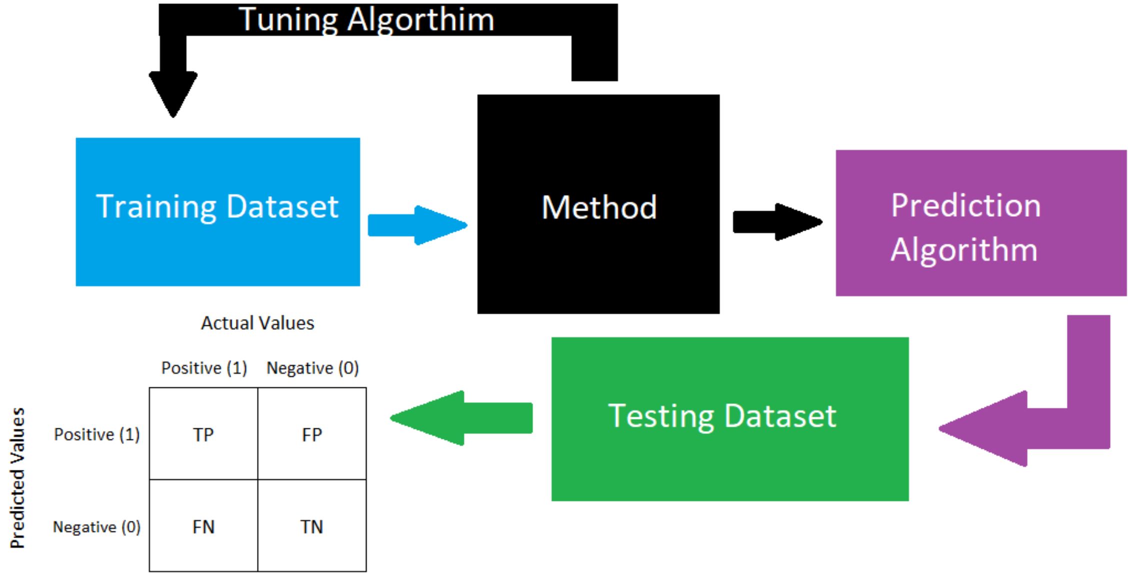

High Bias
Low Variance
Low Bias
High Variance
Prediction Error
Test Sample
Training Sample
Low
High
Model Complexity

Training and Testing

1. Training and Tuning



2. Training, Tuning, and Testing


Tuning Algorthim
Training Dataset
Method
Prediction Algorithm
Actual Values
Positive (1)
Negative (0)
Predicted Values
Positive (1)
Negative (0)
TP
FP
FN
TN
Testing Dataset

Testing error

- Various ways have been developed to estimate this testing error:

1. "Correct" training set error to be more generalizable

- **Idea**: $Error = f(MSE) + \lambda * ModelComplexity$ where $\lambda > 0$
- Ex. *Mallow's Cp, AIC, BIC*

2. Use large, independent and separate test set

- Often not available, though best option

3. Generate test set using **hold out**

- Randomly split available data into 2 partitions
- Use one partition for training, other for testing
- Testing = predict outcome on test set, compute prediction error (ex. MSE or misclassification rate)

Hold out

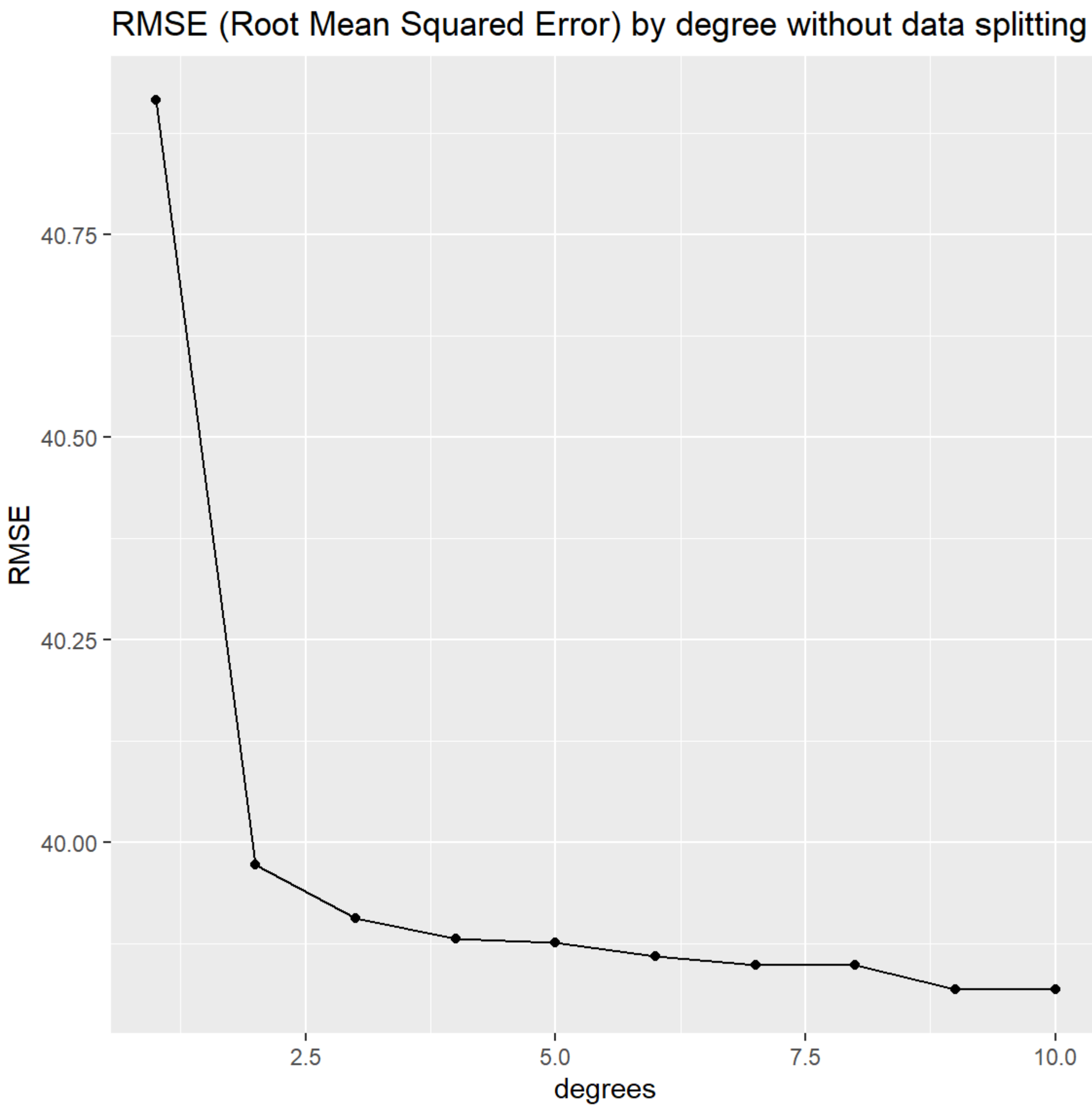
A random splitting into two halves: left part is training set, right part is validation set

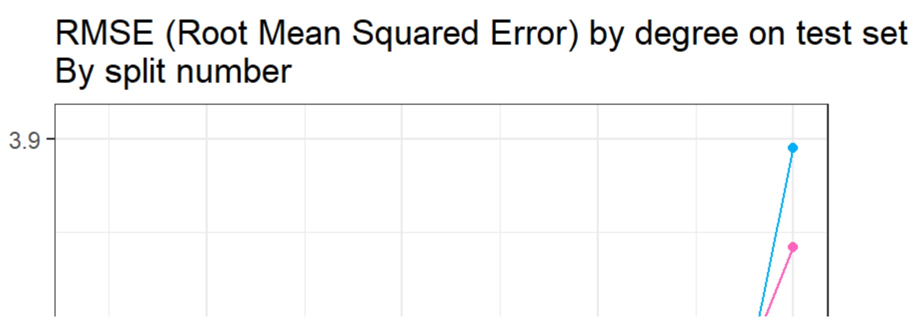
```r
wage_data <- Wage # contained in ISLR package
# Holdout 40% for tesing
tt_indicies <- createDataPartition(y=wage_data$wage, p=0.6, list = FALSE)
wage_data_train <- wage_data[tt_indicies,]
wage_data_test <- wage_data[-tt_indicies,]

# Look at datasets
paged_table(wage_data_train)
```

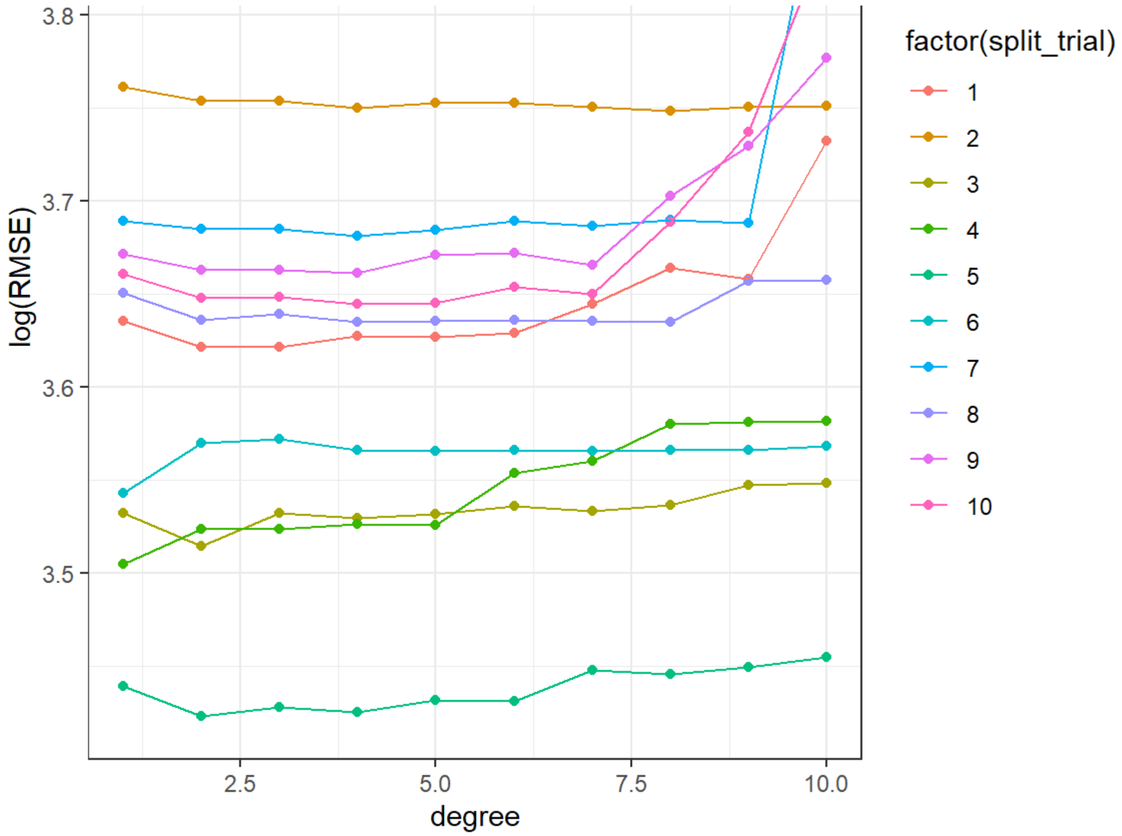
```r
paged_table(wage_data_test)
```

Training and testing

- Consider fitting nonlinear polynomial to wage data
- Using training error vs. testing error to choose spline order


RMSE (Root Mean Squared Error) by degree without data splitting
40.75
40.50
40.25
40.00
RMSE
2.5
5.0
7.5
10.0
degrees


RMSE (Root Mean Squared Error) by degree on test set
By split number
3.9



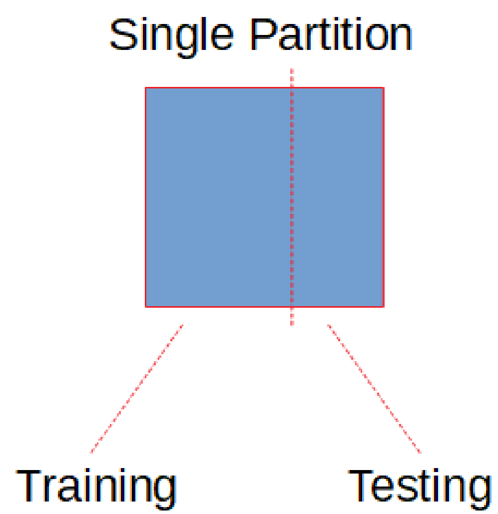
factor(split_trial)
1
2
3
4
5
6
7
8
9
10
log(RMSE)
3.8
3.7
3.6
3.5
degree
2.5
5.0
7.5
10.0

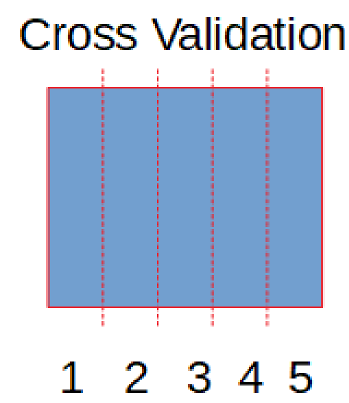
Drawbacks of holdout

- Test set error can be highly dependent on split
  - *Thus **highly variable***
  - *Especially for small dataset or **small group sizes***
- Only subset of data used to train algorithm
  - *May result in poorer algorithm*
  - $\rightarrow$ *may **overestimate** test error*
- Can we **aggregate results over multiple test sets?**

K-fold cross validation

- **Widely used** approach for estimating test error
- **Idea**: Still use entire data for training but evaluate **average** performance by aggregating over multiple test sets
  - *Test sets still must be **independent***
  - *Example: 5-fold CV*





1) Training : 1-4, Testing : 5
2) Training : 1-3+4, Testing : 4
3) Training : 1-2+4-5, Testing : 3
4) Training : 1+3-5, Testing : 2
5) Training : 2-5, Testing : 1

K-fold cross validation

- Denote K folds by $C_1, C_2, \ldots, C_K$, each with n_k observations
- For a given fold l:

  1. *Train algorithm on data in other folds: $\{C_k\}$ s.t. $k \neq l$*
  2. *Test by computing predicted values for data in C_l* ***only***
  3. *Repeat for each fold $l = 1, \ldots, K$, average error (ex. MSE_l)*

- K fold CV error rate

$$CV_{(K)} = \sum_{k=1}^{K} \frac{n_k}{n} MSE_k$$

where $MSE_k = \sum_{i \in C_k} (y_i - \hat{y}_i)^2 / n_k$ where y_i is outcome and $\hat{y}_i$ is predicted outcome from training on C_k **only**

- $K = n$ yields $n - fold$ or *leave-one out cross-validation*

- $CV_{(K)}$ is accurate measure of generalized error rate for algorithm trained on whole sample

K-fold CV in R

```
# 5 fold CV partitions
cv_folds <- createFolds(y=wage_data_subset$wage, k=5)
# Can see whose in fold 1
cv_folds$Fold1
```

```
##  [1]   1  13  20  25  27  28  34  39  46  48  56  62  68  69  72  76  79  86  87
## [20]  88  97 101 102 104 109 111 112 116 125 129 130 148 150 155 161 163 164 167
## [39] 169 179 185 188 193 215 217 229 233 234 235 246 251 264 272 277 279 282 293
## [58] 298 300 304 309 311 324 325 326 337 344 348 352 356 357 362 373 374 377 378
## [77] 380 383 384 386 398
```

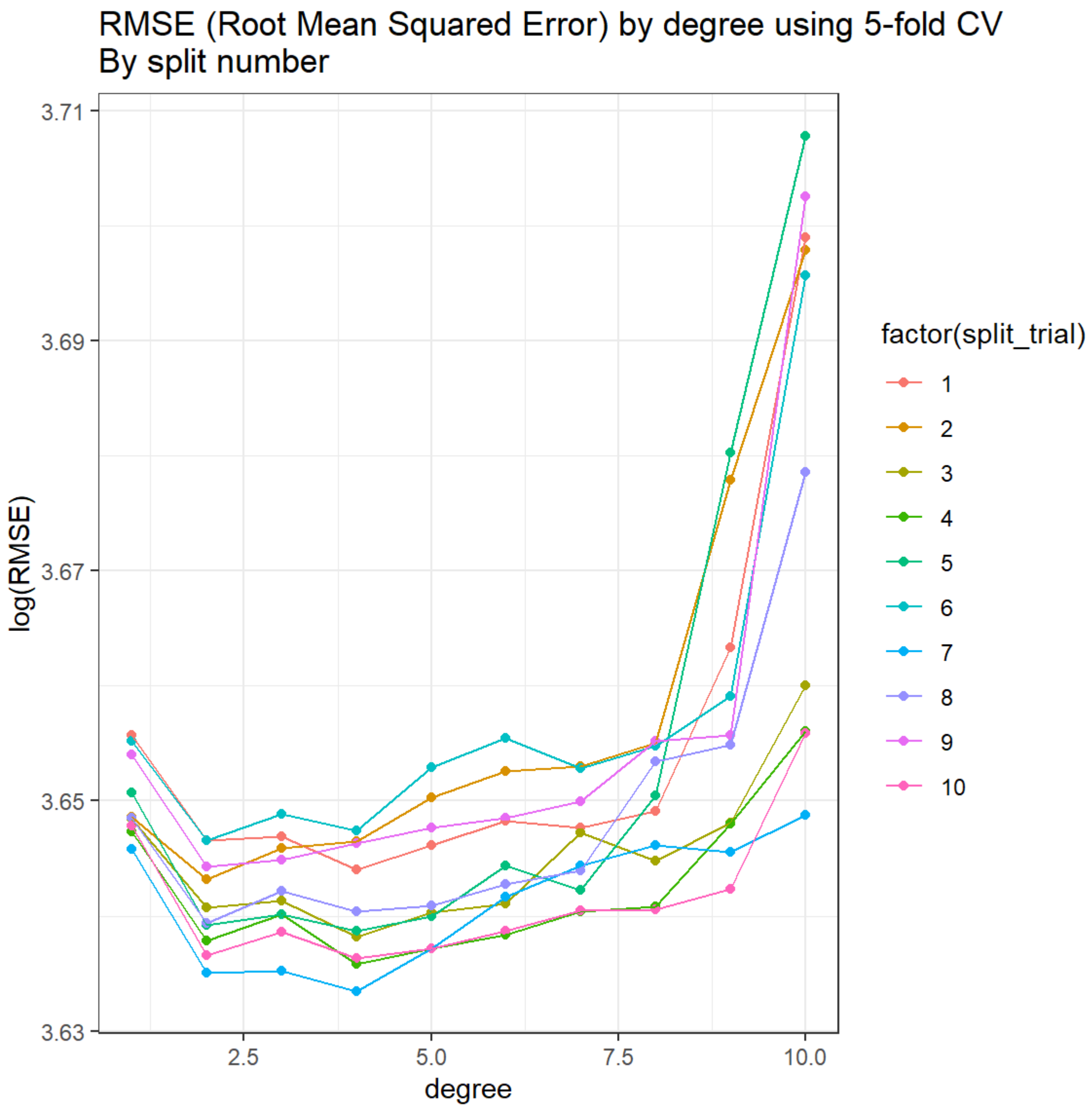
```
# Look at dataset for fold 1
wage_data_fold_1 <- wage_data_subset[cv_folds$Fold1,]
paged_table(wage_data_fold_1)
```

K-fold CV analysis

- Let's look back at the nonlinear fitting example from before. Instead of using a holdout testing method, we use 5-fold CV

```
# Fit model for each degree considered, compute RMSE (on training in this ex.)
poly_reg_fit <- list()
predict_wages <- list()
residuals_wages <- list()
rmse_poly_reg <- list()
mae_poly_reg <- list()
error_rates_degrees <- list()

counter <- 1
trials <- 10 # Look at 10 different 60:40 splits

for(j in 1:trials){
  set.seed(j) # Set seed to get different splits

  tt_indicies <- createFolds(y=wage_data_subset$wage, k=5)

    for(i in 1:length(degrees)){
      for(f in 1:length(tt_indicies)){
        wage_data_train <- wage_data_subset[-tt_indicies[[f]],]
        wage_data_test <- wage_data_subset[tt_indicies[[f]],]

        poly_reg_fit[[f]] <- lm(wage~poly(age, degrees[i]),
                                 data=wage_data_train)
```

```
        predict_wages[[f]] <- predict(poly_reg_fit[[f]], newdata = wage_data_test)
        residuals_wages[[f]] <- wage_data_test$wage-predict_wages[[f]]
        rmse_poly_reg[[f]] <- sqrt(mean(residuals_wages[[f]]^2))
        mae_poly_reg[[f]] <- mean(abs(residuals_wages[[f]]))
      }

      # Save in data frame
      error_rates_degrees[[counter]] <-
        data.frame("RMSE"=mean(unlist(rmse_poly_reg)),
                   "MAE"=mean(unlist(mae_poly_reg)),
                   "degree"=degrees[i],
                   "split_trial"=j)
      counter <- counter+1
    }
}

# Bind all degree-specific results together into single data frame/table
error_rates_degrees_df <- do.call("rbind", error_rates_degrees)

# Plot results as function of degree
ggplot(data=error_rates_degrees_df,
       mapping=aes(x=degree, y=log(RMSE), color=factor(split_trial)))+
  geom_point()+
  geom_line()+
  labs(title="RMSE (Root Mean Squared Error) by degree using 5-fold CV\nBy split number")+
  theme_bw()
```


RMSE (Root Mean Squared Error) by degree using 5-fold CV
By split number
log(RMSE)
3.71
3.69
3.67
3.65
3.63
2.5
5.0
7.5
10.0
degree
factor(split_trial)
1
2
3
4
5
6
7
8
9
10

Choosing K: bias-variance tradeoff

- **Recall**: Holdout method uses only portion of data for training
  - $\rightarrow$ *test/validation performance* ***overestimate***
  - $\rightarrow$ *more folds* $\rightarrow$ *more data in training folds* $\rightarrow$ *better algorithm* $\rightarrow$ *lower mean error*
  - $\rightarrow$ *LOOCV least biased estimate of test error*
- Compared to hold out, each training set in K-fold contains $\frac{(k-1)n}{k}$ obs
  - *Generally more then in holdout* $\rightarrow$ *less biased estimate*

Choosing K: bias-variance tradeoff

- **Recall**: Test set performance from holdout method can vary a lot depending on split
  - $\rightarrow$ *not a **precise** measure of test set error*
- Can decrease variance using aggregate method like K-fold CV
  - *With LOOCV, averaging performance of n trained algorithms*
  - *Testing folds differ, but training sets have almost identical set of observations*
  - $\rightarrow$ *test fold performances **highly correlated***
  - *Using K-fold CV with $K < n$ decrease training set overlap $\rightarrow$ less correlated*
  - $\rightarrow$ *variance of K-fold CV < LOOCV*
- This creates a **bias-variance** tradeoff when choosing K
  - *K=5 or 10 generally chosen (based on simulation studies)*

CV for classification

- Same process as before, divide data into K partitions $C_1, \ldots, C_K$
- Choose error/accuracy rate of interest
  - *E.g. sensitivity, specificity, classification error, etc.*
- For classification error
  - *Compute CV error*

$$CV_K = \sum_{k=1}^{K} \frac{n_k}{n} \text{Error}_k = \frac{1}{K} \sum_{k=1}^{K} \text{Error}_k$$

where $\text{Error}_k = \sum_{i \in C_k} I(y_i \neq \hat{y}_i)/n_k$

- Can we estimate the **variability** of this estimate?
  - *Commonly used estimate of standard error:*

$$\hat{\mathrm{SE}}(\mathrm{CV}_K) = \sqrt{\sum_{k=1}^{K} (\mathrm{Error}_k - \overline{\mathrm{Error}_k})^2 / (K-1)}$$

- While useful, not accurate (**Why?**)
- Also can be used in continuous prediction CV (using MSE for example)

CV for classification

In R: heart disease prediction with LDA (see lecture 6)

```
heart_data <- read_csv(file="../data/heart_disease/Correct_Dataset.csv") %>%
  mutate(heart_disease =
           relevel(factor(ifelse(Target>0, "Yes", "No")),
                   ref = "No"))

# Create lists to hold results
lda_fit <- list()
estimted_probs <- list()
accuracy_rates <- list()

# Create 5 folds
tt_indicies <- createFolds(y=heart_data$heart_disease, k=5)

# Run LDA for each fold, store results
for(f in 1:length(tt_indicies)){
  heart_data_train <- heart_data[-tt_indicies[[f]],]
  heart_data_test <- heart_data[tt_indicies[[f]],]

  lda_fit[[f]] <- train(heart_disease~Age+Sex+Chest_Pain+Resting_Blood_Pressure+
                             Colestrol+MAX_Heart_Rate+Exercised_Induced_Angina,
                           data = heart_data_train, method = "lda")

  estimted_probs[[f]] <- predict(lda_fit[[f]], newdata=heart_data_test, type = "prob")$Yes
  pred_heart_disease <-
    relevel(factor(ifelse(estimted_probs[[f]]>0.5,
                          "Yes", "No")), ref = "No")
```

```r
  # Get accuracy rates from output
  accuracy_rates[[f]] <-
    c(confusionMatrix(pred_heart_disease,
                reference = heart_data_test$heart_disease,
                positive = "Yes")$byClass,
      confusionMatrix(pred_heart_disease,
                reference = heart_data_test$heart_disease,
                positive = "Yes")$overall,
      "fold"=f)
}

accuracy_df <- data.frame(do.call("rbind", accuracy_rates))

# Compute mean and SE for each measure to get CV mean/SE
CV_mean <- accuracy_df %>%
  select(Sensitivity, Specificity, `Pos.Pred.Value`, `Neg.Pred.Value`, Accuracy) %>%
  apply(MARGIN = 2, FUN=mean)

CV_se <- accuracy_df %>%
  select(Sensitivity, Specificity, `Pos.Pred.Value`, `Neg.Pred.Value`, Accuracy) %>%
  apply(MARGIN = 2, FUN=sd)

CV_mean
```

```
##    Sensitivity    Specificity Pos.Pred.Value Neg.Pred.Value       Accuracy
##      0.7116402      0.8482955      0.8022736      0.7766796      0.7855738
```

```r
CV_se
```

```
##    Sensitivity    Specificity Pos.Pred.Value Neg.Pred.Value       Accuracy
##     0.05530303     0.07066323     0.08905437     0.03575939     0.05204986
```

CV with tuning

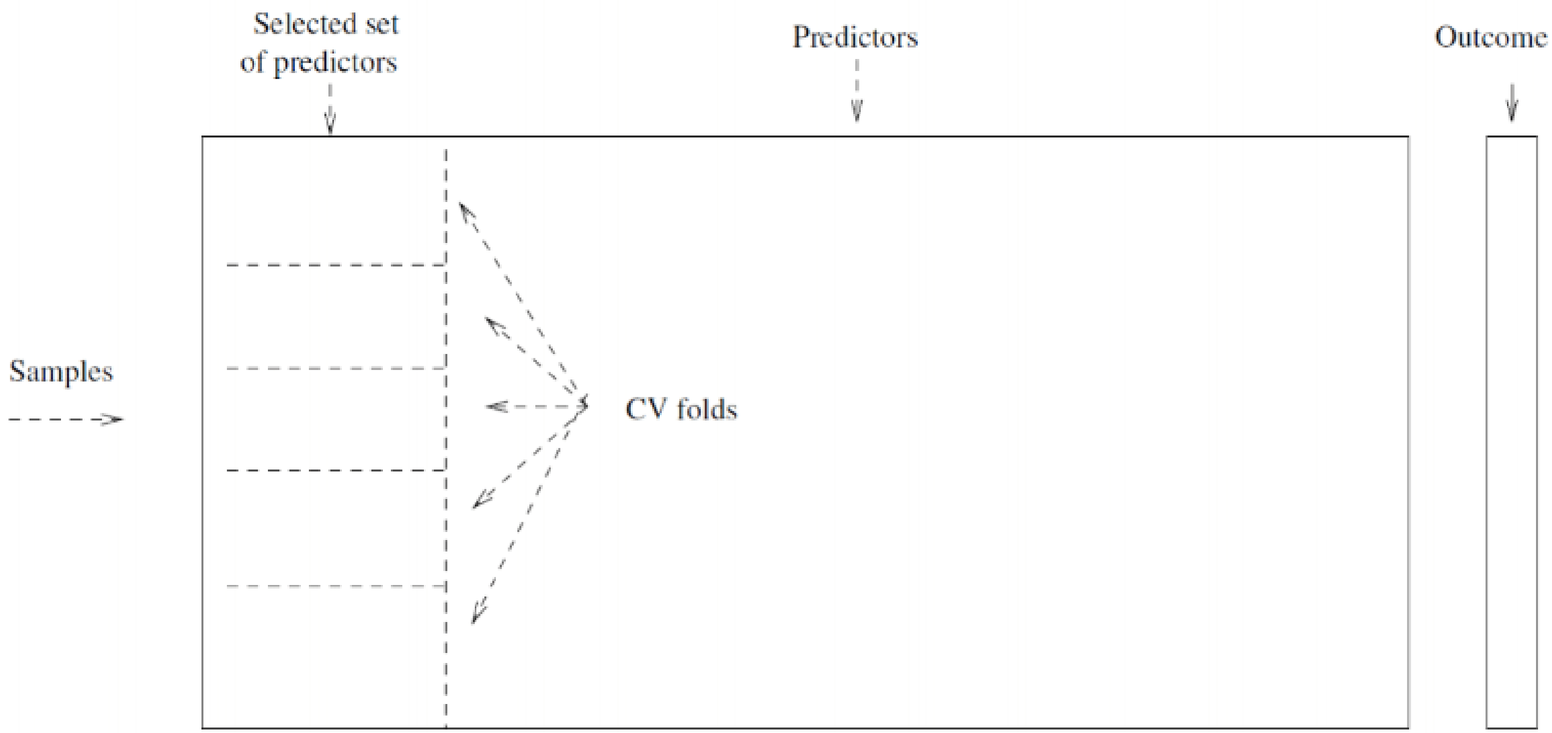
- **Recall**: Often when training a prediction algorithm, need to select **tuning parameters**
  - *Ex. # of neighbors with KNN, number of features with regression, degree in splines, etc.*
  - *Where is tuning implemented in CV?*
- Example: Consider set of 5000 predictors and 50 samples of data
  - *1. Starting with the 5000 predictors and full data, **first** find 100 predictors with largest correlation with outcome*
  - *2. Then train and test an algorithm with only these 100 predictors, using logistic regression as an example*
- How do we estimate the algorithm's test set performance without bias?
- Can we only apply CV in step 2, after the predictors have been chosen using the full data?

NO

- Why?
  - *This selection of parameters greatly impacts the algorithm's performance and thus is a form of tuning*
  - *Tuning needs to be done within the training framework, otherwise you are training and testing on the same dataset*
  - *Thus, need to do step 1 within your CV scheme*

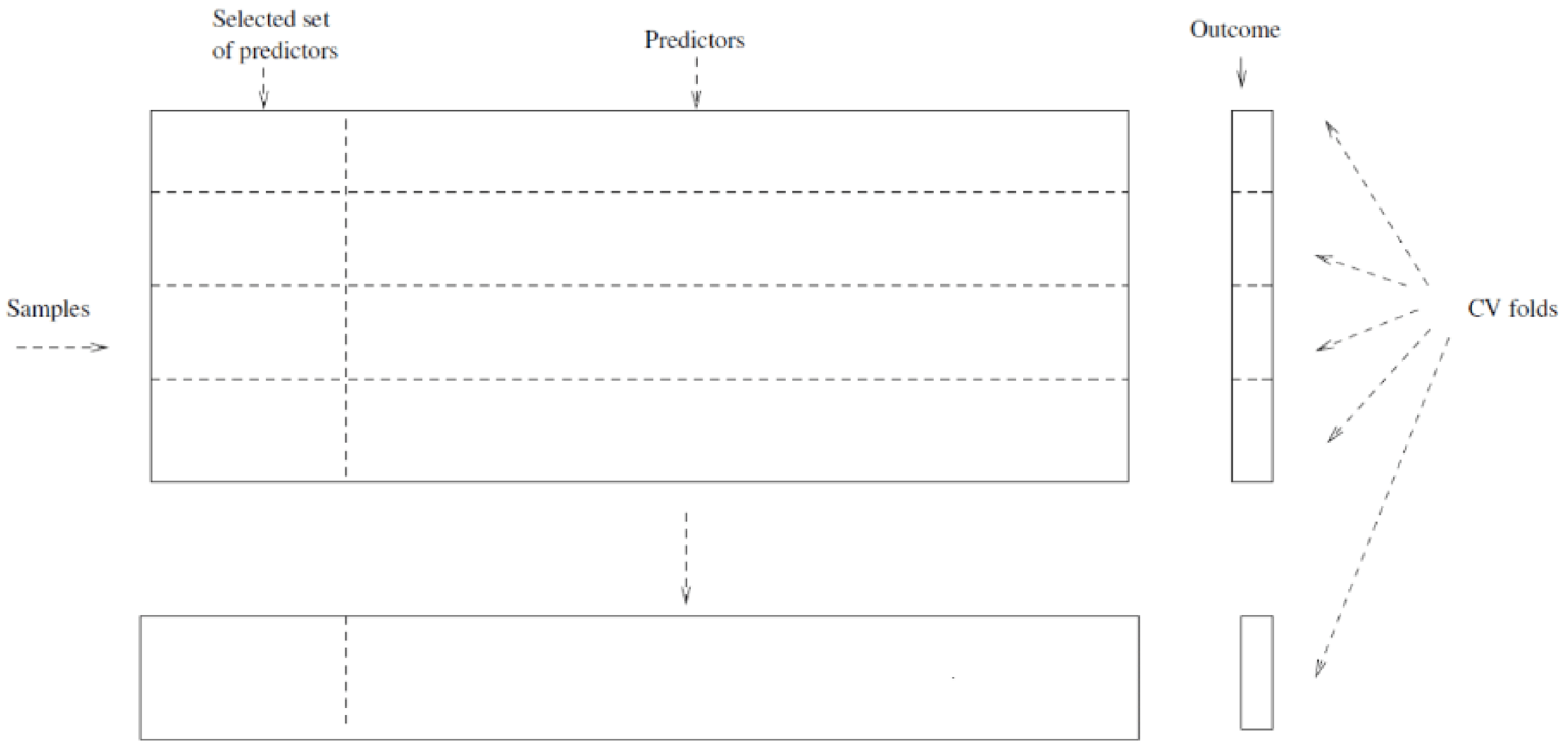
Wrong way: visual

- Only doing step 2 inside CV process



Right way: visual

- Doing both steps 1 and 2 within CV process



Song of the session

Green Eggs and Ham by Princess Nokia

Everything is Beautiful by Princess Nokia