

# 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.

## 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.

# Multiple Linear Regression

# Multiple Linear Regression

## 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 ( $Y$ ).

# Multiple Linear Regression

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

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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.

# Multiple Linear Regression

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

## General Model

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \cdots + \beta_p X_p + \epsilon,$$

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

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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*.

# Multiple Linear Regression

## 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

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

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

$$Y = X\beta + \epsilon,$$

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.

# Multiple Linear Regression

## Example (Multiple Linear Regression Model)

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_3 + \epsilon, \quad \epsilon \sim N(0, \sigma^2)$$

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 ( $X_3$ ) with

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

# Multiple Linear Regression

## Example

Case	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
⋮	⋮	⋮	⋮	⋮
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



# Multiple Linear Regression

## 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

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

# Parameter Estimation

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

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

which provide predictions

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

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

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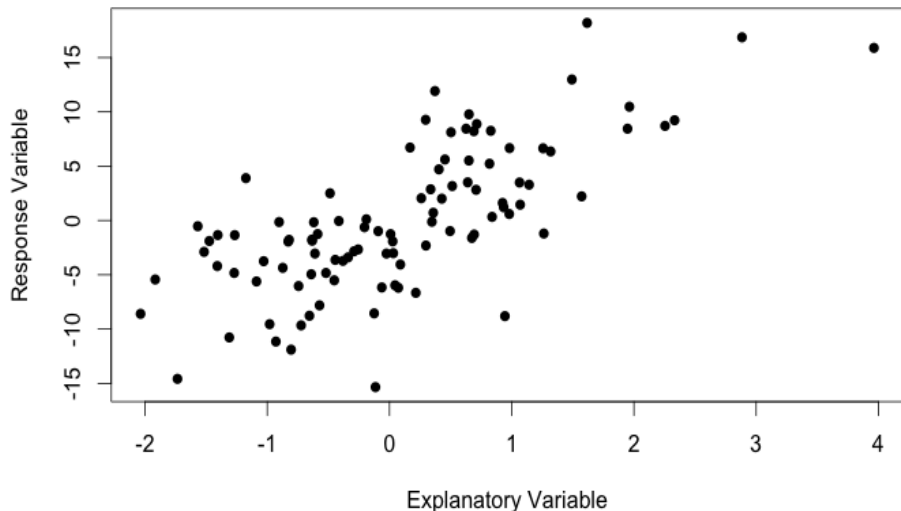
$$\hat{Y} = \hat{\beta}_0 + \hat{\beta}_1 X_1 + \hat{\beta}_2 X_2 + \dots + \hat{\beta}_p X_p? \quad (1)$$

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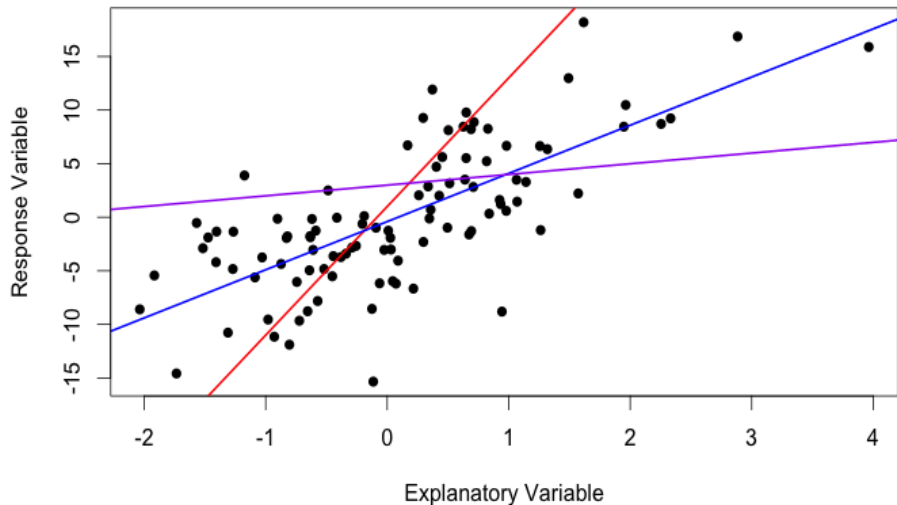
## Least Squares Estimate

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.

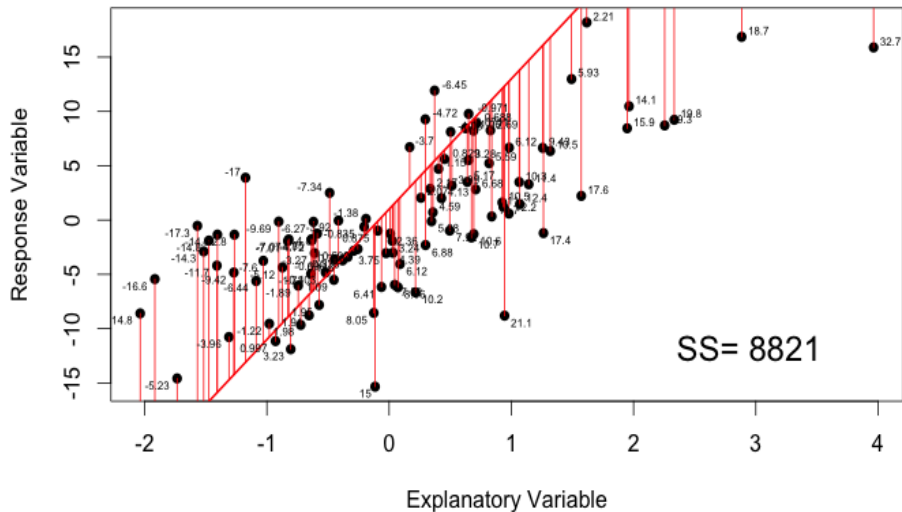
# The Least Squares Line



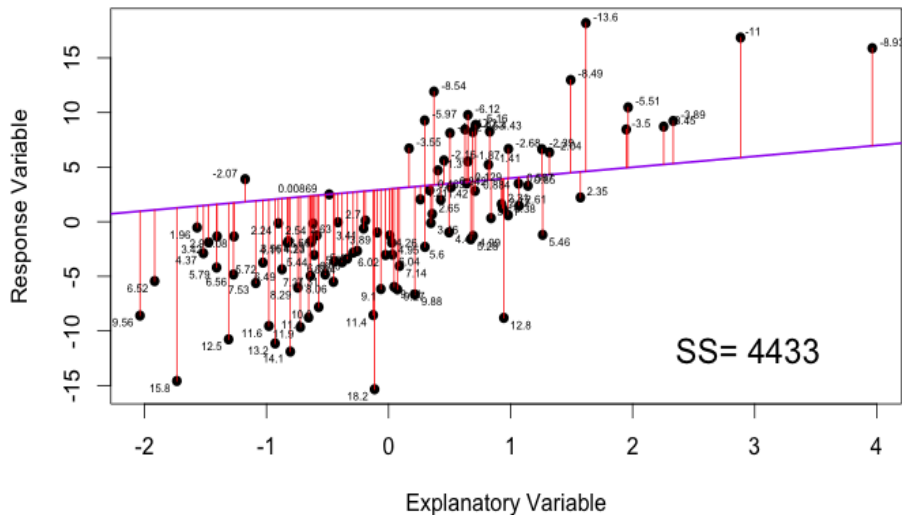
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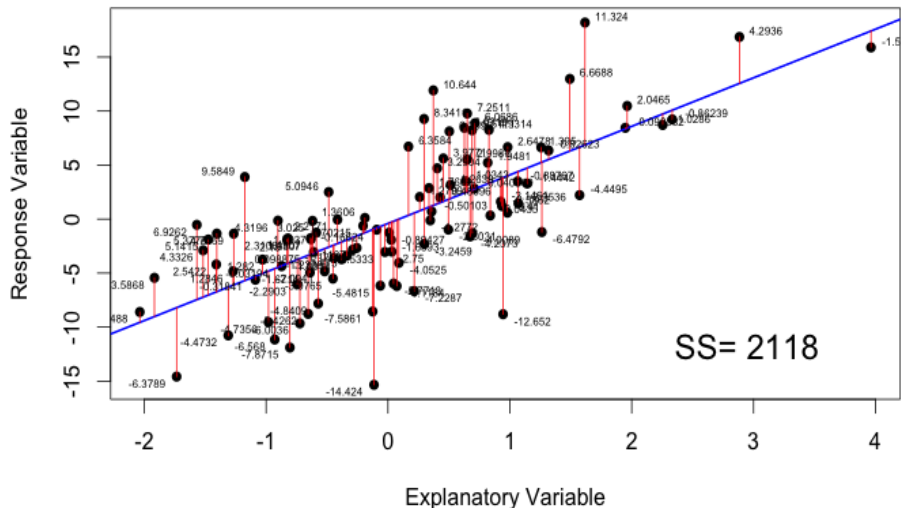
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# The Least Squares Line





## Least Squares Estimate

Define an objective function  $Q(b)$  as follows.

$$\begin{aligned} Q(b_0, b_1, \dots, b_p) &:= \sum_{i=1}^n (Y_i - (b_0 + b_1 X_{i1} + b_2 X_{i2} + \dots + b_p X_{ip}))^2 \\ &= \|Y - Xb\|^2, \end{aligned}$$

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

# Parameter Estimation

## 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?

# Parameter Estimation

## Sketch of Theorem Proof

First note,

$$\begin{aligned}Q(b) &= \|Y - Xb\|^2 = (Y - Xb)^T(Y - Xb) \\&= Y^T Y - Y^T Xb + (Xb)^T Y + (Xb)^T Xb \\&= b^T X^T Xb - 2Y^T Xb + Y^T Y.\end{aligned}$$

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

$$2X^T Xb - 2X^T Y = 0.$$

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

# Parameter Estimation

## 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)
```

# Parameter Estimation

## 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?

# Parameter Estimation

## Example

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

What is the estimated model?

$$\hat{Y} = 4149.89 + 0.79X_1 - 13.17X_2 + 623.56X_3$$

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

# Parameter Estimation

Estimated Model:

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

## 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**?

# Parameter Estimation

Estimated Model:

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## 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**?

$$\widehat{\text{Labor.Hours}} = 4149.89 + 0.79(\mathbf{350000}) - 13.17(\mathbf{8.5}) + 623.56(\mathbf{1}) \\ = 4938.01 \text{ hours} .$$



# 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

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

- 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)
> residuals(lm0)[1:5]
```

1	2	3	4	5
-32.06348	169.20509	-21.82543	-54.11955	75.93372

```
> fitted(lm0)[1:5]
```

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 ***
X1	0.7871	0.3646	2.159	0.0359 *
X2	-13.1660	23.0917	-0.570	0.5712
X3	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

# Linear Algebra Review

# Rank

## Definition

The **rank** of a matrix  $A$ , denoted  $\text{rank}(A)$ , is the number of linearly independent columns of  $A$ .

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## Example

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

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

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



## Theorem

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

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

## Theorem

*If  $X$  is a  $n \times p$  matrix with  $\text{rank}(X) = p$ , then  $\text{rank}(X^T X) = p$*

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## Theorem

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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  $i = 1, 2, \dots, 52$  weeks,

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

$$X_{i3} = \begin{cases} 1 & \text{holiday week} \\ 0 & \text{otherwise} \end{cases} \quad X_{i4} = \begin{cases} 1 & \text{not holiday week} \\ 0 & \text{otherwise} \end{cases}$$

For week  $i$ ,

- Total labor hours ( $Y_i$ )
- Number of cases shipped ( $X_{i1}$ )
- Indirect costs of the total labor hours as a percentage ( $X_{i2}$ )
- Holiday ( $X_{i3}$ )
- Not holiday ( $X_{i4}$ )

# 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:  $col_1 = col_4 + col_5 \rightarrow \text{rank}(X) = 4, \text{rank}(X^T X) = 4.$

# The Bootstrap

# The Bootstrap Principle

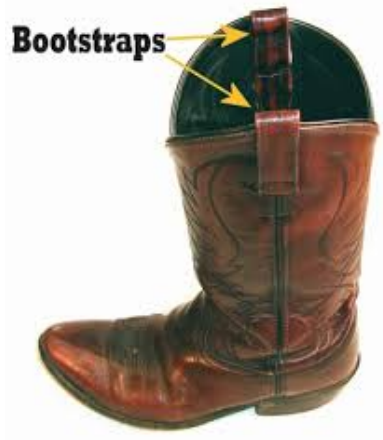
- If we could repeat an experiment over and over again, we could actually find a very good approximation to the sampling distribution.
- Grocery example: If I had 1000 years of data, run the regression model on each year to see how estimates change.

# 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.

# Bootstrap Methods

“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.

# Bootstrap Methods

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  $b = 1, \dots, B$ ,
  - 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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  - 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  $\hat{\Theta}^{(b)}$ .
2. The collection  $(\hat{\Theta}^{(b)} - \hat{\Theta})_{b=1}^B$  estimates the sampling distribution of  $\hat{\Theta} - \Theta$ .

## Example: Gaussian Random Variables

You sample  $n = 100$  data points,  $x_1, \dots, x_{100} \sim N(\mu, 1)$ . (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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- What's a good estimator for  $\mu$ ?

```
> mean(vec)
```

```
[1] 0.1088874
```

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

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

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

## Example: Gaussian Random Variables

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

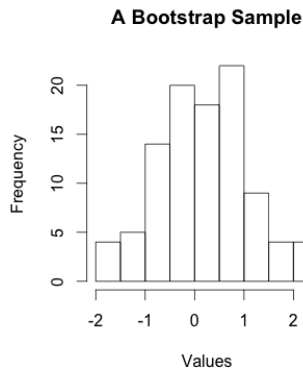
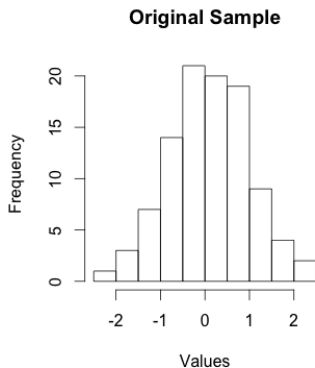
- Resample  $x_1, \dots, x_{100}$  *with replacement* to get  $x_1^{(b)}, \dots, x_{100}^{(b)}$ .
- Compute  $\hat{\mu}^{(b)} = \frac{1}{100} \sum_{i=1}^{100} x_i^{(b)}$ .

```
> B <- 1000
> estimates <- vector(length = B)
> 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
```

# Example: Gaussian Random Variables

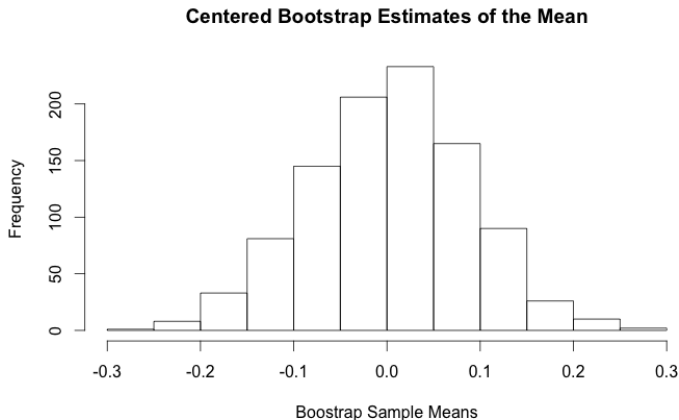
A histogram of the original sample and a histogram of a single resampled bootstrap sample.





# Example: Gaussian Random Variables

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



# Example: Gaussian Random Variables

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

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

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

# Regular Bootstrap Intervals

## Regular Bootstrap Interval Formula:

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

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

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

```
> L <- 2*mean(vec)-quantile(estimates,.975);L
```

```
97.5%  
-0.05218752
```

```
> U <- 2*mean(vec)-quantile(estimates,.025);U
```

```
2.5%  
0.2797513
```

# Regular Bootstrap Intervals (Derivation)

# Regular Bootstrap Intervals (Derivation)

# Percentile Based Bootstrap Intervals

## Percentile Based Bootstrap Formula:

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

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

- 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

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

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

```
> L <- quantile(estimates,.025);L
```

```
2.5%  
-0.0619766
```

```
> U <- quantile(estimates,.975);U
```

```
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.