

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

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# 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.



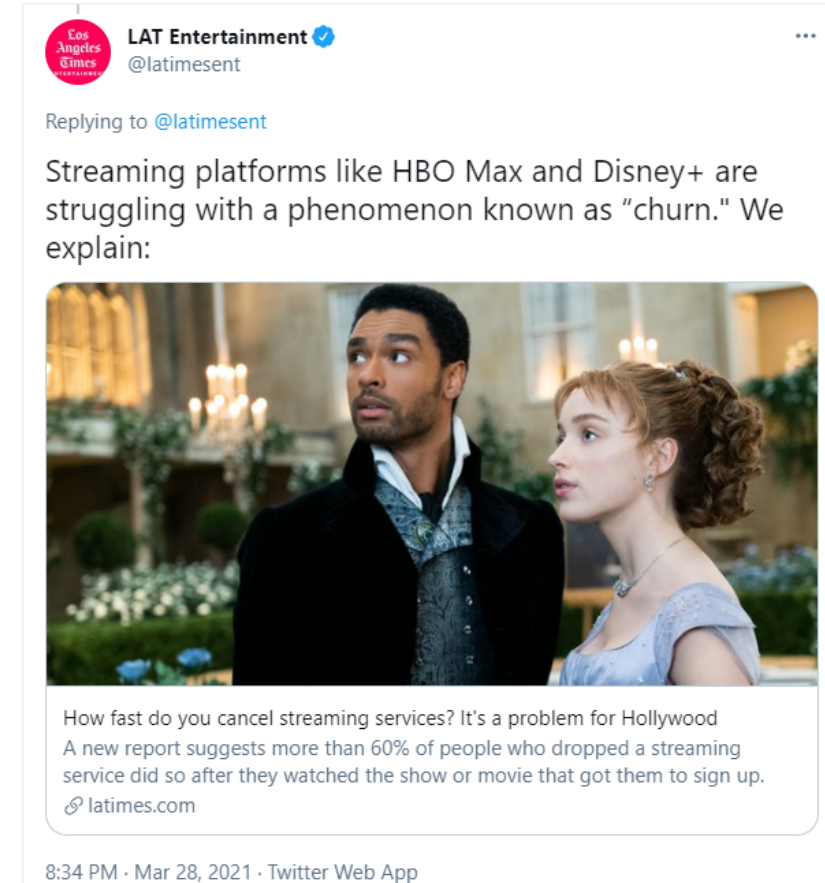
# Differences between inference and prediction

- Inference → focus on **covariate**
  - **Interpretability** of model.
- Prediction → focus on **outcome variable**
  - **Accuracy** of model.

**Both can be complementary!**

# Example: What is churn?

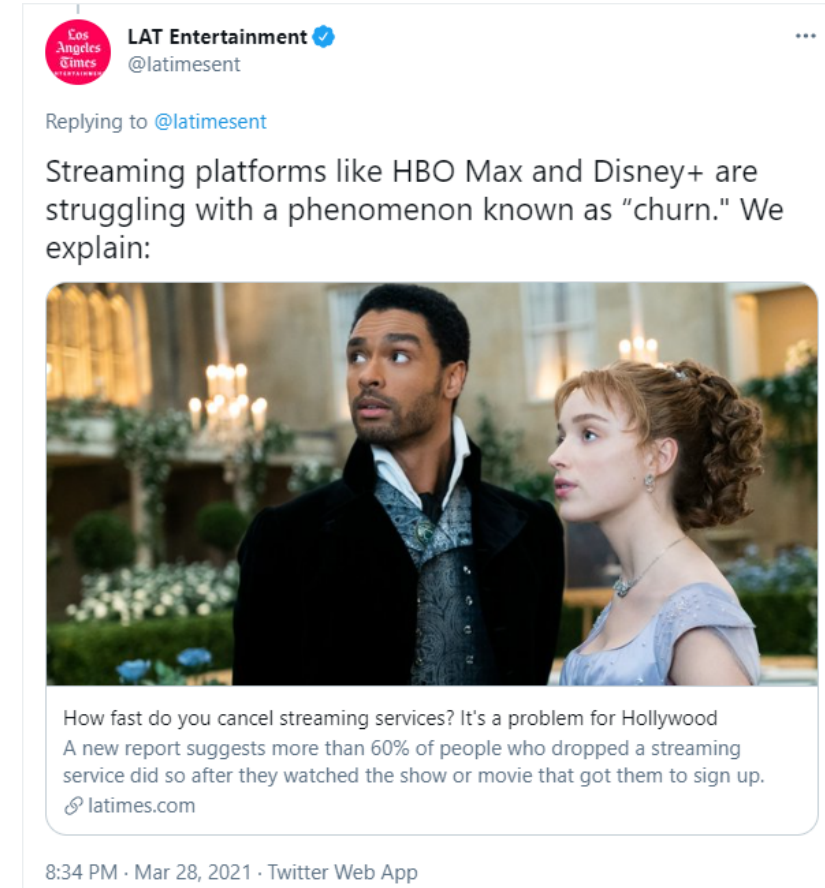
- **Churn:** Measure of how many customers stop using your product (e.g. cancel a subscription).



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**Less costly to keep a customer  
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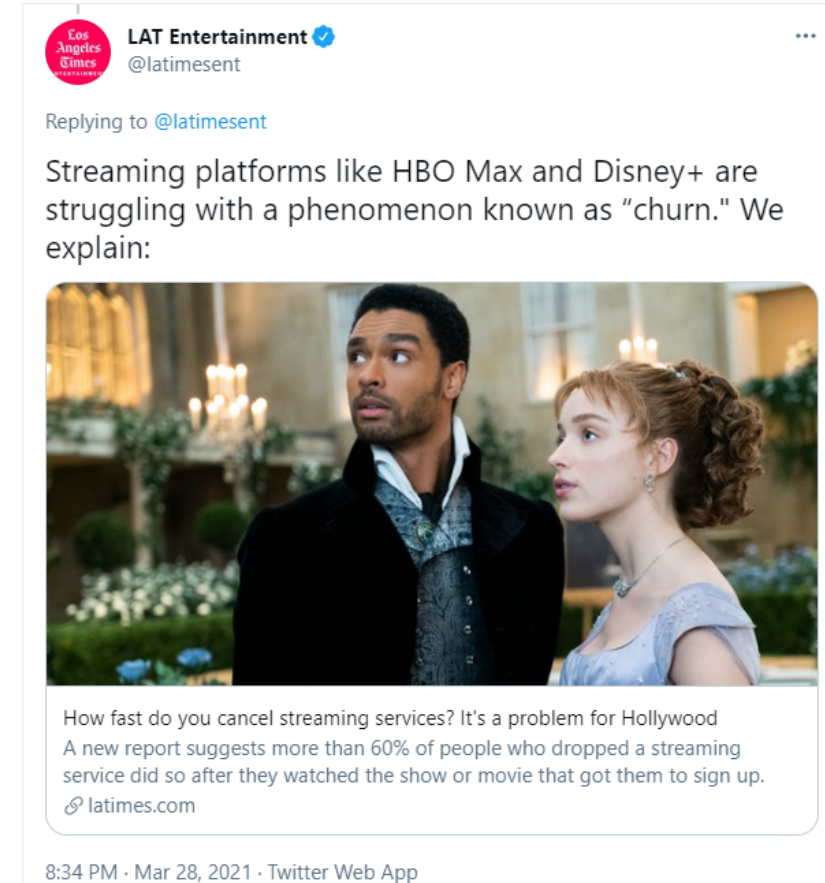


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- **Churn:** Measure of how many customers stop using your product (e.g. cancel a subscription).

**Less costly to keep a customer  
than bring a new one**

**Prevent churn**



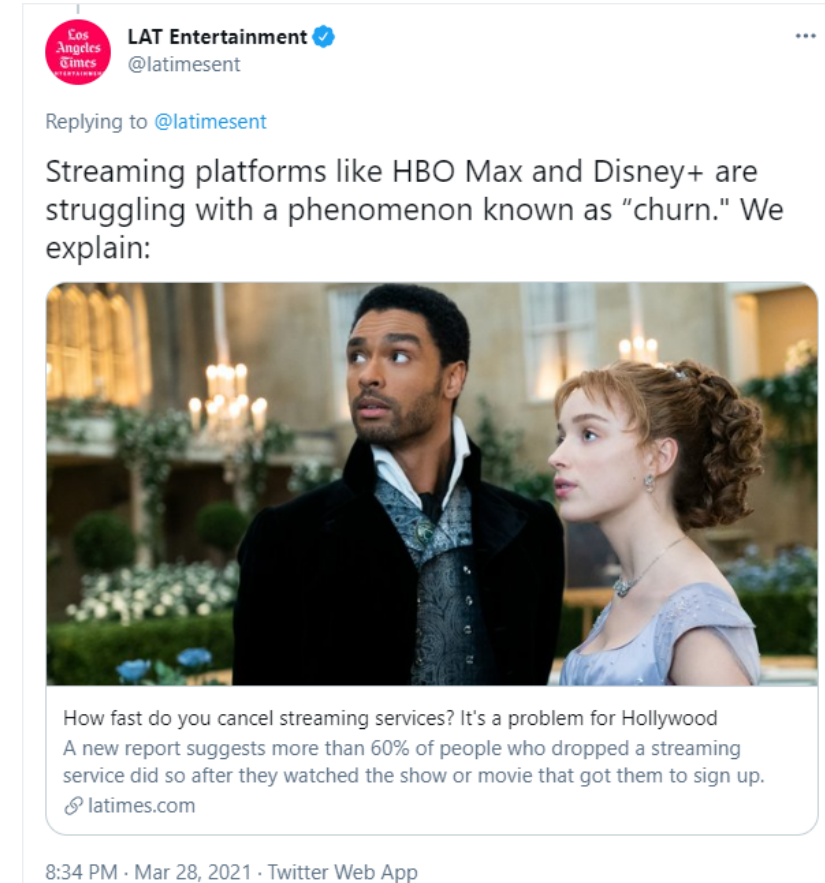
# Example: What is churn?

- **Churn:** Measure of how many customers stop using your product (e.g. cancel a subscription).

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*

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

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

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

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

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

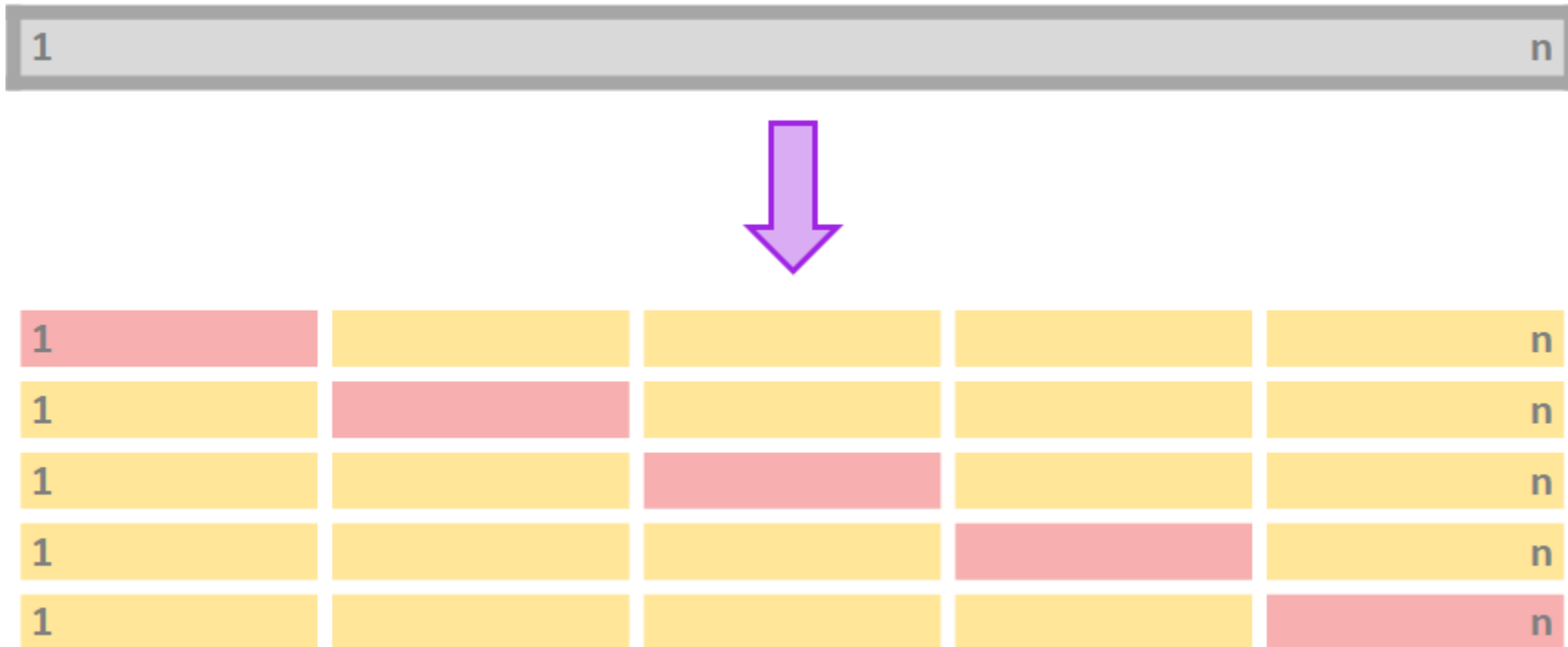
- Complex Model:

$$\logins_i = \beta_0 + \beta_1 \times mandalorian + \beta_2 \times age + \beta_3 \times age^2 + \beta_4 \times city + \beta_5 \times female + \varepsilon_i$$

**Let's go to R**

# 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  $k = 2, \dots, K$  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)

**Do you think 5-fold CV is better or worse than a 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.control)

lm_simple
```



# How do we do CV in R?

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library(caret)
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```
set.seed(100)
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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  $k = 0, \dots, p - 1$ : (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  $M_0, \dots, M_p$  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?

```
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?

```
set.seed(100)

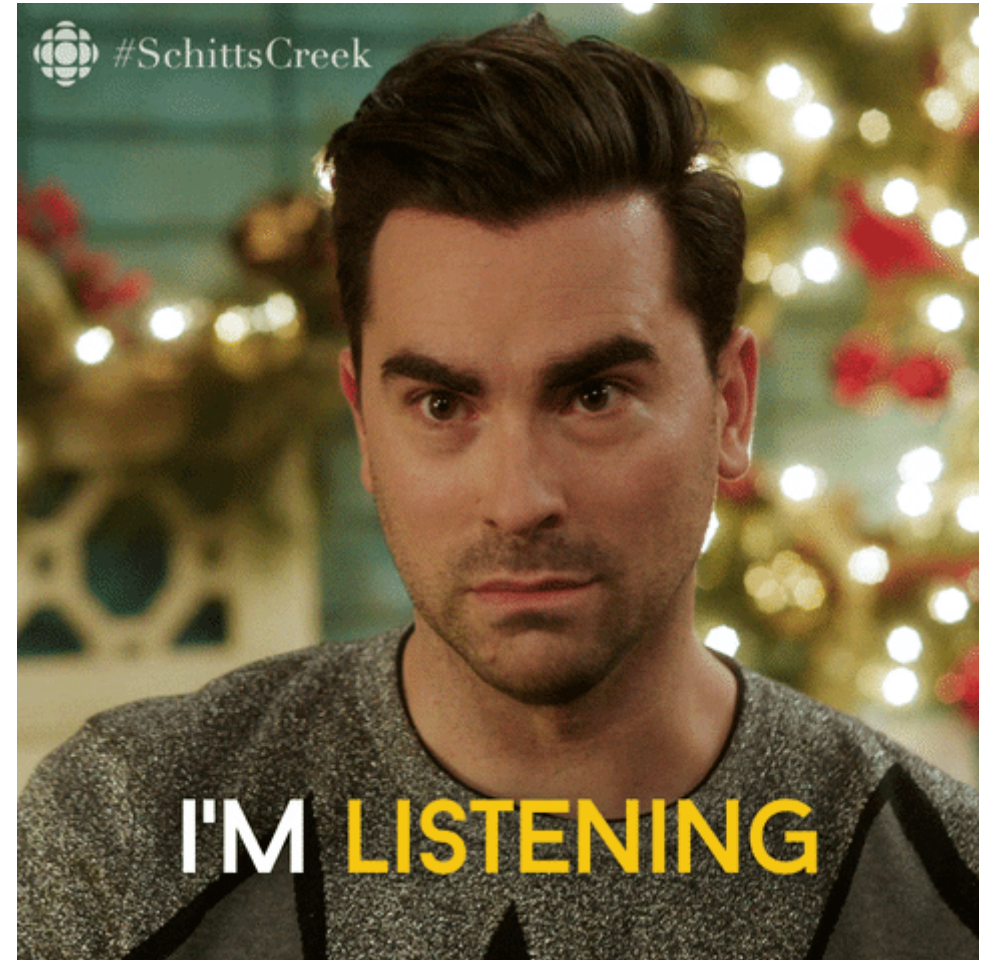
train.control <- trainControl(method = "cv", number = 10) #set up a 10-fold cv

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

# 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."