# Set 4: Linear Regression, Linear Algebra Review and The Bootstrap

STAT GU4206/GR5206 Statistical Computing & Introduction to Data Science

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#### Last Time

- Exploratory Data Analysis.
- Base R Graphics.

### Section I

### Class Notes

### Check Yourself (Warm Up)

#### Iris

- Use the built-in iris dataset:
- This famous (Fisher's or Anderson's) iris data set gives the measurements in centimeters of the variables sepal length and width and petal length and width, respectively, for 50 flowers from each of 3 species of iris. The species are Iris setosa, versicolor, and virginica.

### Check Yourself (Warm Up)

### Tasks: Plotting Data

Use the built-in iris dataset:

- Use the hist() function to plot a histogram of iris sepal width. Label the axes properly.
- Create a scatterplot of iris sepal width vs. iris sepal length. Color the points by whether or not the species is versicolor.
- Create side-by-side boxplots of iris petal length for each species.

### Example

A large national grocery retailer tracks productivity and costs of its facilities closely. Consider a data set obtained from a single distribution center for a one-year period. Each data point for each variable represents one week of activity. The variables included are number of cases shipped in thousands  $(X_1)$ , the indirect costs of labor as a percentage of total costs  $(X_2)$ , a qualitative predictor called holiday that is coded 1 if the week has a holiday and 0 otherwise  $(X_3)$ , and total labor hours (Y).

Suppose, as statisticians, we are asked to build a model to predict total labor hours in the future using this dataset.

### What information would be useful to provide such a model?

- Is there a relationship between holidays and total labor hours? What about number of cases shipped? Indirect costs?
- How strong are these relationships?
- Is the relationship linear?

Suppose, as statisticians, we are asked to build a model to predict total labor hours in the future using this dataset.

### What information would be useful to provide such a model?

- Is there a relationship between holidays and total labor hours? What about number of cases shipped? Indirect costs?
- How strong are these relationships?
- Is the relationship linear?

Multiple linear regression can be used to answer each of these questions.

Models a relationship between two or more **explanatory** variables and a **response** variable by fitting a linear equation to observed data.

General Model 
$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \dots + \beta_p X_p + \epsilon,$$
 with  $\epsilon \sim N(0, \sigma^2)$ .

- . Think of Xj as fixed (not random) . If  $X_{\bar{1}}$  is random, then we assume  $X_{\bar{1}}$  ind. of E

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with  $\epsilon \sim N(0, \sigma^2)$ .

Coefficient  $\beta_j$  quantifies the association between the predictor and the response.

Interpret  $\beta_j$  as the average effect on Y of one unit increase of  $X_j$ , holding all other predictors fixed.

#### Matrix Formulation

Using a set of training observations (data):  $(Y_i, X_{i1}, X_{i2}, \dots, X_{ip})$  for  $i = 1, 2, \dots, n$ , we want to estimate the model

$$Y_i = \beta_0 + \beta_1 X_{i1} + \beta_2 X_{i2} + \cdots + \beta_p X_{ip} + \epsilon_i,$$

with  $\epsilon \sim N(0, \sigma^2)$ . We can represent this with matrices as follows:

$$Y = X\beta + \epsilon, \qquad \begin{bmatrix} 1 & \chi_{11} & \chi_{12} & \cdots & \chi_{1p} \\ 1 & \chi_{21} & \chi_{22} & \cdots & \chi_{2p} \\ \vdots & \vdots & \ddots & \ddots \\ 1 & \chi_{n1} & \chi_{n2} & \cdots & \chi_{np} \end{bmatrix}$$

where

$$Y = (Y_1, Y_2, \dots, Y_n)^T \in \mathbb{R}^n, \quad X = \text{design matrix} \in \mathbb{R}^{n \times (p+1)}$$
  
 $\beta = (\beta_0, \beta_1, \dots, \beta_p)^T \in \mathbb{R}^{p+1}, \quad \epsilon = (\epsilon_1, \epsilon_2, \dots, \epsilon_n)^T \in \mathbb{R}^n.$ 



### The Training Set

Note that we refer to the observations as the **training data** because we will use these training data observations to **train**, or teach, our method how to estimate the model.

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Note that we refer to the observations as the **training data** because we will use these training data observations to **train**, or teach, our method how to estimate the model.

This is in contrast to the **test set** which is data that isn't used to estimate (or train) the model, but rather to test how well the model is at prediction.

### Example (Multiple Linear Regression Model)

$$Y_{\hat{i}} = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_3 + \epsilon_{\hat{i}} \quad \epsilon \sim N(0, \sigma^2)$$

#### where,

- Total labor hours (Y).
- Number of cases shipped (in thousands)  $(X_1)$ .
- Indirect costs of labor as a percentage of total costs  $(X_2)$ .
- Holiday (X<sub>3</sub>) with

$$X_{i3} = \begin{cases} 1 & \text{holiday week,} \\ 0 & \text{otherwise.} \end{cases}$$

### Example

Case	Y	<i>X</i> 1	<i>X</i> 2	<i>X</i> 3
1	4264	305.657	7.17	0
2	4496	328.476	6.20	0
3	4317	317.164	4.61	0
4	4292	366.745	7.02	0
5	4945	265.518	8.61	1
6	4325	301.995	6.88	0
:	:	:	:	:
48	4993	442.782	7.61	1
49	4309	322.303	7.39	0
50	4499	290.455	7.99	0
51	4186	411.750	7.83	0
52	4342	292.087	7.77	0

### Design Matrix

$$X = \begin{pmatrix} 1 & X_{11} & X_{12} & \cdots & X_{1p} \\ 1 & X_{21} & X_{22} & \cdots & X_{2p} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & X_{n1} & X_{n2} & \cdots & X_{np} \end{pmatrix}$$

What is the dimension of the design matrix?

#### Example

$$X = \begin{pmatrix} 1 & 305.657 & 7.17 & 0 \\ 1 & 328.476 & 6.20 & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 1 & 411.750 & 7.83 & 0 \\ 1 & 292.087 & 7.77 & 0 \end{pmatrix}$$

Using the training data, how do we estimate the parameters of the linear regression model? How do we find

$$\hat{\beta} = \left(\hat{\beta}_0, \hat{\beta}_1, \dots, \hat{\beta}_p\right)^T$$

which provide predictions

$$\hat{Y} = \hat{\beta}_0 + \hat{\beta}_1 X_1 + \hat{\beta}_2 X_2 + \dots + \hat{\beta}_p X_p?$$
 (1)

We say, how do we fit or how do we train the model?

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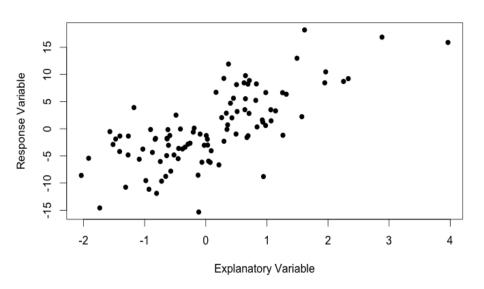
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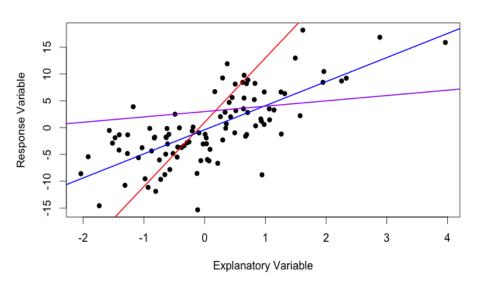
$$\hat{Y} = \hat{\beta}_0 + \hat{\beta}_1 X_1 + \hat{\beta}_2 X_2 + \dots + \hat{\beta}_p X_p?$$
 (1)

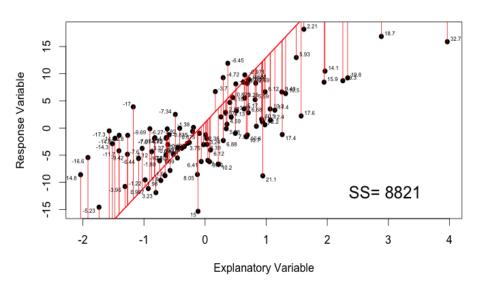
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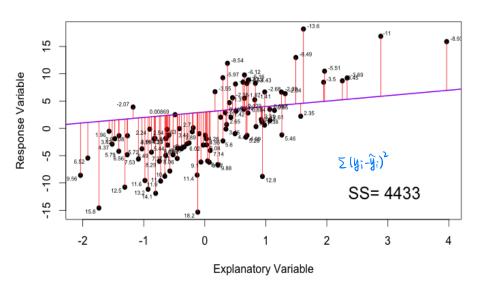
### Least Squares Estimate

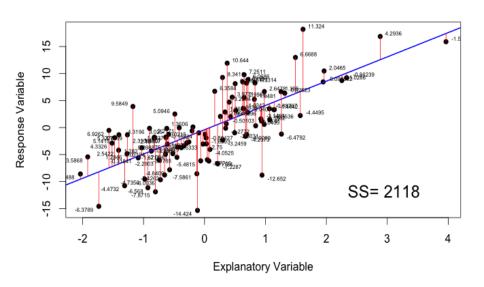
The **least squares line** is calculated from the training data by minimizing the sum of the squares of the vertical deviations from each data point to the line.











#### Least Squares Estimate

Define an objective function Q(b) as follows.

$$Q(b_0,b_1,\ldots,b_p):=\sum_{i=1}^n(Y_i-(b_0+b_1X_{i1}+b_2X_{i2}+\cdots+b_pX_{ip}))^2$$

$$=\|Y-Xb\|^2, \text{ Vector in }\omega I(\underline{X})$$

which we minimize with respect to  $b = (b_0, b_1, b_2, \dots, b_p) \in \mathbb{R}^{p+1}$ .



#### **Theorem**

If design matrix X has full column rank, then the global minimizer of

$$Q(b) = \|Y - Xb\|^2$$

with respect to  $b = (b_0, b_1, \dots, b_{p-1})^T$  is

$$\hat{\beta} = (X^T X)^{-1} X^T Y.$$

#### To come:

- What do we mean by full column rank?
- Is there a geometric interpretation of this result?

#### Sketch of Theorem Proof

First note,

$$Q(b) = ||Y - Xb||^{2} = (Y - Xb)^{T} (Y - Xb)$$
  
=  $Y^{T} Y - Y^{T} Xb + (Xb)^{T} Y + (Xb)^{T} Xb$   
=  $b^{T} X^{T} Xb - 2Y^{T} Xb + Y^{T} Y$ .

Taking the first derivative of Q(b) with respect to b and equating the derivative equal to zero gives

$$2X^TXb - 2X^TY = 0.$$

Solving the expression for b yields  $b = (X^T X)^{-1} X^T Y$ .

The second derivative is a positive definite matrix which implies that Q(b) achieves its minimum at  $\hat{\beta} = (X^T X)^{-1} X^T Y$ .

### Example

```
> Grocery <- read.table("Kutner_6_9.txt", header=T)
> head(Grocery)
```

```
Y X1 X2 X3
1 4264 305.657 7.17 0
2 4496 328.476 6.20 0
3 4317 317.164 4.61 0
4 4292 366.745 7.02 0
5 4945 265.518 8.61 1
6 4325 301.995 6.88 0
```

```
> # Construct design matrix
> X <- cbind(rep(1,52), Grocery$X1, Grocery$X2, Grocery$X3)
```

### Example

```
Least Square Estimator: \hat{\beta} = (X^T X)^{-1} X^T Y
```

```
> beta_hat <- solve((t(X) %*% X)) %*% t(X) %*% Grocery$Y
> round(t(beta_hat), 2)
```

```
[,1] [,2] [,3] [,4]
[1,] 4149.89 0.79 -13.17 623.55
```

What is the estimated model?

### Example

Least Square Estimator: 
$$\hat{\beta} = (X^T X)^{-1} X^T Y$$

> beta\_hat <- solve((t(X) %\*% X)) %\*% t(X) %\*% Grocery\$Y
> round(t(beta\_hat), 2)

What is the estimated model?

$$\hat{Y} = 4149.89 + 0.79X_1 - 13.17X_2 + 623.56X_3$$
 
$$\widehat{\text{Labor.Hours}} = 4149.89 + 0.79 \times \text{Cases.Shipped}$$
 
$$-13.17 \times \text{Indirect.Costs} + 623.56 \times \text{Holiday}.$$

#### Estimated Model:

$$\widehat{\mathsf{Labor.Hours}} = 4149.89 + 0.79 \times \mathsf{Cases.Shipped} \\ -13.17 \times \mathsf{Indirect.Costs} + 623.56 \times \mathsf{Holiday}.$$

### **Example: Prediction**

How many labor hours does our model predict for a **holiday** week with **350000 cases** shipped and indirect costs at **8.5 percent**?

#### Estimated Model:

$$\widehat{\mathsf{Labor.Hours}} = 4149.89 + 0.79 \times \mathsf{Cases.Shipped} \\ -13.17 \times \mathsf{Indirect.Costs} + 623.56 \times \mathsf{Holiday}.$$

#### **Example: Prediction**

How many labor hours does our model predict for a **holiday** week with **350000 cases** shipped and indirect costs at **8.5 percent**?

Labor. Hours = 
$$4149.89 + 0.79(350000) - 13.17(8.5) + 623.56(1)$$
  
=  $4938.01$  hours .

### Fitting Linear Models in R

lm(formula,data) is used to fit linear models.

### Example

```
> lm0 <- lm(Y ~ X1 + X2 + X3, data = Grocery)
> lm0
```

#### Call:

```
lm(formula = Y ~ X1 + X2 + X3, data = Grocery)
```

#### Coefficients:

(Intercept) X1 X2 X3 4149.8872 0.7871 -13.1660 623.5545

#### Fitted Values and Residuals

• The  $i^{th}$  fitted value is denoted  $\hat{Y}_i$  and defined by

$$\hat{Y}_i = \hat{\beta}_0 + \hat{\beta}_1 X_{i1} + \hat{\beta}_2 X_{i2} + \dots + \hat{\beta}_{p-1} X_{i,p-1}.$$

• Denote the fitted values by the  $n \times 1$  vector

$$\hat{Y} = (\hat{Y}_1, \hat{Y}_2, \dots, \hat{Y}_n)^T = X\hat{\beta}.$$

- The  $i^{th}$  residual denoted  $e_i$  is the difference between the actual response value and its corresponding fitted value:  $e_i = Y_i \hat{Y}_i$ .
- Denote the residuals by the  $n \times 1$  vector

$$e = (e_1, e_2, \dots, e_n)^T = Y - \hat{Y}.$$

#### Fitted Values and Residuals

### For an estimated linear model in R,

- Compute residuals with residuals().
- Compute **fitted values** with fitted().

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### Example

```
> lm0 <- lm(Y ~ X1 + X2 + X3, data = Grocery)
```

1 2 3 4 5 4296.063 4326.795 4338.825 4346.120 4869.066

# **Model Summary**

```
> summary(lm0)
Residuals:
   Min 1Q Median 3Q
                           Max
-264.05 -110.73 -22.52 79.29 295.75
Coefficients:
          Estimate Std. Error t value Pr(>|t|)
(Intercept) 4149.8872 195.5654 21.220 < 2e-16 ***
Х1
           X2 -13.1660 23.0917 -0.570 0.5712
Х3
        623.5545 62.6409 9.954 2.94e-13 ***
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 '' 1
```

Residual standard error: 143.3 on 48 degrees of freedom Multiple R-squared: 0.6883, Adjusted R-squared: 0.6689 F-statistic: 35.34 on 3 and 48 DF, p-value: 3.316e-12

#### Section III

# Linear Algebra Review

#### Rank

#### **Definition**

The **rank** of a matrix A, denoted rank(A), is the number of linearly independent columns of A.

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#### Example

$$A = (v_1 \quad v_2 \quad v_3) = \begin{pmatrix} 3 & -2 & 8 \\ -2 & 12 & -16 \\ 7 & 9 & 5 \end{pmatrix}.$$

rank(A) = 2 because  $v_1$  and  $v_2$  are linearly independent, but

$$0 = 2v_1 - v_2 - v_3 = 2\begin{pmatrix} 3 \\ -2 \\ 7 \end{pmatrix} - \begin{pmatrix} -2 \\ 12 \\ 9 \end{pmatrix} - \begin{pmatrix} 8 \\ -16 \\ 5 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}.$$

#### **Inverse**

#### Theorem

The following statements are equivalent if A is a  $p \times p$  matrix

- A is invertible.
- $C(A) = \mathbb{R}^p$
- rank(A) = p

#### Theorem

If X is a  $n \times p$  matrix with rank(X) = p, then rank $(X^TX) = p$ 

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#### **Theorem**

If X is a  $n \times p$  matrix with rank(X) = p, then  $rank(X^TX) = p$ 

Why do we care about the above result?

$$\hat{\beta} = (X^T X)^{-1} X^T Y$$

In the Grocery retailer example consider introducing another variable *not holiday*.

#### Example

For i = 1, 2, ..., 52 weeks,

$$Y_i = \beta_0 + \beta_1 X_{i1} + \beta_2 X_{i2} + \beta_3 X_{i3} + \beta_4 X_{i4} + \epsilon_i, \quad \epsilon_i \sim N(0, \sigma^2)$$

$$X_{i3} = egin{cases} 1 & ext{holiday week} \ 0 & ext{otherwise} \end{cases} \qquad X_{i4} = egin{cases} 1 & ext{not holiday week} \ 0 & ext{otherwise} \end{cases}$$

For week i,

- Total labor hours (Y<sub>i</sub>)
- Number of cases shipped  $(X_{i1})$
- Indirect costs of the total labor hours as a percentage  $(X_{i2})$
- Holiday (X<sub>i3</sub>)
- Not holiday (X<sub>i4</sub>)

# Multiple Linear Regression

## Example

$$X = \begin{pmatrix} 1 & 305657 & 7.17 & 0 & 1 \\ 1 & 328476 & 6.20 & 0 & 1 \\ 1 & 317164 & 4.61 & 0 & 1 \\ 1 & 366745 & 7.02 & 0 & 1 \\ 1 & 265518 & 8.61 & 1 & 0 \\ 1 & 301995 & 6.88 & 0 & 1 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & 442782 & 7.61 & 1 & 0 \\ 1 & 322303 & 7.39 & 0 & 1 \\ 1 & 290455 & 7.99 & 0 & 1 \\ 1 & 411750 & 7.83 & 0 & 1 \\ 1 & 292087 & 7.77 & 0 & 1 \end{pmatrix}$$

Notice:  $col_1 = col_4 + col_5 \longrightarrow rank(X) = 4$ ,  $rank(X^TX) = 4$ .

#### Section IV

# The Bootstrap

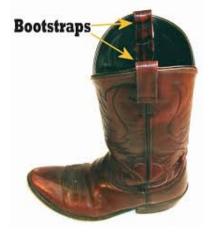
# The Bootstrap Principle

- If we could repeat an experiment over and over again, we could actually find a very good approximation to the sampling distribution.
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# The Bootstrap Principle

- If we could repeat an experiment over and over again, we could actually find a very good approximation to the sampling distribution.
- Grocery example: If I had 1000 years of data, run the regression model on each year to see how estimates change.
- Often too expensive or time-consuming.
- Bradley Efron's Idea (1979): Use computers to **simulate** replication.
- Instead of repeatedly obtaining new, independent datasets from the population, we repeatedly obtain datasets from the sample itself, the original dataset.

"Pull yourself up by your bootstraps!"



#### To get a bootstrap estimate,

- 1. Resample from the original data *n* times *with replacement* (note an original data observation could be in the new sample more than once),
- 2. Use the new dataset to compute a bootstrap estimate,
- 3. Repeat this to create B new datasets, and B new estimates.

Formally, you have original data  $(x_i)_{i=1}^n$  and you are interested in estimating a population parameter  $\Theta$  from the data. Label the estimate  $\hat{\Theta}$ .

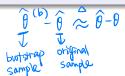
#### Procedure

- 1. For b = 1, ..., B,
  - Create a new dataset  $\mathcal{B}_b = (x_i^{(b)})_{i=1}^n$  by sampling from original dataset with replacement.
  - Use the new dataset to find an estimate  $\hat{\Theta}^{(b)}$ .

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  - Use the new dataset to find an estimate  $\hat{\Theta}^{(b)}$ .
- 2. The collection  $(\hat{\Theta}^{(b)} \hat{\Theta})_{b=1}^{B}$  estimates the sampling distribution of  $\hat{\Theta} \Theta$ .



You sample n=100 data points,  $x_1,\ldots,x_{100}\sim \textit{N}(\mu,1)$ . (Recall, Lab 1.)

```
> n <- 100

> vec <- rnorm(n, mean = mu)

> head(vec)

[1] -0.6264538  0.1836433 -0.8356286  1.5952808  0.3295078

[6] -0.8204684
```

• What's a good estimator for  $\mu$ ?

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\[ [6] \quad -0.8204684 \]
```

• What's a good estimator for  $\mu$ ? Sample mean

```
> mean(vec)
[1] 0.1088874 \(\frac{\chi}{\chi}\frac{\lambda}{\chi}
```

Set  $\hat{\mu} = 0.11$ . Recall,  $\hat{\mu} \sim N(\mu, 1/100)$ .

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• What's a good estimator for  $\mu$ ?

```
> mean(vec)
```

Set  $\hat{\mu} = 0.11$ . Recall,  $\hat{\mu} \sim N(\mu, 1/100)$ .

• How can we estimate  $Var(\hat{\mu})$ ?

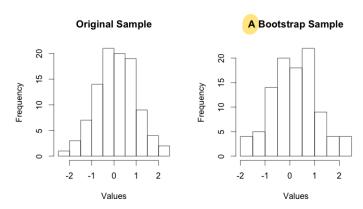
We'll use the bootstrap to estimate the variance! For b = 1 : B,

- Resample  $x_1, \ldots, x_{100}$  with replacement to get  $x_1^{(b)}, \ldots, x_{100}^{(b)}$ .
- Compute  $\hat{\mu}^{(b)} = \frac{1}{100} \sum_{i=1}^{100} x_i^{(b)}$ .

```
> B <- 1000
> estimates <- vector(length = B) Pep(NA, B) NULL
> for (b in 1:B) {
+ new_sample <- sample(vec, size = n, replace = TRUE)
+ estimates[b] <- mean(new_sample)
+ }
> head(estimates)
```

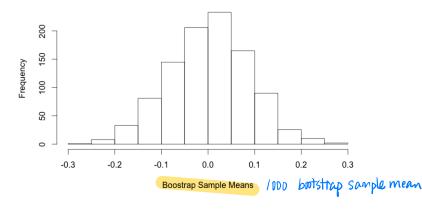
```
[1] 0.12250487 0.10894538 0.21117547 0.05405239 0.16694190 [6] 0.13804749
```

A histogram of the original sample and a histogram of a single resampled bootstrap sample.



The Bootstrap Distribution of the Statistic. Recall  $(\hat{\mu}^{(b)} - \hat{\mu})_{b=1}^{B}$  approximates the sampling distribution of  $\hat{\mu} - \mu$ .

#### Centered Bootstrap Estimates of the Mean



We'll use the bootstrap to estimate the variance!

# Estimating the Variance

> var(estimates)

[1] 0.007380355



True variance:  $Var(\hat{\mu}) = \frac{\sigma^2}{n} = \frac{1}{100} = 0.01$ .

# Regular Bootstrap Intervals

#### Regular Bootstrap Interval Formula:

• The 95% bootstrap interval is (L, U), where

$$L=2\hat{\Theta}-\hat{\Theta}_{0.975}^*$$
 and  $U=2\hat{\Theta}-\hat{\Theta}_{0.025}^*$ 

• Note that  $\hat{\Theta}_p^*$  is the  $p^{th}$  percentile of  $\hat{\Theta}_{b=1}^B$ 

# Regular Bootstrap Intervals

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• The 95% bootstrap interval is (L, U), where

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 and  $U=2\hat{\Theta}-\hat{\Theta}_{0.025}^*$ 

• Note that  $\hat{\Theta}_p^*$  is the  $p^{th}$  percentile of  $\hat{\Theta}_{b=1}^B$  0.975 % % % 0.905 % %

97.5% -0.05218752

2.5%

0.2797513

# Regular Bootstrap Intervals (Derivation)

$$0.95 = P(\hat{\theta}_{0.005}^* \le \hat{\theta}^* \le \hat{\theta}_{0.975}^*)$$

$$= P(\hat{\theta}_{0.005}^* - \hat{\theta} \le \hat{\theta}^* = \hat{\theta}_{0.975}^*)$$

$$\approx P(\hat{\theta}_{0.005}^* - \hat{\theta} \le \hat{\theta}^* = \hat{\theta}_{0.975}^* - \hat{\theta})$$

$$= P(\hat{\theta}_{0.005}^* - \hat{\theta} \le \hat{\theta}^* = \hat{\theta}_{0.975}^* - \hat{\theta})$$

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# Regular Bootstrap Intervals (Derivation)

# Percentile Based Bootstrap Intervals

#### Percentile Based Bootstrap Formula:

• The 95% percentile bootstrap interval is (L, U), where

$$L = \hat{\Theta}^*_{0.025}$$
 and  $U = \hat{\Theta}^*_{0.975}$ 

• Note that  $\hat{\Theta}_p^*$  is the  $p^{th}$  percentile of  $\hat{\Theta}_{b=1}^B$ 

# Percentile Based Bootstrap Intervals

## Percentile Based Bootstrap Formula:

• The 95% percentile bootstrap interval is (L, U), where

$$L = \hat{\Theta}_{0.025}^*$$
 and  $U = \hat{\Theta}_{0.975}^*$ 

• Note that  $\hat{\Theta}_p^*$  is the  $p^{th}$  percentile of  $\hat{\Theta}_{b=1}^B$ 

2.5%

-0.0619766

97.5%

0.2699623

# **Bootstrap Intervals**

## Nonparametric Testing

# **Bootstrapping Summary**

### Bootstrapping is very flexible!

- Bootstrapping gives you a distribution over estimators.
- This can be used to:
  - · Approximate more complicated metrics (medians, quantiles, etc.).
  - Approximate distributional properties.
  - Create confidence intervals.
- By resampling  $(x_i, y_i)_{i=1}^n$  pairs, we could create bootstrap estimators for linear model regression parameters.

#### Intervals

- Intervals can be used as a nonparametric hypothesis testing procedure.
- Both the regular and percentile based intervals are common techniques.
- The percentile based bootstrap interval is more intuitive to construct.

# **Optional Reading**

- Chapter 3 (3.1, 3.2, 3.6) from An Introduction to Statistical Learning.
- Chapter 1 (Vectors and Vector Spaces) found here from G. Donald Allen's Linear Algebra course (class website) at Texas A & M.
- Chapter 6 (The Bootstrap) in Advanced Data Analysis from an Elementary Point of View.