STA 235H - Model Selection I:
Bias vs Variance, Cross-Validation, and Stepwise

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McCombs School of Business, UT Austin

Introduction to prediction

- So far, we had been focusing on causal inference:
  - Estimating an effect and "predicting" a counterfactual (what if?)
- Now, we will focus on prediction:
  - Estimate/predict outcomes under specific conditions.

Differences between inference and prediction

- Inference $\rightarrow$ focus on covariate
  - Interpretability of model.
- Prediction $\rightarrow$ focus on outcome variable
  - Accuracy of model.

Both can be complementary!

Example: What is churn?

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LAT Entertainment
@latimesent

Replying to @latimesent

Streaming platforms like HBO Max and Disney+ are struggling with a phenomenon known as "churn." We explain:

How fast do you cancel streaming services? It's a problem for Hollywood
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8:34 PM · Mar 28, 2021 · Twitter Web App

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Less costly to keep a customer than bring a new one

Prevent churn

Identify customer that are likely to cancel/quit/fail to renew

Bias vs Variance

"There are no free lunches in statistics"

- Not one method dominates others: Context/dataset dependent.
- Remember that the goal of prediction is to have a method that is accurate in predicting outcomes on previously unseen data.
  - Validation set approach: Training and testing data

Balance between flexibility and accuracy

Bias vs Variance

Variance

"[T]he amount by which f would change if we estimated it using a different training dataset"

Bias

"[E]rror introduced by approximating a real-life problem with a model"

Which models do you think are higher variance: More flexible models or less flexible models?

Bias vs. Variance: The ultimate battle

- In inference, bias >> variance
- In prediction, we care about both:
  - Measures of accuracy will have both bias and variance.

Trade-off at different rates

How do we measure accuracy?

Different measures:

- Remember $Adj - R^2$?
- Mean Squared Error (MSE): *Can be decomposed into variance and bias terms*

$$MSE = \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{f}(x_i))^2$$

How do we measure accuracy?

Different measures:

- Akaike Information Criterion (AIC): *Balances goodness of fit while penalizing for number of predictors*

$$AIC = 2(d+1) - 2\log(\hat{L}) \overset{OLS}{=} \frac{1}{n\hat{\sigma}^2}(RSS + 2d\hat{\sigma}^2)$$

- Bayesian Information Criterion (BIC): *Balances goodness of fit while penalizing for number of predictors*

$$BIC = (d+1)\log(n) - 2\log(\hat{L}) \overset{OLS}{=} \frac{1}{n\hat{\sigma}^2}(RSS + \log(n)d\hat{\sigma}^2)$$

where $\hat{\sigma}^2$: Estimate of the error variance (full model), d: Number of predictors, $\hat{L}$: Maximum likehood estimate.

Is flexibility always better?

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Example: Let's predict pre-churn!

- You work at Disney+ and you know that a good measure for someone at risk of unsubscribing is the times they've logged in the past week:

```
disney <- read.csv("https://raw.githubusercontent.com/maibennett/sta235/main/exampleSite/content/Cla

head(disney)
```

```
##   id female city age logins mandalorian unsubscribe
## 1  1      1    1  53     10           0           1
## 2  2      1    1  48      7           1           0
## 3  3      0    1  45      7           1           0
## 4  4      1    1  51      5           1           0
## 5  5      1    1  45     10           0           0
## 6  6      1    0  40      0           1           0
```

Two candidates: Simple vs Complex

- **Simple Model**:

$$logins_i = \beta_0 + \beta_1 \times mandalorian + \beta_2 \times city + \varepsilon_i$$

- **Complex Model**:

$$\begin{aligned} logins_i = & \beta_0 + \beta_1 \times mandalorian + \beta_2 \times age + \beta_3 \times age^2 + \\ & \beta_4 \times city + \beta_5 \times female + \varepsilon_i \end{aligned}$$

Create Validation Sets

```r
set.seed(100) #Always set seed for replication!

n <- nrow(disney)

train <- sample(1:n, n*0.8) #randomly select 80% of the rows for our training sample

train.data <- disney %>% slice(train)
test.data <- disney %>% slice(-train)
```

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Estimate Accuracy Measure

```
library(modelr)

lm_simple <- lm(logins ~ mandalorian + city, data = train.data)

lm_complex <- lm(logins ~ female + city + age + I(age^2) + mandalorian, data = train.data)

# For simple model:
rmse(lm_simple, test.data)
```

```
## [1] 2.089868
```

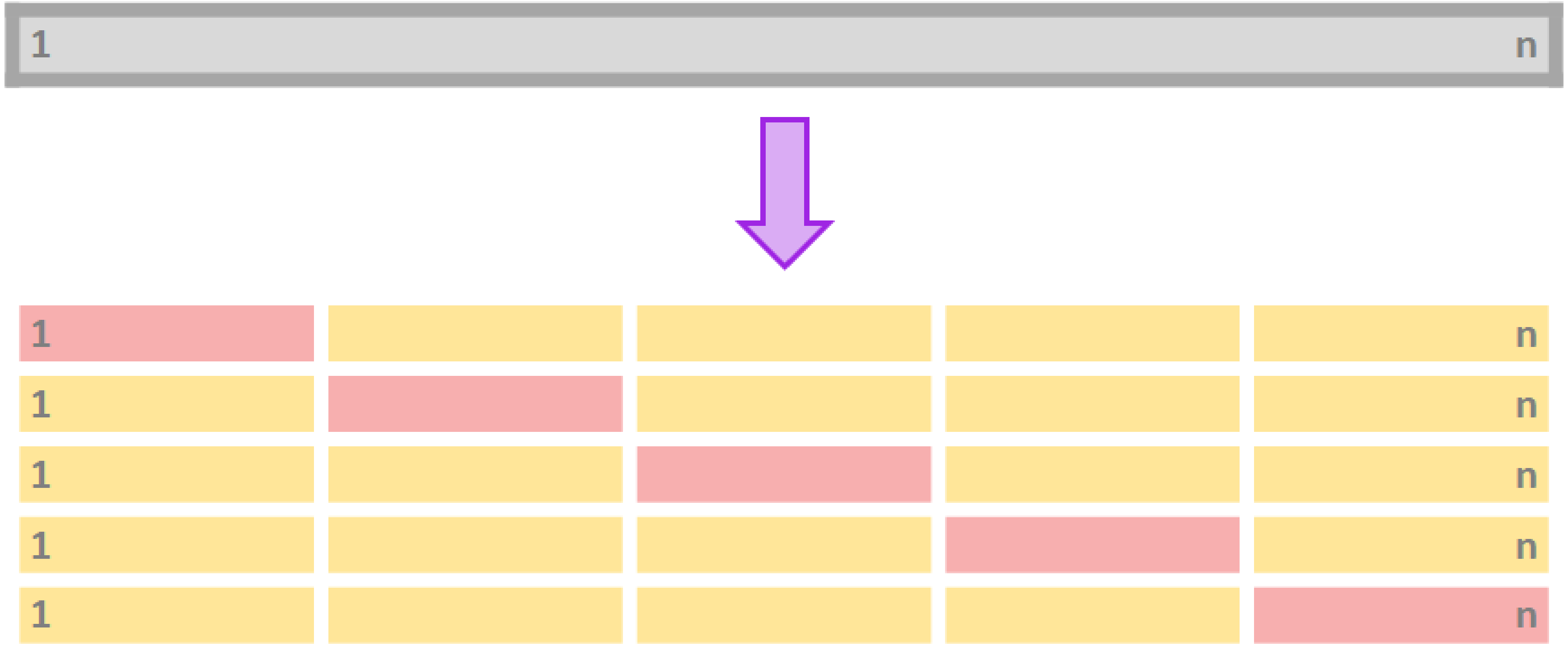
```
# For complex model:
rmse(lm_complex, test.data)
```

```
## [1] 2.093429
```

- Which one would you prefer?

Cross-Validation

- To avoid using only **one training and testing dataset**, we can iterate over *k-fold* division of our data:



Cross-Validation

Procedure for *k-fold* cross-validation:

1. Divide your data in *k-folds* (usually, $K = 5$ or $K = 10$).
2. Use $k = 1$ as the testing data and $k = 2, .., K$ as the training data.
3. Calculate the accuracy measure A_k on the testing data.
4. Repeat for each k.
5. Average A_k for all $k \in K$.

Main advantage: Use the entire dataset for training AND testing.

Extreme scenario: $K = n \rightarrow$ Leave One Out Cross-Validation (LOOCV)

How do we do CV in R?

```
library(caret)

set.seed(100)

train.control <- trainControl(method = "cv", number = 10)

lm_simple <- train(logins ~ mandalorian + city, data = disney, method="lm", trControl = train.contro

lm_simple
```

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lm_simple
```

```
## Linear Regression
##
## 5000 samples
##    2 predictor
##
## No pre-processing
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 4500, 4501, 4499, 4500, 4500, 4501, ...
## Resampling results:
##
##   RMSE      Rsquared   MAE
##   2.087314  0.6724741  1.639618
##
## Tuning parameter 'intercept' was held constant at a value of TRUE
```

Stepwise selection

- We have seen how to choose between some given models. **But what if we want to test all possible models?**
- **Stepwise selection**: Computationally-efficient algorithm to select a model based on the data we have (subset selection).

Algorithm for forward stepwise selection:

1. Start with the *null model*, M_0 (no predictors)
2. For $k = 0, \ldots, p-1$: (a) Consider all $p-k$ models that augment M_k with one additional predictor. (b) Choose the *best* among these $p-k$ models and call it M_{k+1}.
3. Select the single best model from $M_0, \ldots, M_p$ using CV.

Backwards stepwise follows the same procedure, but starts with the full model.

Will forward stepwise subsetting yield the same results as backwards stepwise selection?

How do we do stepwise selection in R?

```r
library(leaps)

regfit.fwd <- regsubsets(logins ~ . - unsubscribe, data=disney, method = "forward")
summary(regfit.fwd)
```

```
## Subset selection object
## Call: regsubsets.formula(logins ~ . - unsubscribe, data = disney, method = "forward")
## 5 Variables  (and intercept)
##             Forced in Forced out
## id              FALSE      FALSE
## female          FALSE      FALSE
## city            FALSE      FALSE
## age             FALSE      FALSE
## mandalorian     FALSE      FALSE
## 1 subsets of each size up to 5
## Selection Algorithm: forward
##          id  female city age mandalorian
## 1  ( 1 ) " " " "    " "  " " "*"
## 2  ( 1 ) " " " "    "*"  " " "*"
## 3  ( 1 ) " " " "    "*"  "*" "*"
## 4  ( 1 ) " " "*"    "*"  "*" "*"
## 5  ( 1 ) "*" "*"    "*"  "*" "*"
```

How do we do stepwise selection in R?

```r
set.seed(100)

train.control <- trainControl(method = "cv", number = 10) #set up a 10-fold cv

lm.fwd <- train(logins ~ . - unsubscribe, data = disney, method = "leapForward",
                tuneGrid = data.frame(nvmax = 1:5), trControl = train.control)
lm.fwd$results
```

```
##   nvmax     RMSE  Rsquared      MAE     RMSESD RsquaredSD      MAESD
## 1     1 2.273269 0.6113410 1.847755 0.04250683 0.01688996 0.04353289
## 2     2 2.087314 0.6724741 1.639618 0.04920703 0.01434646 0.04889721
## 3     3 2.087994 0.6722625 1.640315 0.04919353 0.01436182 0.04904907
## 4     4 2.088156 0.6722088 1.640489 0.04919301 0.01435653 0.04904416
## 5     5 2.088235 0.6721845 1.640525 0.04925197 0.01438207 0.04908729
```

- Which one would you choose out of the 5 models? Why?

How do we do stepwise selection in R?

```r
# We can see the number of covariates that is optimal to choose:
lm.fwd$bestTune
```

```
##   nvmax
## 2     2
```

```r
# And how does that model looks like:
summary(lm.fwd$finalModel)
```

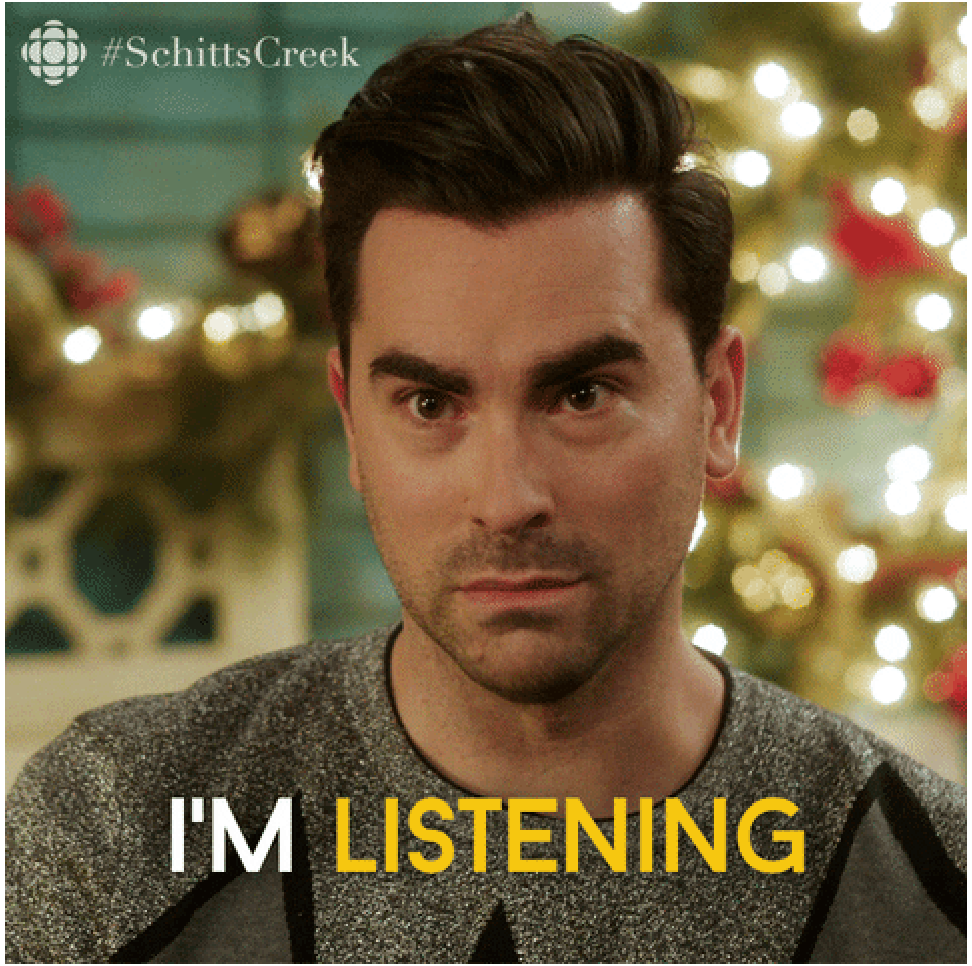
```
## Subset selection object
## 5 Variables  (and intercept)
##             Forced in Forced out
## id              FALSE      FALSE
## female          FALSE      FALSE
## city            FALSE      FALSE
## age             FALSE      FALSE
## mandalorian     FALSE      FALSE
## 1 subsets of each size up to 2
## Selection Algorithm: forward
##          id  female city age mandalorian
## 1  ( 1 ) " " " "    " "  " " "*"
## 2  ( 1 ) " " " "    "*"  " " "*"
```

```r
# If we want to recover the coefficient names, we can use the coef() function:
coef(lm.fwd$finalModel, lm.fwd$bestTune$nvmax)
```

```
## (Intercept)        city mandalorian
##    7.026494    2.577163   -6.265728
```

Takeaway points

- In prediction, everything is going to be about **bias vs variance**.
- Importance of **validation sets**.
- We have methods to **select models**.



Next class

- Continue with prediction and model selection
- **Shrinkage methods**:
  - Ridge regression and Lasso.

References

- James, G. et al. (2021). "Introduction to Statistical Learning with Applications in R". *Springer. Chapter 2, 5, and 6.*
- STDHA. (2018). "Stepwise Regression Essentials in R."
- STDHA. (2018). "Cross-Validation Essentials in R."