STA 235 - Model Selection II: Shrinkage

Spring 2021

McCombs School of Business, UT Austin

Some reminders

Homework 3 is due this Wednesday

No questions will be answered after 7pm 4/13

Some reminders (Cont.)

Highlight sessions on Thur. 5:00-5:30pm

- Same link every week.
- If you feel you are **falling behind**, I highly encourage you to attend.
- Same as last class, extra point will be given for **participation**:
    - That means **answering polls** AND **participating in class** (e.g. asking/answering a questions, etc.)

Coming soon: Prediction project

Data Challenge!

- Will be posted this week.
- You will be allowed to work **pairs**:
    - That means that your group can be one (1) or two (2) persons (I encourage you to find a partner).
    - **Don't email me asking me if you can be a group of 3, 4, etc.**

Continuing our journey

Last class:

- Bias vs Variance
- Validation sets and cross-validation
- Model selection: Stepwise

Today:

- Regularization and model selection: Shrinkage
- Prediction: K-nearest neighbors

Honey, I shrunk the coefficients!

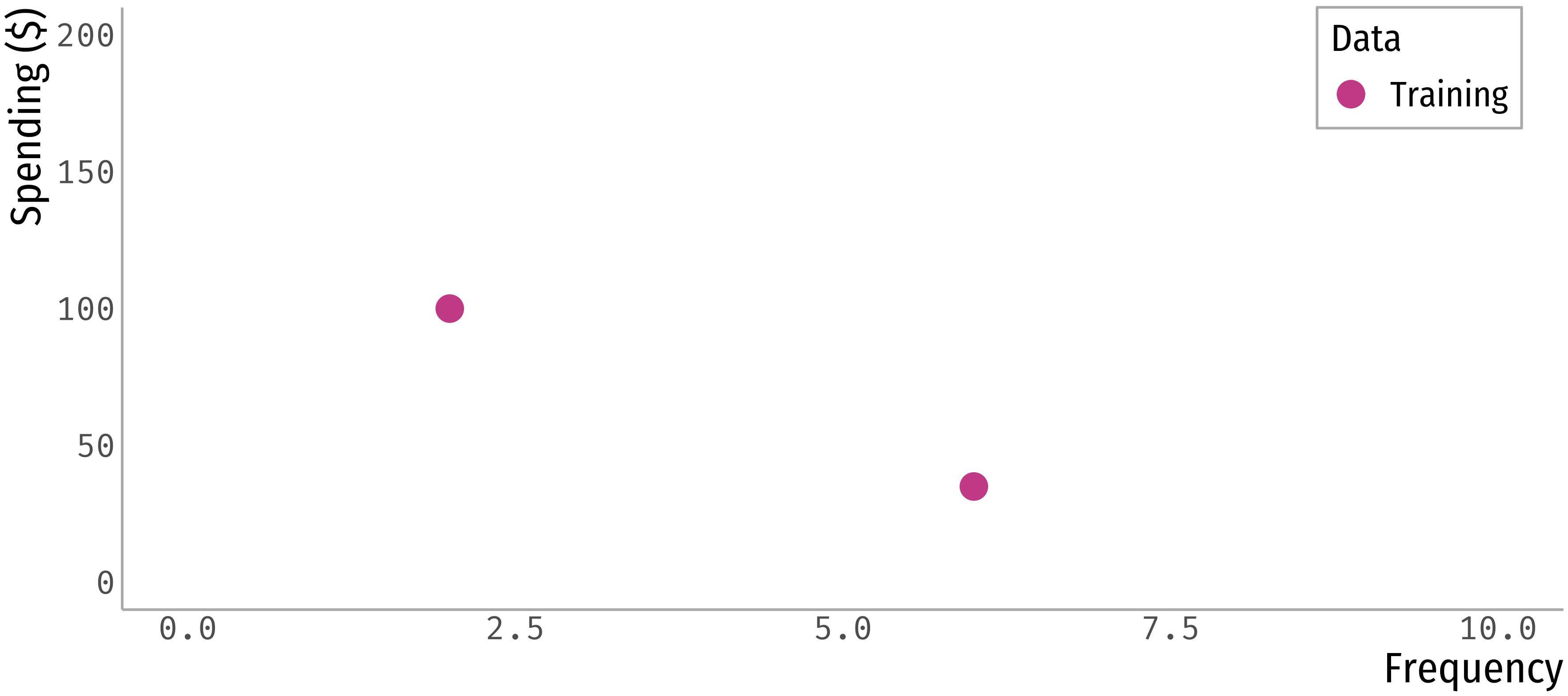
What is shrinkage?

- Last class, we saw **stepwise procedure**: Subsetting model selection approach.
    - Select k out of p total predictors
- **Shrinkage** *(a.k.a Regularization)*: Fitting a model with all p predictors, but introducing bias (i.e. shrinking coefficients towards 0) for improvement in variance.
    - Ridge regression
    - Lasso regression

Let's build a ridge.

Ridge Regression: An example

- Remember the JITT example? Window-shoppers vs. High rollers

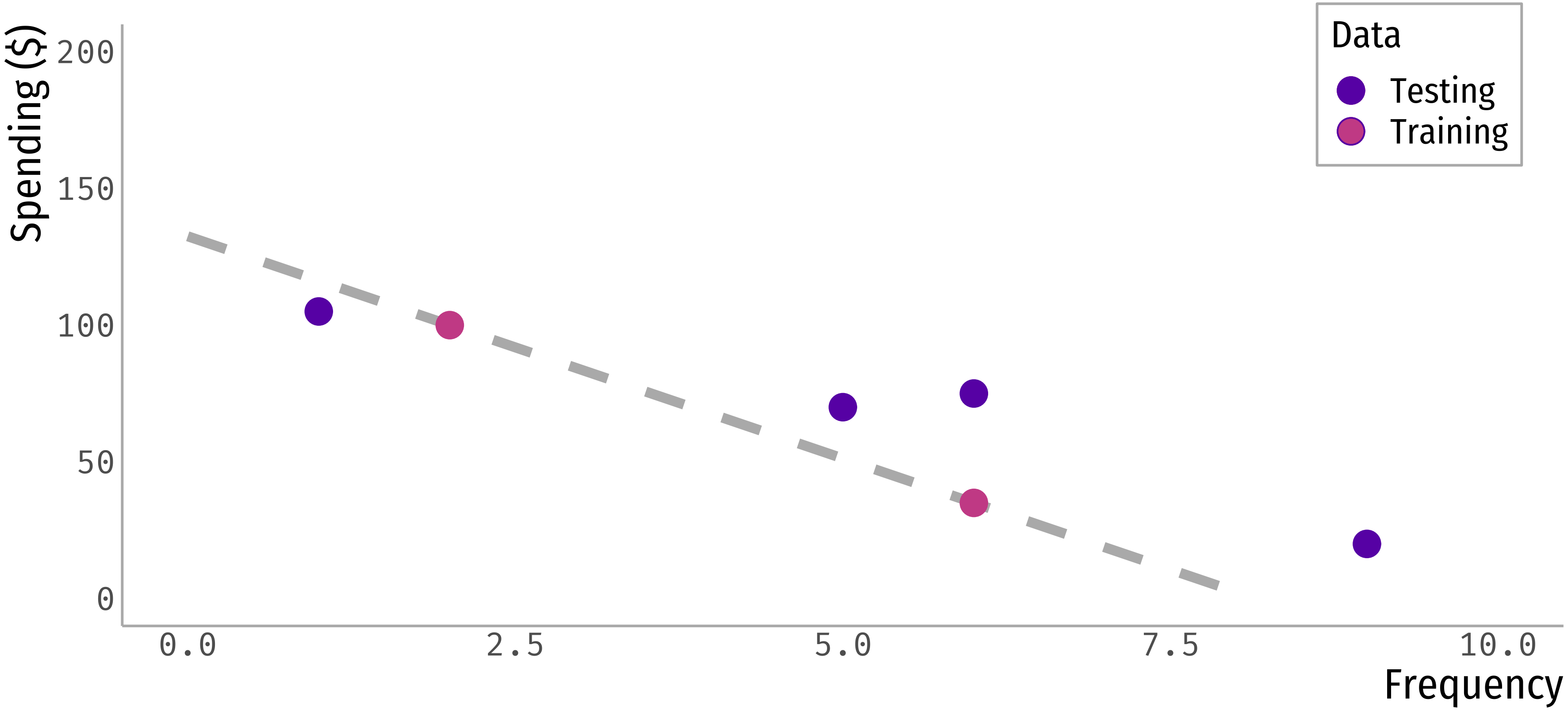


Ordinary Least Squares

- In an **OLS**: Minimize sum of squared-errors, i.e. $\min_\beta \sum_{i=1}^n (\mathbf{spend}_i - \mathbf{freq}_i \beta)^2$

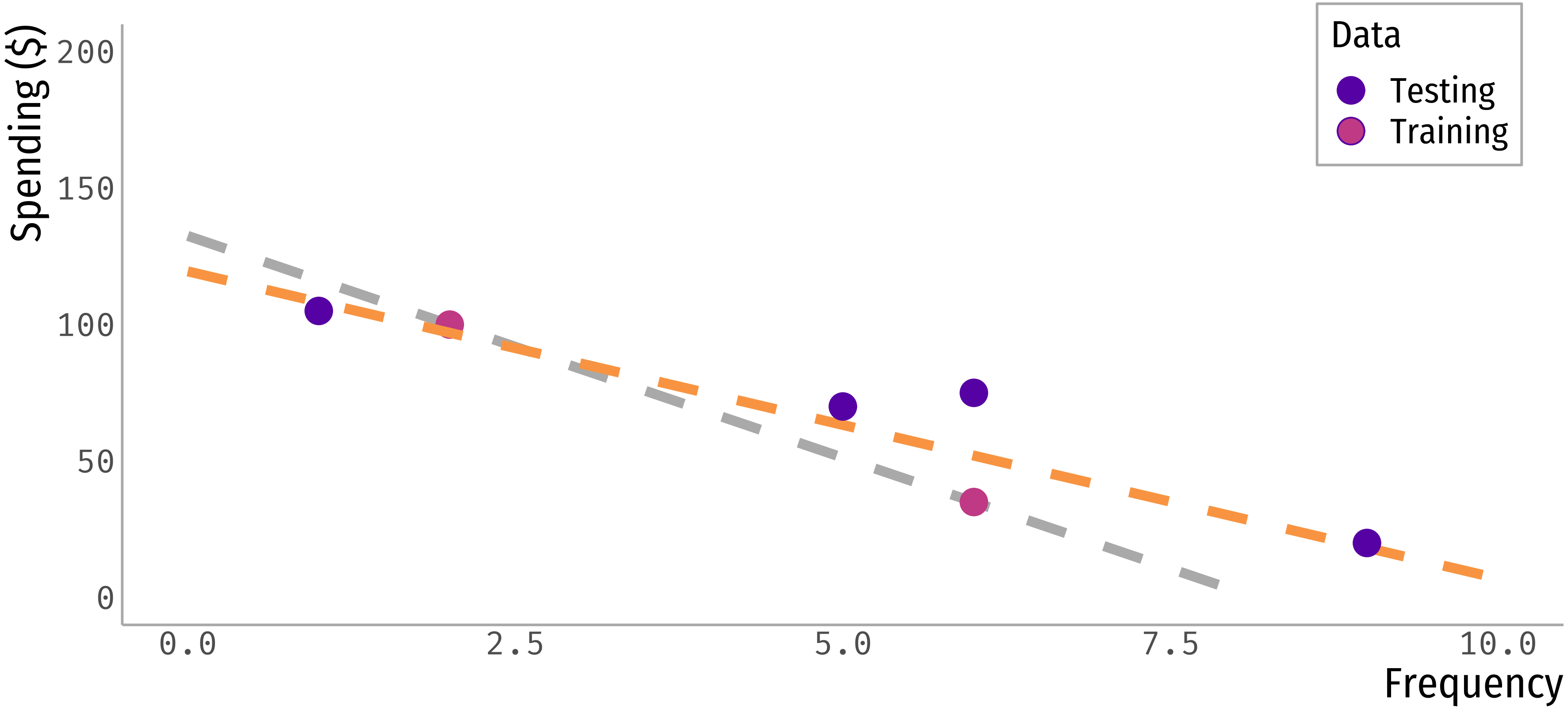
What about fit?

- Does the OLS fit the testing data well?



Ridge Regression

- Let's shrink the coefficients!: **Ridge Regression**



Poll time!

Why does Ridge Regression reduce its slope compared to OLS?

Ridge Regression: What does it do?

- Ridge regression **introduces bias to reduce variance** in the testing data set.
- In a simple regression (i.e. one regressor/covariate):

$$\min_{\beta} \sum_{i=1}^{n} \underbrace{(y_i - x_i\beta)^2}_{OLS}$$

Ridge Regression: What does it do?

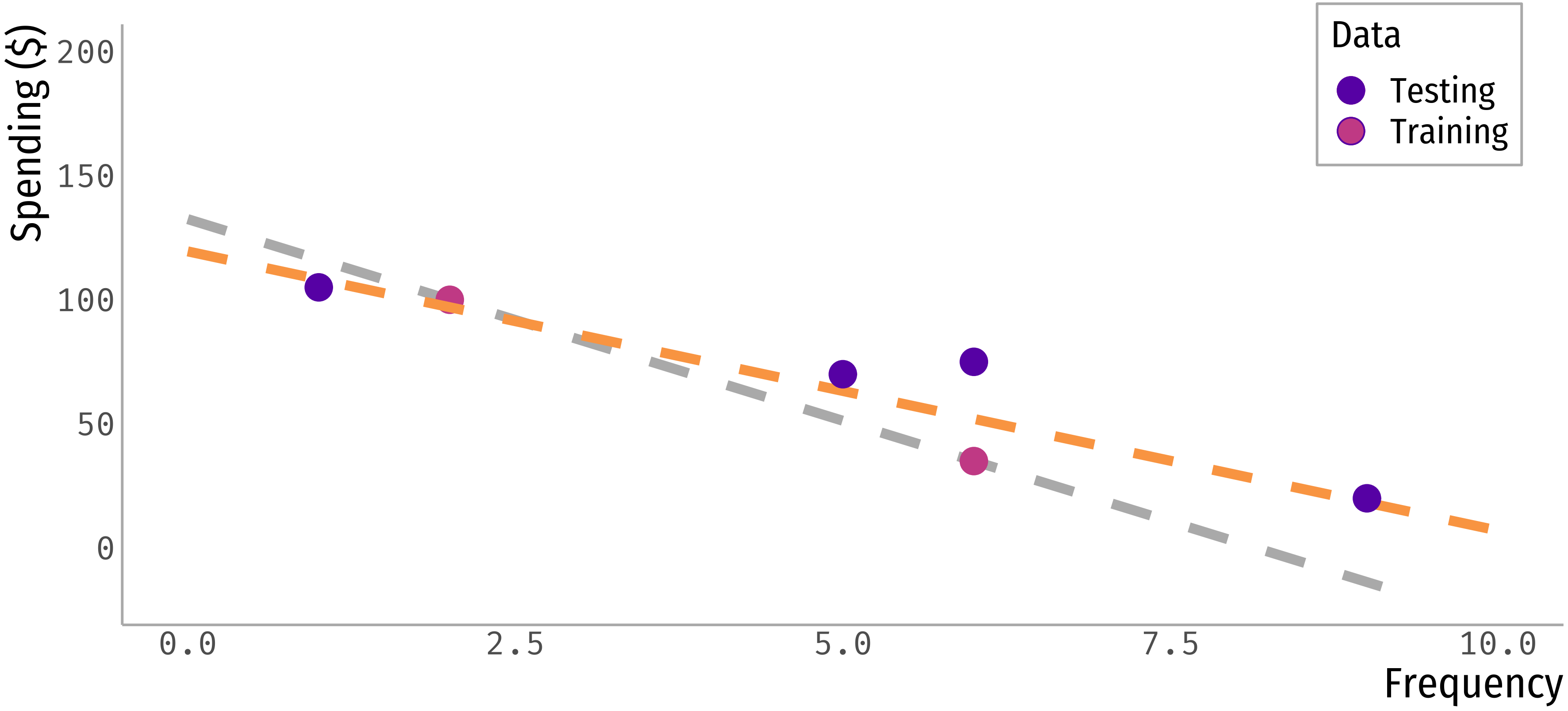
- Ridge regression **introduces bias to reduce variance** in the testing data set.
- In a simple regression (i.e. one regressor/covariate):

$$\min_{\beta} \sum_{i=1}^{n} \underbrace{(y_i - x_i\beta)^2}_{OLS} + \underbrace{\lambda \cdot \beta^2}_{RidgePenalty}$$

- λ is the **penalty factor** $\longrightarrow$ indicates how much we want to shrink the coefficients.

Back to the plots...

- Let's solve the minimization problem for ridge regression. **What line do we choose?**



For the OLS line

$$0 + \lambda \cdot (-16.25)^2 = 264.1\lambda$$

For the OLS line

$$0 + \lambda \cdot (-16.25)^2 = 264.1 \times 3 = 792.3$$

Now, for the ridge regression line

$$(3^2 + (-17)^2) + \lambda \cdot (-11.25)^2 = 298 + 126.6 \times 3 = 677.8$$

But remember... we care about accuracy in the testing dataset!

RMSE on the testing dataset: OLS

$$RMSE = \sqrt{\frac{1}{4}\sum_{i=1}^{4}(\text{spend}_i - (132.5 - 16.25 \cdot \text{freq}_i))^2} = 28.36$$

RMSE on the testing dataset: Ridge Regression

$$RMSE = \sqrt{\frac{1}{4}\sum_{i=1}^{4}(\text{spend}_i - (119.5 - 11.25 \cdot \text{freq}_i))^2} = 12.13$$

Poll time!

What problem is Ridge Regression looking to fix?

Ridge Regression in general

- For regressions that include **more than one regressor**:

$$\min_{\beta} \sum_{i=1}^{n} \underbrace{(y_i - \sum_{k=0}^{p} x_i \beta_k)^2}_{OLS} + \underbrace{\lambda \cdot \sum_{k=1}^{p} \beta_k^2}_{RidgePenalty}$$

- In our previous example, if we had two regressors, $female$ and $freq$:

$$\min_{\beta} \sum_{i=1}^{n} (\text{spend}_i - \beta_0 - \beta_1 \text{female}_i - \beta_2 \text{freq}_i)^2 + \lambda \cdot (\beta_1^2 + \beta_2^2)$$

- Because the ridge penalty includes the β's coefficients, **scale matters**:
  - Standardize coefficients to $SD = 1 \rightarrow x'_{ij} = \frac{x_{ij}}{\sqrt{\frac{1}{n}(x_{ij} - \bar{x}_j)^2}}$

Some jargon

- Ridge regression is also referred to as l_2 regularization:
  - l_2 norm $\rightarrow$ $||\beta||_2 = \sum_{k=1}^{p} \beta^2$
- Some important notes:
  - $||\hat{\beta}_\lambda^R||_2$ will always decrease in λ.
  - $||\hat{\beta}_\lambda^R||_2/||\hat{\beta}||_2$ will always decrease in λ.

Poll time!

If $\lambda=0$, what is the value of l_2 norm for the ridge regression over the l_2 norm of OLS?

How do we choose λ?

Cross-validation!

1) Choose a grid of λ values

2) Compute cross-validation error (e.g. RMSE) for each

3) Choose the smallest one.

λ vs RMSE?

λ vs RMSE? A zoom

How do we do this in R?

```
library(caret)

set.seed(100)

data <- read.csv("https://raw.githubuserconten

lambda_seq <- 10^seq(-3, 3, length = 100)

cv <- train(spend ~., data = train.data,
            method = "glmnet",
            preProcess = "scale",
            trControl = trainControl("cv", numl
            tuneGrid = expand.grid(alpha = 0,
                         lambda = lambda_seq)
  )

cv_lambda <- data.frame(lambda = cv$results$lar
                      rmse = cv$results$RMSE
```

- We will be using the `caret` package

How do we do this in R?

```r
library(caret)

set.seed(100)

data <- read.csv("https://raw.githubuserconten

lambda_seq <- 10^seq(-3, 3, length = 100)

cv <- train(spend ~., data = train.data,
            method = "glmnet",
            preProcess = "scale",
            trControl = trainControl("cv", numb
            tuneGrid = expand.grid(alpha = 0,
                          lambda = lambda_seq)
  )

cv_lambda <- data.frame(lambda = cv$results$lan
                        rmse = cv$results$RMSE
```

- We will be using the `caret` package
- We are doing **cross-validation**, so remember to set a seed!

How do we do this in R?

```
library(caret)

set.seed(100)

data <- read.csv("https://raw.githubuserconten

lambda_seq <- 10^seq(-3, 3, length = 100)

cv <- train(spend ~., data = train.data,
            method = "glmnet",
            preProcess = "scale",
            trControl = trainControl("cv", num
            tuneGrid = expand.grid(alpha = 0,
                         lambda = lambda_seq)
  )

cv_lambda <- data.frame(lambda = cv$results$la
                        rmse = cv$results$RMSE
```

- We will be using the `caret` package
- We are doing **cross-validation**, so remember to set a seed!
- You need to create a grid for the λ's **that will be tested**

How do we do this in R?

```
library(caret)

set.seed(100)

data <- read.csv("https://raw.githubuserconten

lambda_seq <- 10^seq(-3, 3, length = 100)

cv <- train(spend ~., data = train.data,
            method = "glmnet",
            preProcess = "scale",
            trControl = trainControl("cv", num
            tuneGrid = expand.grid(alpha = 0,
                                   lambda = lambda_seq)
  )

cv_lambda <- data.frame(lambda = cv$results$la
                        rmse = cv$results$RMSE
```

- We will be using the `caret` package
- We are doing **cross-validation**, so remember to set a seed!
- You need to create a grid for the λ's **that will be tested**
- The function we will use is `train`: Same as before
  - `method="glmnet"` means that it will run an elastic net.
  - `alpha=0` means is a **ridge regression**
  - `lambda = lambda_seq` is not necessary (you can provide your own grid)

How do we do this in R?

```
library(caret)

set.seed(100)

data <- read.csv("https://raw.githubuserconten

lambda_seq <- 10^seq(-3, 3, length = 100)

cv <- train(spend ~., data = train.data,
            method = "glmnet",
            preProcess = "scale",
            trControl = trainControl("cv", numl
            tuneGrid = expand.grid(alpha = 0,
                          lambda = lambda_seq)
  )

cv_lambda <- data.frame(lambda = cv$results$la
                        rmse = cv$results$RMSE
```

- We will be using the `caret` package
- We are doing **cross-validation**, so remember to set a seed!
- You need to create a grid for the λ's **that will be tested**
- The function we will use is `train`: Same as before
- Important objects in `cv`:
  - `results$lambda`: Vector of λ that was tested
  - `results$RMSE`: RMSE for each λ
  - `bestTune$lambda`: λ that minimizes the error term.

How do we do this in R?

OLS regression:

```
lm1 <- lm(spend ~ freq + female,
          data = train.data)

coef(lm1)
```

```
## (Intercept)        freq      female
## 118.2605090  -3.4339875  -0.6391956
```

```
pred.lm <- lm1 %>% predict(test.data)

RMSE(pred.lm, test.data$spend)
```

```
## [1] 22.79557
```

Ridge regression:

```
coef(cv$finalModel, cv$bestTune$lambda)
```

```
## 3 x 1 sparse Matrix of class "dgCMatrix"
##                       1
## (Intercept) 117.4837717
## freq         -9.4095221
## female       -0.2773666
```

```
pred.ridge <- cv %>% predict(test.data)

RMSE(pred.ridge, test.data$spend)
```

```
## [1] 22.7896
```

Throwing a lasso

Lasso regression

- Very similar to ridge regression, except it **changes the penalty term**:

$$\min_{\beta} \sum_{i=1}^{n} \underbrace{(y_i - \sum_{k=0}^{p} x_i \beta_k)^2}_{OLS} + \underbrace{\lambda \cdot \sum_{k=1}^{p} |\beta_k|}_{Lasso Penalty}$$

- In our previous example:

$$\min_{\beta} \sum_{i=1}^{n} (\text{spend}_i - \beta_0 - \beta_1 \text{female}_i - \beta_2 \text{freq}_i)^2 + \lambda \cdot (|\beta_1| + |\beta_2|)$$

- Lasso regression is also called l_1 regularization:

$$||\beta||_1 = \sum_{k=1}^{p} |\beta|$$

Ridge vs Lasso

Ridge

- Final model will have p coefficients
- Usually better with multicollinearity

Lasso

- Can set coefficients = 0
- Improves interpretability of model
- Can be used for model selection

And how do we do Lasso in R?

```r
library(caret)

set.seed(100)

data <- read.csv("https://raw.githubuserconten

lambda_seq <- 10^seq(-3, 3, length = 100)

cvl <- train(spend ~., data = train.data,
             method = "glmnet",
             trControl = trainControl("cv", numb
             tuneGrid = expand.grid(alpha = 1,
                                    lambda = lambda_seq)
  )

cvl_lambda <- data.frame(lambda = cvl$results$l
                         rmse = cvl$results$RMS
```

Exactly the same!

- … But change `alpha=1`!!

And how do we do Lasso in R?

Ridge regression:

```
coef(cv$finalModel, cv$bestTune$lambda)
```

```
## 3 x 1 sparse Matrix of class "dgCMatrix"
##                       1
## (Intercept) 117.4837717
## freq         -9.4095221
## female       -0.2773666
```

```
pred.ridge <- cv %>% predict(test.data)

RMSE(pred.ridge, test.data$spend)
```

```
## [1] 22.7896
```

Lasso regression:

```
coef(cvl$finalModel, cvl$bestTune$lambda)
```

```
## 3 x 1 sparse Matrix of class "dgCMatrix"
##                      1
## (Intercept) 117.032965
## freq         -3.296245
## female        .
```

```
pred.lasso <- cvl %>% predict(test.data)

RMSE(pred.lasso, test.data$spend)
```

```
## [1] 22.79291
```

Main takeway points

- You can **shrink coefficients** to introduce bias and decrease variance.
- Ridge and Lasso regression are **similar**:
    - Lasso can be used for model selection.
- Importance of understanding **how to estimate the penalty coefficient**.

References

- James, G. et al. (2013). "Introduction to Statistical Learning with Applications in R". *Springer. Chapter 6.*
- STDHA. (2018). "Penalized Regression Essentials: Ridge, Lasso & Elastic Net"