# Lesson 15: Model Building

With an emphasis on prediction

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# Learning Objectives

- 1. Understand the place of LASSO regression within association and prediction modeling for binary outcomes.
- 2. Recognize the process for tidymodels
- 3. Understand how penalized regression is a form of model/variable selection.
- 4. Perform LASSO regression on a dataset using R and the general process for classification methods.

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#### Some important definitions

- Model selection: picking the "best" model from a set of possible models
  - Models will have the same outcome, but typically differ by the covariates that are included, their transformations, and their interactions
  - "Best" model is defined by the research question and by how you want to answer it!

- Model selection strategies: a process or framework that helps us pick our "best" model
  - These strategies often differ by the approach and criteria used to the determine the "best" model

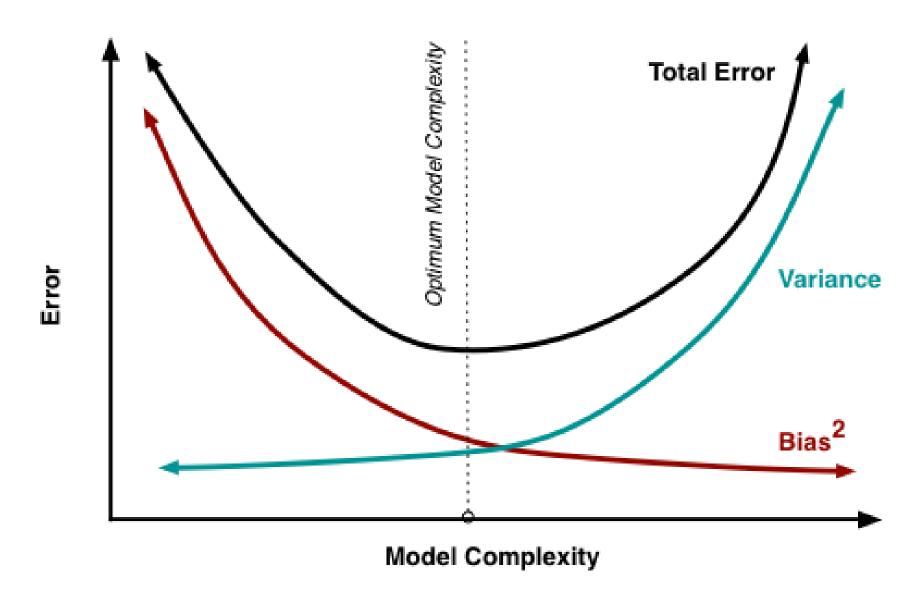
• Overfitting: result of fitting a model so closely to our *particular* sample data that it cannot be generalized to other samples (or the population)

#### Bias-variance trade off

 Recall from 512/612: MSE can be written as a function of the bias and variance

$$MSE = \mathrm{bias}ig(\widehat{eta}ig)^2 + \mathrm{variance}ig(\widehat{eta}ig)$$

- We no longer use MSE in logistic regression to find the best fit model, BUT the idea between the bias and variance trade off holds!
- For the same data:
  - More covariates in model: less bias, more variance
    - Potential overfitting: with new data does our model still hold?
  - Less covariates in model: more bias, less variance
    - More bias bc more likely that were are not capturing the true underlying relationship with less variables



Source: http://scott.fortmann-roe.com/docs/BiasVariance.html

### The goals of association vs. prediction

#### Association / Explanatory / One variable's effect

- Goal: Understand one variable's (or a group of variable's) effect on the response after adjusting for other factors
- Mainly interpret odds ratios of the variable that is the focus of the study

#### Prediction

- **Goal:** to calculate the most precise prediction of the response variable
- Interpreting coefficients is not important
- Choose only the variables that are strong predictors of the response variable
  - Excluding irrelevant variables can help reduce widths of the prediction intervals

#### Model selection strategies for categorical outcomes

#### Association / Explanatory / One variable's effect

 Selection of potential models is tied more with the research context with some incorporation of prediction scores

- Pre-specification of multivariable model
- Purposeful model selection
  - "Risk factor modeling"
- Change in Estimate (CIE) approaches
  - Will learn in Survival Analysis (BSTA 514)

#### Prediction

 Selection of potential models is fully dependent on prediction scores

- Logistic regression with more refined model selection
  - Regularization techniques (LASSO, Ridge, Elastic net)
- Machine learning realm
  - Decision trees, random forest, k-nearest neighbors, Neural networks

#### Before I move on...

- We CAN use purposeful selection from last quarter in any type of generalized linear model (GLM)
  - This includes logistic regression!

- The best documented information on purposeful selection is in the Hosmer-Lemeshow textbook on logistic regression
  - Textbook in student files is linked here
  - Purposeful selection starts on page 89 (or page 101 in the pdf)

- I will not discuss purposeful selection in this course
  - Be aware that this is a tool that you can use in any regression!

### Okay, so prediction of categorical outcomes

- Classification: process of predicting categorical responses/outcomes
  - Assigning a category outcome based on an observation's predictors

- Note: we've already done a lot of work around predicting probabilities within logistic regression
  - Can we take those predicted probabilities one step further to predict the binary outcome??

- Common classification methods (good site on brief explanation of each)
  - Logistic regression
  - Naive Bayes
  - k-Nearest Neighbor (KNN)
  - Decision Trees
  - Support Vector Machines (SVMs)
  - Neural Networks

### Logistic regression is a classification method

• But to be a good classifier, our logistic regression model needs to built a certain way

- Prediction depends on type of variable/model selection!
  - This is when it can become machine learning

- So the big question is: how do we select this model??
  - Regularized techniques, aka penalized regression

## Poll Everywhere Question 1

# Learning Objectives

1. Understand the place of LASSO regression within association and prediction modeling for binary outcomes.

#### 2. Recognize the process for tidymodels

- 3. Understand how penalized regression is a form of model/variable selection.
- 4. Perform LASSO regression on a dataset using R and the general process for classification methods.

### Before I get really into things!!

- tidymodels is a great package when we are performing prediction
- One problem: it uses very different syntax for model fitting than we are used to...
- tidymodels syntax dictates that we need to define:
  - A model
  - A recipe
  - A workflow

### tidymodels with GLOW

To fit our logistic regression model with the interaction between age and prior fracture, we use:

term	estimate	std.error	statistic	p.value	conf.low	conf.high
(Intercept)	-1.376	0.134	-10.270	0.000	-1.646	-1.120
age_c	0.063	0.015	4.043	0.000	0.032	0.093
priorfrac_Yes	1.002	0.240	4.184	0.000	0.530	1.471
age_c_x_priorfrac_Yes	-0.057	0.025	-2.294	0.022	-0.107	-0.008

#### Same as results from previous lessons

term	estimate	std.error	statistic	p.value	conf.low	conf.high
(Intercept)	-1.376	0.134	-10.270	0.000	-1.646	-1.120
priorfracYes	1.002	0.240	4.184	0.000	0.530	1.471
age_c	0.063	0.015	4.043	0.000	0.032	0.093
priorfracYes:age_c	-0.057	0.025	-2.294	0.022	-0.107	-0.008

#### Interaction model:

$$\begin{array}{ll} \text{logit}\left(\widehat{\pi}(\mathbf{X})\right) = \widehat{\beta}_0 & +\widehat{\beta}_1 \cdot I(\text{PF}) & +\widehat{\beta}_2 \cdot Age & +\widehat{\beta}_3 \cdot I(\text{PF}) \cdot Age \\ \text{logit}\left(\widehat{\pi}(\mathbf{X})\right) = -1.376 & +1.002 \cdot I(\text{PF}) & +0.063 \cdot Age & -0.057 \cdot I(\text{PF}) \cdot Age \end{array}$$

Reminder of main effects and interactions

# Learning Objectives

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### Penalized regression

- Basic idea: We are running regression, but now we want to incentivize our model fit to have less predictors
  - Include a penalty to discourage too many predictors in the model

• Also known as *shrinkage* or *regularization* methods

• Penalty will reduce coefficient values to zero (or close to zero) if the predictor does not contribute much information to predicting our outcome

- ullet We need a tuning parameter that determines the amount of shrinkage called lambda/ $\lambda$ 
  - How much do we want to penalize additional predictors?

## Poll Everywhere Question 2

### Three types of penalized regression

Main difference is the type of penalty used

#### Ridge regression

- Penalty called L2 norm, uses sqaured values
- Pros
  - Reduces overfitting
  - lacksquare Handles p>n
  - Handles collinearity
- Cons
  - Does not shrink coefficients to 0
  - Difficult to interpret

#### Lasso regression

 Penalty called L1 norm, uses absolute values

- Pros
  - Reduces overfitting
  - Shrinks coefficients to 0
- Cons
  - Cannot handle p > n
  - Does not handle multicollinearity well

#### Elastic net regression

- L1 and L2 used, best of both worlds
- Pros
  - Reduces overfitting
  - lacksquare Handles p>n
  - Handles collinearity
  - Shrinks coefficients to 0
- Cons
  - More difficult to do than other two

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## Overview of the process

1. Split data into training and testing datasets

- 2. Perform our classification method on training set
  - This is where we will use penalized regression!

3. Measure predictive accuracy on testing set

### Example to be used: GLOW Study

• From GLOW (Global Longitudinal Study of Osteoporosis in Women) study

• Outcome variable: any fracture in the first year of follow up (FRACTURE: 0 or 1)

- Risk factor/variable of interest: history of prior fracture (PRIORFRAC: 0 or 1)
- Potential confounder or effect modifier: age (AGE, a continuous variable)
  - Center age will be used! We will center around the rounded mean age of 69 years old

- Crossed out because we are no longer attached to specific predictors and their association with fracture
  - Focused on predicting fracture with whatever variables we can!

### Step 1: Splitting data

- Training: act of creating our prediction model based on our observed data
  - Supervised: Means we keep information on our outcome while training

• **Testing:** act of measuring the predictive accuracy of our model by trying it out on *new* data

- When we use data to create a prediction model, we want to test our prediction model on *new* data
  - Helps make sure prediction model can be applied to other data outside of the data that was used to create it!

• So an important first step in prediction modeling is to split our data into a training set and a testing set!

### Step 1: Splitting data

#### Training set

- Sandbox for model building
- Spend most of your time using the training set to develop the model
- Majority of the data (usually 80%)

#### Testing set

- Held in reserve to determine efficacy of one or two chosen models
- Critical to look at it once at the end, otherwise it becomes part of the modeling process
- Remainder of the data (usually 20%)

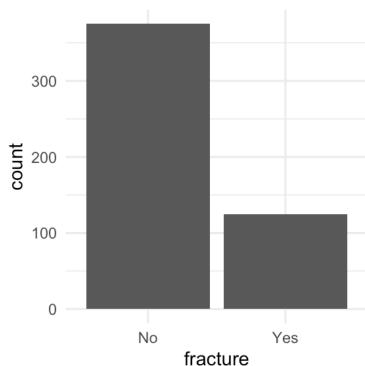
• Slide content from Data Science in a Box

## Poll Everywhere Question 3

#### Step 1: Splitting data

- When splitting data, we need to be conscious of the proportions of our outcomes
  - Is there imbalance within our outcome?
  - We want to randomly select observations but make sure the proportions of No and Yes stay the same
  - We stratify by the outcome, meaning we pick Yes's and No's separately for the training set

```
1 ggplot(glow1, aes(x = fracture)) + geom_bar()
```



- Side note: took out bmi and weight bc we have multicollinearity issues
  - Combo of I hate these variables and my previous work in the LASSO identified these as not important

```
1 glow = glow1 %>%
2 dplyr::select(-sub_id, -site_id, -phy_id, -age, -bmi, -weight)
```

### Step 1: Splitting data

- From package rsample within tidyverse, we can use initial\_split() to create training and testing data
  - Use strata to stratify by fracture

```
1 glow_split = initial_split(glow, strata = fracture, prop = 0.8)
2 glow_split
```

```
<Training/Testing/Total> <400/100/500>
```

Then we can pull the training and testing data into their own datasets

```
1 glow_train = training(glow_split)
2 glow_test = testing(glow_split)
```

### Step 1: Splitting data: peek at the split

#### 1 glimpse(glow\_train)

```
Rows: 400
Columns: 10
$ priorfrac <fct> No, No, Yes, No, No, Yes, No, Yes, Yes, No, No,
No, No, No, ...
          <int> 158, 160, 157, 160, 152, 161, 150, 153, 156, 166,
$ height
153, 160, ...
$ premeno
          No, No, No,...
$ momfrac
          <fct> No, No, Yes, No, No, No, No, No, No, No, Yes, No,
No, No, No...
$ armassist <fct> No, No, Yes, No, No, No, No, No, No, No, No, No,
Yes, No, No...
$ smoke
          <fct> No, No, No, No, Yes, No, No, No, Yes, No,
No, No, No...
$ raterisk <fct> Same, Same, Less, Less, Same, Same, Less, Same,
Same, Less, ...
$ fracscore <int> 1, 2, 11, 5, 1, 4, 6, 7, 7, 0, 4, 1, 4, 2, 2, 7,
2, 1, 4, 5,...
No, No, No, ...
$ age_c
          <dbl> -7, -4, 19, 13, -8, -2, 15, 13, 17, -11, -2, -5,
-1, -2, 0, ...
```

#### 1 glimpse(glow test)

```
Rows: 100
Columns: 10
$ priorfrac <fct> No, No, No, No, No, No, No, No, Yes, Yes, No, No,
No, No, No...
$ height
          <int> 167, 162, 165, 158, 153, 170, 154, 171, 142, 152,
166, 154, ...
$ premeno
          <fct> No, No, No, Yes, No, Yes, Yes, Yes, Yes, No, No,
No, No, No,...
$ momfrac
         <fct> No, No, No, No, Yes, No, No, Yes, No, No, No, No,
No, No, No...
$ armassist <fct> Yes, No, Yes, No, Yes, No, Yes, No, No, No, No,
No, No, No, ...
$ smoke
          No, No, No...
$ raterisk <fct> Same, Less, Less, Greater, Same, Same, Same, Same,
Same, Sam...
$ fracscore <int> 3, 1, 5, 1, 8, 3, 7, 1, 6, 7, 0, 2, 0, 0, 1, 2, 2,
8, 4, 3, ...
No, No, No, ...
          <dbl> -13, -10, 3, -8, 17, 0, 6, -5, 1, 17, -11, -6,
$ age c
-10, -12, -6, \dots
```

### Step 2: Fit LASSO penalized logistic regression model

- Using Lasso penalized regression!
- We can simply set up a penalized regression model

```
1 lasso_mod = logistic_reg(penalty = 0.001, mixture = 1) %>%
2
3 set_engine("glmnet")
```

- glmnet takes the basic fitting of glm and adds penalties!
  - In tidymodels we set an engine that will fit the model
- mixture option let's us pick the penalty
  - mixture = 0 for Ridge regression
  - mixture = 1 for Lasso regression
  - 0 < mixture < 1 for Elastic net regression</p>

#### Step 2: Fit LASSO: Main effects

```
glow_rec_main = recipe(fracture ~ ., data = glow_train) %>%

step_dummy(priorfrac, premeno, momfrac, armassist, smoke, raterisk)

glow_workflow_main = workflow() %>%

add_model(lasso_mod) %>% add_recipe(glow_rec_main)

glow_fit_main = glow_workflow_main %>% fit(glow_train)
```

### Step 2: Fit LASSO: Main effects: Identify variables

POS

NEG

POS

Looks like age is removed!

8 armassist Yes

5 smoke Yes

7 fracscore

9 height

3 priorfrac\_Yes 0.493

4 raterisk Same 0.438 POS

6 premeno Yes 0.285 POS

0.376

0.197

0.146 POS

0.0382 NEG

#### Step 2: Fit LASSO: Main effects + interactions

- We want to include interactions in our regression
- The main effect model will be our starting point
  - Otherwise, we may drop main effects but not their interactions
  - Cannot do that: see hierarchy principle
- I remove age\_c from this section because main effects did not include it

```
1 glow_rec_int = recipe(fracture ~ ., data = glow_train) %>%
2    update_role(age_c, new_role = "dont_use") %>%
3
4    step_dummy(priorfrac, premeno, momfrac, armassist, smoke, raterisk) %>%
5
6    step_interact(terms = ~ all_predictors():all_predictors())
7
8    glow_workflow_int = workflow() %>%
9         add_model(lasso_mod) %>% add_recipe(glow_rec_int)
10
11    glow_fit_int = glow_workflow_int %>% fit(glow_train)
```

### Step 2: Fit LASSO: Identify interactions

```
1 vi data int = glow fit int %>%
    pull workflow fit() %>%
     vi(lambda = 0.001) %>%
      filter(Importance != 0)
   vi data int
# A tibble: 34 \times 3
  Variable
                              Importance Sign
                                  <dbl> <chr>
  <chr>
                                   4.29 NEG
1 smoke Yes
 2 smoke Yes x raterisk Greater 3.89 POS
 3 smoke Yes x raterisk Same 3.14 POS
 4 premeno Yes x smoke Yes
                          3.00 NEG
 5 momfrac Yes_x_armassist_Yes 2.82 NEG
 6 priorfrac_Yes_x_premeno_Yes 2.50 NEG
 7 priorfrac Yes
                                  1.82 POS
 8 armassist Yes x smoke Yes
```

1.44 POS

1.31 POS

1.17 POS

This is where things got a little annoying for me...

9 premeno Yes x raterisk Greater

10 momfrac Yes x smoke Yes

# i 24 more rows

### Step 2: Fit LASSO: Identify interactions

• I combed through the column names of the results to find the interactions

```
1 vi data int$Variable
                                         "smoke_Yes_x_raterisk_Greater"
[1] "smoke Yes"
                                         "premeno Yes x smoke Yes"
[3] "smoke Yes x raterisk Same"
                                         "priorfrac Yes x premeno Yes"
    "momfrac Yes x armassist Yes"
    "priorfrac Yes"
                                         "armassist Yes x smoke Yes"
                                         "momfrac Yes x smoke Yes"
[9] "premeno Yes x raterisk Greater"
[11] "priorfrac Yes x momfrac Yes"
                                         "priorfrac Yes x armassist Yes"
                                         "momfrac_Yes_x_raterisk_Same"
[13] "premeno_Yes_x_armassist_Yes"
[15] "priorfrac_Yes_x_raterisk_Greater"
                                         "armassist Yes x raterisk Greater"
                                         "priorfrac Yes x smoke Yes"
[17] "fracscore x momfrac Yes"
                                         "fracscore x priorfrac Yes"
[19] "premeno_Yes_x_raterisk_Same"
    "fracscore_x_premeno_Yes"
                                         "raterisk Same"
    "fracscore"
                                         "fracscore_x_raterisk_Greater"
[23]
                                         "fracscore x smoke Yes"
    "armassist Yes x raterisk Same"
                                         "momfrac Yes x raterisk Greater"
[27]
    "height"
                                         "fracscore_x_raterisk_Same"
[29] "priorfrac Yes x raterisk Same"
                                         "height x premeno Yes"
[31] "height x raterisk Greater"
[33] "height x fracscore"
                                         "height x armassist Yes"
```

### Step 2: Fit LASSO: Identify interactions

- I combed through the column names of the results to find the interactions
  - I used ChatGPT to help me because I'm pretty new to tidymodels: let's view what I asked

### Step 2: Fit LASSO: Create recipe and fit model (from LASSO)

• This is not the typical procedure for LASSO, but the tidymodels framework for interactions did not let me keep all main effects when looking at my interactions

```
glow_rec_int2 = recipe(fracture ~ ., data = glow_train) %>%
     update role(age c, new role = "dont use") %>%
     step dummy(priorfrac, premeno, momfrac, armassist, smoke, raterisk) %>%
 5
     step interact(terms = interaction terms)
 6
   log model = logistic reg()
 9
10
   glow workflow int2 = workflow() %>%
11
         add model(log model) %>% add recipe(glow rec int2)
12
13 glow fit int2 = glow workflow int2 %>% fit(glow train)
```

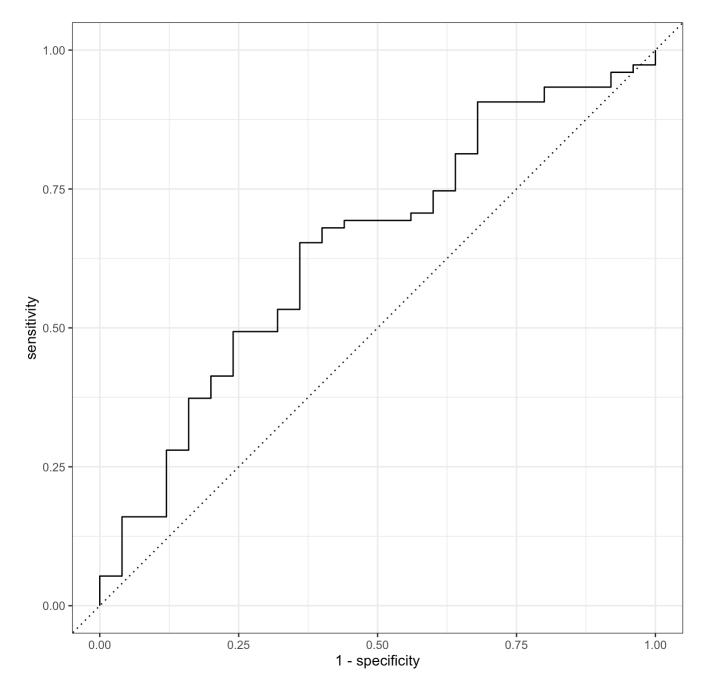
### Step 2: Fit LASSO: Look at model fit

	term	estimate	std.error	statistic	p.value
	<chr></chr>	<dbl></dbl>	<dbl></dbl>	<dbl></dbl>	<dbl></dbl>
1	(Intercept)	3.09	10.3	0.300	0.764
2	height	-0.0415	0.0637	-0.652	0.515
3	fracscore	-2.92	2.15	-1.36	0.175
4	priorfrac_Yes	15.1	8.61	1.75	0.0793
5	premeno_Yes	-0.805	1.14	-0.709	0.478
6	momfrac_Yes	-1.71	1.74	-0.984	0.325
7	armassist_Yes	18.5	10.7	1.73	0.0838
8	smoke_Yes	-22.8	838.	-0.0272	0.978
9	raterisk_Same	16.0	10.1	1.59	0.112
10	raterisk_Greater	1.13	9.16	0.123	0.902
11	height_x_fracscore	0.0215	0.0136	1.58	0.113
12	height_x_priorfrac_Yes	-0.0825	0.0531	-1.55	0.120
13	height_x_armassist_Yes	-0.114	0.0645	-1.77	0.0762
14	height_x_raterisk_Same	-0.0940	0.0623	-1.51	0.131
15	height_x_raterisk_Greater	0.00238	0.0563	0.0423	0.966
16	fracscore_x_priorfrac_Yes	-0.373	0.177	-2.10	0.0353
17	fracscore_x_momfrac_Yes	0.608	0.313	1.94	0.0520
18	fracscore_x_armassist_Yes	-0.111	0.178	-0.626	0.531
19	fracscore_x_smoke_Yes	0.604	0.564	1.07	0.284
20	fracscore_x_raterisk_Same	-0.257	0.209	-1.23	0.217
21	fracscore_x_raterisk_Greater	-0.318	0.212	-1.50	0.133
22	<pre>priorfrac_Yes_x_premeno_Yes</pre>	-2.72 Less	son 15: Mddel <b>Q</b> u <b>6</b> ding	-2.56	0.0104

23	priorfrac_Yes_x_momfrac_Yes	-1.35	1.35	-1.00	0.317
24	<pre>priorfrac_Yes_x_armassist_Yes</pre>	1.45	0.820	1.76	0.0779
25	priorfrac_Yes_x_smoke_Yes	-0.329	1.68	-0.196	0.845
26	<pre>priorfrac_Yes_x_raterisk_Same</pre>	0.122	0.837	0.146	0.884
27	<pre>priorfrac_Yes_x_raterisk_Greater</pre>	0.838	0.916	0.915	0.360
28	premeno_Yes_x_momfrac_Yes	0.304	1.58	0.192	0.848
29	premeno_Yes_x_armassist_Yes	1.73	0.923	1.87	0.0615
30	premeno_Yes_x_smoke_Yes	-3.98	1.84	-2.17	0.0300
31	premeno_Yes_x_raterisk_Same	0.716	1.16	0.620	0.535
32	premeno_Yes_x_raterisk_Greater	1.71	1.19	1.44	0.150
33	momfrac_Yes_x_armassist_Yes	-3.60	1.43	-2.52	0.0118
34	momfrac_Yes_x_smoke_Yes	2.73	2.67	1.02	0.307
35	momfrac_Yes_x_raterisk_Same	1.87	1.33	1.41	0.160
36	momfrac_Yes_x_raterisk_Greater	0.730	1.33	0.548	0.583
37	armassist_Yes_x_smoke_Yes	1.58	1.67	0.948	0.343
38	armassist_Yes_x_raterisk_Same	0.690	0.893	0.774	0.439
39	armassist_Yes_x_raterisk_Greater	-0.247	0.975	-0.253	0.800
40	<pre>smoke_Yes_x_raterisk_Same</pre>	19.5	838.	0.0232	0.981
41	smoke_Yes_x_raterisk_Greater	20.0	838.	0.0239	0.981
42	raterisk_Same_x_raterisk_Greater	NA	NA	NA	NA

## Poll Everywhere Question 4

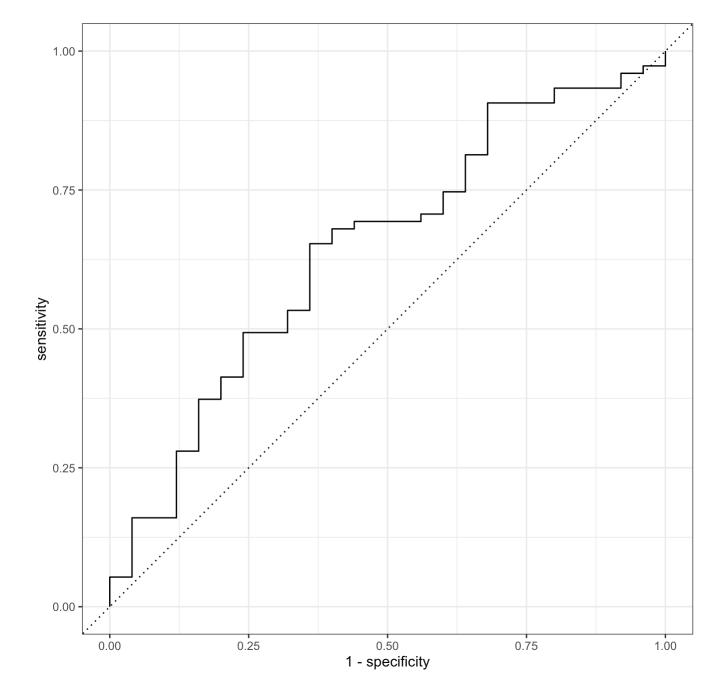
### Step 3: Prediction on testing set



### Step 3: Prediction on testing set

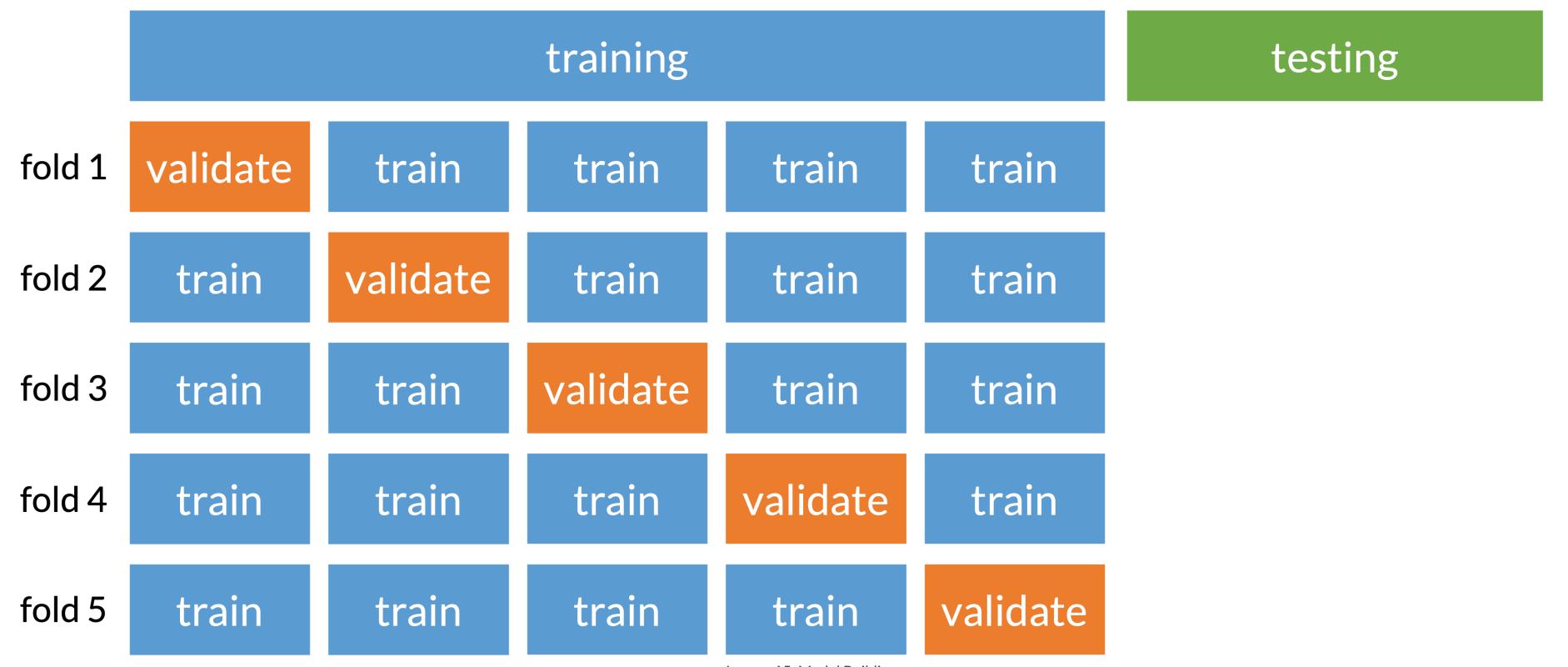
Why is this AUC worse than the one we saw with prior fracture, age, and their interaction?

- Only 1 training and testing set: can overfit training and perform poorly on testing
- We did not tune our penalty
- Our testing set only has 100 observations!



### Cross-validation (specifically k-fold)

- Prevents overfitting to one set of training data
- Split data into folds that train and validate model selection
- Basically subsection of training and testing (called validating) before truly testing on our original testing set



### Solutions / Resources (beyond our class right now)

- Use a tuning parameter for our penalty
  - Basically, we need to figure out what the best penalty is for our model
  - We use the training set to determine the best penality
  - Videos that includes tuning parameter with LASSO
    - TidyTuesday video on LASSO with interactions
- Cross-validation
  - Under Cross validation within Data Science in a Box
- For complete video of machine learning with LASSO, cross-validation, and tuning parameters
  - See "Unit 5 Deck 4: Machine learning" on this Data Science in a Box page
    - Video goes through an example with more complicated data, but can be followed with our work!

#### Summary

- Revisited model selection techniques and discussed how a binary outcome can be treated differently than a continuous outcome
- Discussed association vs prediction modeling
- Discussed classification: a type of machine learning!
- Introduced penalized regression as a classification method
- Performed penalized regression (specifically LASSO) to select a prediction model
- Process presented today has major flaws
  - We did not tune our parameter
  - We did not perform cross validation

### For your Lab 4

- You can use purposeful selection, like we did last quarter
  - If you want to focus on association modeling!
  - A good way to practice this again if you struggled with it previously

- You can try out LASSO regression
  - If you want to focus on prediction modeling!
  - And if you want to stretch your R coding skills