Lesson 15: Model Building

With an emphasis on prediction

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Lesson 15: Model Building

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

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

- 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 $\sqrt{\sim}$
 - "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



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Before I get really into things!!

gln.

- 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:



| | (|
|---------------|------------|
| · dus ~ | \searrow |
| FILL) | |
| (\uparrow) | |

| 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



| lenn | estimate : | stu.enoi | Statistic | p.value | COIII.IOW | com.mgn |
|--------------------|------------|----------|-----------|---------|-----------|---------|
| (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:



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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

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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

- We need a tuning parameter that determines the amount of shrinkage called lambda/ λ
 - 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 <u>L2 norm</u>, uses solution values
- Pros
 - Reduces overfitting
 - 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

A shrink vs regulized

- Pros
 - Reduces overfitting
 - Handles p > n
 - Handles collinearity
 - Shrinks coefficients to 0
- Cons
 - More difficult to do than other two

Desert vain frog



Arabian sand boa



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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**!

create nodel

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

2

- 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



- 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

ane -c

glow = glow1 %>%
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 <u>strata</u> to stratify by fracture



• 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) | 1 glimpse(glow_test) |
|---|---|
| Rows: 400 | Rows: 100 |
| Columns: 10 | Columns: 10 |
| <pre>\$ priorfrac <fct> No, No, Yes, No, No, Yes, No, Yes, Yes, No, No,</fct></pre> | <pre>\$ priorfrac <fct> No, No, No, No, No, No, No, No, Yes, Yes, No, No,</fct></pre> |
| No, No, | No, No, No… |
| \$ height <int> 158, 160, 157, 160, 152, 161, 150, 153, 156, 166,</int> | \$ height <int> 167, 162, 165, 158, 153, 170, 154, 171, 142, 152,</int> |
| 153, 160, | 166, 154, |
| \$ premeno <fct> No, No, No, No, No, No, No, No, No, No,</fct> | \$ premeno <fct> No, No, No, Yes, No, Yes, Yes, Yes, Yes, No, No,</fct> |
| No, No, No, | No, No, No, |
| \$ momfrac <fct> No, No, Yes, No, No, No, No, No, No, No, Yes, No,</fct> | <pre>\$ momfrac <fct> No, No, No, No, Yes, No, No, Yes, No, No, No,</fct></pre> |
| No, No, No… | No, No, No… |
| \$ armassist <fct> No, No, Yes, No, No, No, No, No, No, No, No, No, No</fct> | \$ armassist <fct> Yes, No, Yes, No, Yes, No, Yes, No, No, No, No, No,</fct> |
| Yes, No, No… | No, No, No, |
| \$ smoke <fct> No, No, No, No, Yes, No, No, No, Yes, No,</fct> | \$ smoke <fct> Yes, Yes, No, No, No, No, No, No, No, No, No, No</fct> |
| No, No, No… | No, No, No… |
| <pre>\$ raterisk <fct> Same, Same, Less, Less, Same, Same, Less, Same,</fct></pre> | <pre>\$ raterisk <fct> Same, Less, Less, Greater, Same, Same, Same, Same,</fct></pre> |
| Same, Less, … | Same, Sam |
| \$ fracscore <int> 1, 2, 11, 5, 1, 4, 6, 7, 7, 0, 4, 1, 4, 2, 2, 7,</int> | \$ fracscore <int> 3, 1, 5, 1, 8, 3, 7, 1, 6, 7, 0, 2, 0, 0, 1, 2, 2,</int> |
| 2, 1, 4, 5, | 8, 4, 3, |
| \$ fracture <fct> No, No, No, No, No, No, No, No, No, No,</fct> | \$ fracture <fct> No, No, No, No, No, No, No, No, No, No,</fct> |
| No, No, | No, No, No, … |
| \$ age_c <dbl> -7, -4, 19, 13, -8, -2, 15, 13, 17, -11, -2, -5,</dbl> | \$ age_c <dbl> -13, -10, 3, -8, 17, 0, 6, -5, 1, 17, -11, -6,</dbl> |
| -1, -2, 0, | -10, -12, -6, |





Step 2: Fit LASSO: Main effects: Identify variables

5 >0

| <pre>1 library(vip) 2 vi_data_main = glow fit_main %>% 3 pull_workflow fit() %>% 4 Vi(lambda = 0.001) % 5 filter(Importance != 0) 6 vi_data_main</pre> | vi: variable | importance |
|--|--------------|------------|
| # A tibble: 9 × 3 | | |
| | | |

| <chr></chr> | <db1></db1> | <chr></chr> |
|---|-------------|-------------|
| | 0.559 | POS |
| 2 momfrac_Yes | 0.542 | POS |
| 3 priorfrac_Yes | 0.493 | POS |
| | 0.438 | POS |
| 5 smoke_Yes | 0.376 | NEG |
| 6 premeno_Yes | 0.285 | POS |
| 7 fracscore | 0.197 | POS |
| 8 armassist_Yes | 0.146 | POS |
| 9 height | 0.0382 | NEG |
| | \sim | • |
| Looks like age is ren | noved! | |
| | | |

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





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

Step 2: Fit LASSO: Identify interactions

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

1 vi_data_int\$Variable

[1] "smoke Yes" [3] "smoke Yes x raterisk Same" "momfrac Yes x armassist Yes" [5] "priorfrac Yes" [7] "premeno Yes x raterisk Greater" [9] "priorfrac Yes x momfrac Yes" [11] "premeno Yes x armassist Yes" [13] "priorfrac Yes x raterisk Greater" [15] [17] "fracscore x momfrac Yes" "premeno Yes x raterisk Same" [19] "fracscore x premeno Yes" [21] "fracscore" [23] [25] "armassist Yes x raterisk Same" "height" [27] "priorfrac Yes x raterisk Same" [29] "height x raterisk Greater" [31] "height x fracscore" [33]

"priorfrac Yes x premeno Yes" "armassist Yes x smoke Yes" "momfrac Yes x smoke Yes" "priorfrac Yes x armassist Yes" "momfrac Yes x raterisk Same" "armassist Yes x raterisk Greater" "priorfrac_Yes_x_smoke Yes" "fracscore x priorfrac Yes" "raterisk Same" "fracscore x raterisk Greater" "fracscore x smoke Yes" "momfrac Yes x raterisk Greater" "fracscore x raterisk Same" "height x premeno Yes" "height x armassist Yes"

"smoke Yes x raterisk Greater"

"premeno Yes x smoke 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") %>%
 2
 3
     step dummy(priorfrac, premeno, momfrac, armassist, smoke, raterisk) %>%
 4
 5
     step interact(terms = interaction terms)
 6
   log model = logistic reg()
 8
 9
   glow workflow int2 = workflow() %>%
10
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

1 print(tidy(glow_fit_int2), n=60)

.

| # 1 | A tibble: 42 × 5 | | | | |
|-----|--------------------------------------|-------------|------------------------|-------------|-------------|
| | 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 | <pre>fracscore_x_priorfrac_Yes</pre> | -0.373 | 0.177 | -2.10 | 0.0353 |
| 17 | <pre>fracscore_x_momfrac_Yes</pre> | 0.608 | 0.313 | 1.94 | 0.0520 |
| 18 | <pre>fracscore_x_armassist_Yes</pre> | -0.111 | 0.178 | -0.626 | 0.531 |
| 19 | <pre>fracscore_x_smoke_Yes</pre> | 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 | priorfrac Yes x premeno Yes | -2.72 Less | son 15: Madel Buchling | -2.56 | 0.0104 |

| 23 | priorfrac_Yes_x_momfrac_Yes | -1.35 | 1.35 | -1.00 | 0.317 |
|----|---|--------|-------|--------|--------|
| 24 | priorfrac_Yes_x_armassist_Yes | 1.45 | 0.820 | 1.76 | 0.0779 |
| 25 | priorfrac_Yes_x_smoke_Yes | -0.329 | 1.68 | -0.196 | 0.845 |
| 26 | priorfrac_Yes_x_raterisk_Same | 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 | <pre>momfrac_Yes_x_armassist_Yes</pre> | -3.60 | 1.43 | -2.52 | 0.0118 |
| 34 | <pre>momfrac_Yes_x_smoke_Yes</pre> | 2.73 | 2.67 | 1.02 | 0.307 |
| 35 | <pre>momfrac_Yes_x_raterisk_Same</pre> | 1.87 | 1.33 | 1.41 | 0.160 |
| 36 | <pre>momfrac_Yes_x_raterisk_Greater</pre> | 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 | <pre>smoke_Yes_x_raterisk_Greater</pre> | 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

```
1 glow_test_pred = predict(glow_fit_int2, new_data = glow_test, type = "prob") %>%
2 bind cols(glow test)
```

```
1 glow_test_pred %>%
2 roc_auc(truth = fracture,
3 .pred_No)
```

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!

```
1 glow_test_pred %>%
```

```
2 roc_curve(truth = fracture, .pred_No) %>%
```

```
3 autoplot()
```



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