

Crackers

Getting hungry just thinking about learning some statistical analysis? If you are like many, you might reach for a box of crackers as a "healthy alternative" to more sugar-laden foods. But just how healthy are crackers? FOr instance, the Los Angeles Unified School District Obesity Prevention Motion identified Pepperidge Farm's Cheddar Goldfish as an unapproved snack food. ¹ To investigate what is contained in a crackers box, we learn the tools of exploratory data analysis.

1 The crackers data set

We'll use a data set containing various nutritional information (see Table 1) gleaned from the website www.dietfacts.com and the sides of cracker boxes at a supermarket in Oberlin Ohio 2 .

To access the data we download it from a website by issuing the command:

> crackers = read.csv("http://www.math.csi.cuny.edu/st/R/crackers.csv")

The variable crackers contains the data. The data set contains measurements on 11 variables with 92 different types. How might we view this data? We can see all the values at once by typing the name of the data set, crackers. However, the values will quickly scroll by. The edit() function provides a better alternative:

> edit(crackers)

A basic spread-sheet like window should open showing the data set. A warning: you will be unable to proceed until this window is closed.

Question 1: Scroll through the Company variable and note any companies you do not recognize.

Question 2: Which company seems to have the most cracker products on the shelves? Guess how many different products are on the shelves?

What we would like to be able to do is access the data in the variables. In order to do this easily, we attach() the data set:

> attach(crackers)

¹http://cafe-la.lausd.k12.ca.us/usnacks.htm

² This data set has been contributed to the Journal of Statistical Education by Carolyn Cuff of Westminster College. Many of the question in this project follow those outlined in an accompanying paper. Some of the variable names were shortened from the original. The data is census data for all crackers sold at this grocery chain. Can you tell what the chain is?



Now we can refer to the variables by name, such as Product (case is important).

The numeric variables are all per-serving measurements. To see what variables are available, the variable names can be read off from the spread sheet, or printed out using the names() function:

> names(crackers)

[1]	"Company"	"Product"	"Crackers"
[4]	"Grams"	"Calories"	"Fat.Calories"
[7]	"Fat.Grams"	"Saturated.Fat.Grams"	"Sodium"
[10]	"Carbohydrates"	"Fiber"	

For instance, the variable Crackers records the crackers per serving and the variable Fat. Calories records the calories due to fat per serving.

Nutrition Facts Serving Size 55 crackers (55g) Servings Per Container 12		
Amount Per Serving		
Calories 150 Calories F	rom Fat 60	
%Dai	ily Values*	
Total Fat 6g	11%	
Saturated Fat 1.5g	7%	
Sodium 250mg	10%	
Total Carbohydrates 19g		
Dietary Fiber 0g	0%	
* Percent Daily Values are based on a 2,0	000	
calorie diet	000	

Table 1: Example of a nutritional label. This one for Pepperidge Farm's Cheddar Goldfish.

2 Numeric variables

Most of the variables in the data set are numeric. For such data, we have numeric summaries and graphical summaries available. Each has there place. Graphical summaries allow us to quickly see several features of a distribution at once, whereas numeric summaries allow us to quantitatively compare our data to some other data set or pre-conceived notion about our data.



2.1 Numeric summaries

Numeric summaries we use summarize the center (mean() and median()), the spread (range(), sd() and IQR()), or even the position within a data set (quantile() and scale()).

Question 3: Apply the functions mean(), median(), range(), IQR(), and sd() above to the Calories data set. What values do you get?

Question 4: Of the five numbers found in the previous exercise, which one is not available from the output of summary() applied to the data set Calories().

Question 5: The grams per serving variable, **Grams**, has missing data. You can verify this by typing the command

> Grams

The missing values are code NA, read "not available." When there are missing values, the extra argument na.rm=TRUE is often needed. Verify that mean(Grams) is not what is wanted, but

> mean(Grams, na.rm = TRUE)

provides the expected answer.

2.2 Graphical summaries of numeric data

There are a number of graphical means to summarize a data set. For instance stem-and-leaf diagrams, dotplots, histograms, densities, and boxplots. All of these devices allow us to quickly visualize the following: the center of the distribution, a sense of spread, the minimum value of the data, the maximum value, the range, where the bulk of the data sits, if there are any values far from the bulk, and the general shape of the data.

The R functions used to produce these graphics are stem(), stripchart(), hist(), density(), and boxplot()

2.3 Stem and Leaf diagrams

For instance, a stem-and-leaf diagram of the calories per serving is made as follows:

> stem(Calories)

The decimal point is 1 digit(s) to the right of the |

- 4 | 00
- 8 | 00000000000
- 10 | 00
- 12 | 0000000000000
- 16 | 000

From the diagram we can see that the smallest number is 40, the largest 160, the range is 120. The "shape" of this data set is *bimodal*— that is, there are two distinct "peaks" (around 60 and 140).

Question 6: Issue the command

> stem(Grams)

To make a simple stem-and-leaf diagram of the grams per serving. What is the range of values, as read from the stem-and-leaf diagram? Describe the shape of the data set.

Question 7: The choice of stem is automatically determined by stem(). It may not always produce the best results. However, you can override the choice by using an extra scale= argument. For instance, try the command

> stem(Grams, scale = 1/2)

Find the range of the data and compare to your previous answer. Does this make a better stem and leaf diagram than before? Explain why?

Question 8: Make a stem-and-leaf diagram of the crackers per serving variable Crackers. What is the range of the data? This shape of this data set is skewed right. What type of cracker do you think has 55 or more per serving? Check your answer by quickly scrolling through the data set.

2.4 Dotplots

A dotplot can be produced with the stripchart() function. ³

The simplest use of stripchart() will not stack points when there are ties, you must ask for this behavior. For example, to make the dotplot (Figure 1) of the data in Grams (grams per serving), we issue the following command: ⁴

> stripchart(Grams, method = "stack")

Some things we can quickly see from Figure 1 are that the range is roughly 13 to 31, the mean is around 20 (balance point), the median is somewhere in the left cluster of values, and the shape is bimodal. To check our guesses on the mean and median we have:

> summary(Grams)

Min. 1st Qu. Median Mean 3rd Qu. Max. NA's 13.0 15.0 16.0 22.1 30.0 31.0 11.0

Question 9: Make a stripchart of the data in the variable Calories.

³ Alternatively, you can use the DOTplot() function that may be installed using source("http://www.math.csi.cuny.edu/st/R/DOTplot.R")

⁴If you use DOTplot() the graphic is produced by DOTplot(Grams).

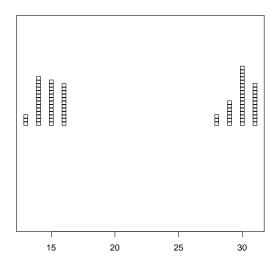


Figure 1: Dotplot of grams per serving

- 1. What is the range of the data?
- 2. What is the shape of the data?
- 3. Estimate the mean of the data using the idea of balancing.
- 4. Are there any crackers that are "average" by this measure?
- 5. Check your estimate, by computing the mean.

2.5 Histograms

The dotplots made with this much data are pretty busy, a histogram may better show the key features of the data set.

Histograms are made using the function hist(), as in its use to produce a histogram of the amount of sodium per serving:

> hist(Sodium)

Question 10: Based on the histogram in Figure 2 do the following:

- 1. Estimate the range of the data
- 2. Estimate the mean of the data set
- 3. Estimate the median of the data set
- 4. Describe the shape of the data

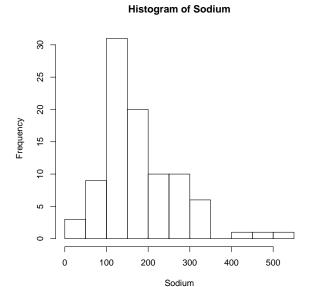


Figure 2: Histogram of sodium amount in crackers.

Check your numeric answers using the appropriate function.

Question 11: Produce a histogram of the number of crackers per serving. Based on the histogram do the following

- 1. Estimate the range of the data
- 2. Estimate the mean of the data set
- 3. Estimate the median of the data set
- 4. Describe the shape of the data

Check your numeric answers using the appropriate function.

Density estimates

A density estimate is similar to a histogram, in that it visually summarizes the shape of a distribution. However, they have advantages, in that they are more directly related to the population density and many may be used simultaneously.

Density estimates are generated using the density() command. This command simply produces the numbers, to visualize the density it may be added to a histogram or plotted by itself.

To plot a density by itself we use the plot() function in combination with density(). For instance, to plot the density of crackers per serving (Figure 3):

> plot(density(Crackers))

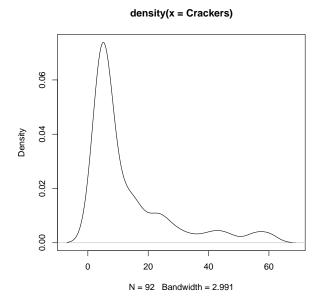


Figure 3: Density plot of crackers per serving

To add data to a graphic ⁵ we use the function points() and lines(). The former adds the data as points, the latter connects the points with lines. We want to plot a curve, so we would use lines():

> lines(density(Crackers))

(That is, replace plot() with lines().)

When adding a density on top of histogram, one first needs to make the histogram having a total area of 1. This is achieved using the extra argument probability=TRUE to hist(). We abbreviate this to prob=T.

For instance, a histogram with density estimate of the crackers per serving is generated (Figure 4), as with:

- > hist(Crackers, prob = T)
- > lines(density(Crackers))

Question 12: Based on Figure 3 answer the following:

- 1. Is the data set symmetric or skewed?
- 2. Are there long tails? If so, which?
- 3. Estimate the mean and median. Which is greater and why.
- 4. Check your estimates using the functions mean() and median(). Were you close?

⁵If you close the graphics window before adding the line, you will get an error message.

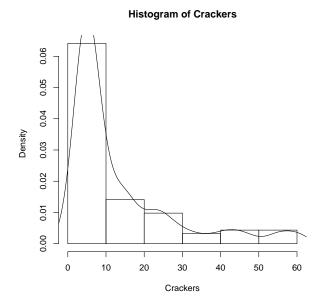


Figure 4: Histogram and density estimate of the number of crackers per serving

Question 13: Make a density plot of the variable Sodium. Based on this, is the population skewed or symmetric? Long tailed?

Question 14: One can add the actual data points to the histogram and density estimate using the rug() function. To see what is done, with the density plot for Sodium still open issue the following:

> rug(Sodium)

2.6 Boxplots

Boxplots succinctly describe a numeric data set in a manner that lends itself to multiple comparisons. From a boxplot we can quickly identify all of the following: the center, the spread, the range, symmetry or skew, and tail length.

Boxplots are produced with the boxplot() function. For example, a boxplot of the number of crackers per serving (Figure 5) may be made with

- > boxplot(Crackers)
- > title("Number of crackers per serving")
- Question 15: From Figure 5 answer the following:
 - 1. What is the "center" of the variable?
 - 2. What is the spread?

Number of crackers per serving

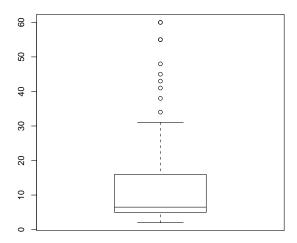


Figure 5: Boxplot of number of crackers per serving

- 3. Is the data set skewed?
- 4. Do you expect the mean or median to be the largest? Why? Check it.
- 5. Are there any "outliers?" If so, how many?

Question 16: Make a boxplot of the Fat.Grams variable. From your figure answer the following:

- 1. What is the "center" of the variable?
- 2. What is the spread?
- 3. Is the data set skewed?
- 4. Do you expect the mean or median to be the largest? Why? Check it.
- 5. Are there any "outliers?" If so, how many?

Question 17: If there are two variables, one numeric and one categorical (numeric will also work) of the same size, it is easy to produce parallel boxplots for each level of the categorical variable. The syntax is to use numeric ~ categorical for the argument. For instance: ⁶

⁶The extra argument las=2 is optional. It turns the labels so that they are easier to read. You can also enlarge the plot window to see more text.

> boxplot(Calories ~ Company, las = 2)

Based on your plot, answer the following:

- 1. Which company has the widest range?
- 2. Which company has the largest median?
- 3. Which company has the largest IQR?
- 4. Why do some companies have just a short horizontal line?

3 Using just some of the data

A nice feature of R is the ability to easily extract just part of the data in a variable. The cracker data set lends itself to analysis of the sub-populations. For example, a histogram of calories per serving shows two distinct modes—one near 60 and one near 130. What causes this? Could it be the difference between low-fat crackers and non-dietetic crackers?

3.1 Extraction by index

A look at the variable Product in the data set shows that the following indices are low fat and low sodium crackers:

low fat: 10 12 19 23 28 30 42 50 51 54 58 68 73 86 90

low sodium: 8 24 29 31 41 55 56 66 71 80 92

We enter these into vectors for storage as follows:

```
> low.fat = c(10, 12, 19, 23, 28, 30, 42, 50, 51, 54, 58, 68, 73, 86, 90)
> low.sodium = c(8, 24, 29, 31, 41, 55, 56, 66, 71, 80, 92)
```

To refer to the values in the Calories variable that correspond to the low fat crackers is done by extraction. To extract just the specified indices is made possible using the square-bracket notation, []. For instance:

> Calories[low.sodium]

```
[1] 70 80 70 70 150 60 60 140 150 150 60
```

Just the 11 values for which there are indices are printed.

Question 18: Make a stem and leaf diagram of the Calories variable for the low-sodium crackers. Is the data still bimodal?

Question 19: Make a stem and leaf diagram of the Calories variable for the low-fat crackers. Is the data still bimodal?

Question 20: You can combine indices using c(), or eliminate potential duplicates with union(low.fat,low.sodium)(). Do so, then make a histogram of the Calories variable for this larger restricted data set. Describe the data set, and contrast it to the full data stored in Calories.

Question 21: Parallel boxplots of the calories per serving for low-fat crackers and other crackers can be produced as follows

> boxplot(Calories[low.fat], Calories[-low.fat])

This uses the special convention for negative indices—to exclude the values.

Produce the boxplot. The first boxplot refers to the first variable, etc. Does it appear that the distribution of the number of Calories is dependent on whether the cracker is labeled as low in fat? Explain.

Question 22: The crackers with extra cheese or bacon flavor are

Make parallel boxplots of the crackers with these extra flavors and those without. Does it appear that the distribution of the number of Calories is dependent on whether the cracker has a "cheesy" or "bacony" flavor? Explain.

Question 23: Use extraction to find the products where the calories per serving are more than 140. Are there any surprises in the data set? Explain what you expected and describe what you see.

3.2 Extraction using logical data

Extraction may also be done in response to a "question." A sample question would be "Which indices correspond to values where the calories per serving are less than 100?" R is a little more succinct. This is "asked" as:

> Calories < 100

Question 24: Run the above command and interpret the output. What is computed for each value?

The actual indices are found in combination with the which() function:

> which(Calories < 100)

[1] 1 2 3 4 5 6 7 8 9 10 17 18 19 20 21 22 23 24 29 30 31 32 33 34 35 [26] 36 53 54 55 56 58 59 61 62 64 70 74 75 76 77 78 84 88 89 90 91 92

The which() function returns the index for each TRUE value. A vector of TRUE and FALSE values is called a logical vector. Many functions are adapted to use logical vectors. For instance, the sum() function adds up all the TRUE values:

> sum(Calories < 100)

[1] 47

For extraction, only those values corresponding to TRUE are returned:

- > low.cal = Calories < 100
- > Calories[low.cal]
- [1] 60 60 60 60 70 60 70 70 70 70 80 80 60 80 80 80 70 80 70 50 70 60 70 80 80 [26] 80 60 60 60 60 70 80 60 70 80 60 60 60 60 70 60 70 70 50 60 60

Variables that have only two values (TRUE and FALSE), say, or 0 and 1 are referred to as indicator variables. They can often make many computations easier to organize.

The negation operator, !, reverses the TRUE's and FALSE's. For instance, the command

> Calories[!low.cal]

```
[1] 130 120 140 140 140 130 140 140 140 140 130 150 150 150 150 140 140 160 140
[20] 160 130 140 130 120 110 150 110 140 130 130 140 140 120 130 150 140 130 150
[39] 150 140 140 120 160 140 150
```

Returns values for which the calories per serving are 100 or more (Calories >= 100)

Question 25: You don't need to use the same variable. For instance to look at the crackers which have just a few per serving we have

> Product[Crackers <= 3]

- [1] Bretton Vinta [3] Vivant Cabaret
- [5] Harvest Bakery Cornbread Harvest Bakery Multigrain
- [7] Harvest Bakery Rye Stoned Wheat Thins
- 92 Levels: Barnum's Animal crackers ... Zesta Soup & Oyster Crackers

Repeat a similar command, only showing those crackers with more than 50 per serving. Which crackers are these?

Question 26: The boxplot() function works well with indicator variables. For example, a histogram of Crackers, the crackers per serving, shows that many are 10 or fewer and others, the small crackers, have many more. To break the data up by the crackers per serving and then plot boxplots for each may be done as follows:

- > small.serv = Crackers <= 10 > boxplot(Calories ~ small.serv)
- (The labels on the boxplots are taken from the values in small.serv. This is in contrast to a more cumbersome expression like

> boxplot(Calories[small.serv], Calories[!small.serv])

)

Run these commands. Do the two boxplots look as though the represent the same population?

Question 27:

Create an indicator variable low.cal as follows

> low.cal = Calories < 100

Now make boxplots of fat grams per serving (Fat.Grams) broken up by the indicator variable low.cal.

Are there any non-low calorie crackers with fewer grams of fat than some low-calories crackers? What part of the boxplots answers this?

4 Bivariate analysis

What can we glean from the Crackers data set when we look at two numeric variables simultaneously. Can we see what determines the calories per serving? Is there a relationship between Sodium and Fiber? etc. To answer these it helps to look at bivariate relationships.

4.1 scatterplots

Looking at two numeric variables simultaneously is often done using a *scatterplot*. These are produced in R with the plot() function. This function can be used several ways. To make a scatterplot, we'll use it with an argument like

If only a subset of the data is desired, you can specify this by the indices, or using a logical expression using syntax like

Simply replace . . . by a logical expression, or a data vector of indices.

For example, a scatterplot of grams per serving on the x axis and calories per serving on the y axis is done, as follows (Figure 6):

> plot(Calories ~ Grams)

The scatterplot shows two distinct clusters of data. Within each cluster there appears to be very little trend.

Question 28:

Verify that the command

> plot(Calories ~ Grams, subset = Calories >= 100)

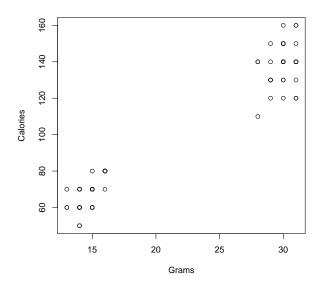


Figure 6: Scatterplot of grams per serving predicting calories per serving

plots just the upper cluster. What subset command using Grams instead of Calories will produce this same graphic?

Question 29: Make a scatterplot with Crackers on the x axis and Calories on the y axis. Does there appear to be any trends?

Question 30: From you graph of Crackers versus Calories there is an "outlier" around (45,90). To identify that in the data set can be done using the mouse. Type the command

> identify(Crackers, Calories, labels = Product)

Now click on a point, and the point will be labeled with the corresponding product name. Right click to stop the process.

What product is the outlier?

Question 31: As an exploratory device, multiple scatterplots can be made at once in a graphic called a scatterplot matrix. The pairs() function will do so. For example, to make all pairs of scatterplots of the variables 5 through 11 we have the command

> pairs(crackers[5:11])

Which relationship is closest to a straight line?

Question 32: Make a scatterplot with Carbohydrates on the x axis and Calories on the y axis. Does the amount of carbohydrates per serving cracker seem to affect the number of calories per serving?

Question 33: Make an indicator variable, low.carb, which is TRUE if the number of Carbohydrates is less than 15. Make parallel boxplots of the number of calories per serving broken up by the values of low.carb. Explain the differences in the boxplot.

4.2 Correlation

The Pearson correlation coefficient is a numeric summary of the strength of a linear relationship between two variables. The Spearman correlation coefficient is a numeric summary of the *monotonic* relationship between two variables. They are both computed by the cor() function. The default is to return the Pearson coefficient. When the extra argument method="spearman" is used the latter is returned.

For instance the correlation between the calories per serving and the carbohydrates per serving is computed with

> cor(Calories, Carbohydrates)

[1] 0.867

Question 34: What is the correlation between Fat.Grams and Fat.Calories? Make a scatterplot and guess the correlation first.

Question 35: What is the correlation between the crackers per serving (Crackers) and calories per serving (Calories)?

Question 36: Make a scatterplot of crackers per serving (Crackers) and calories per serving (Calories). Does the relationship appear to be linear? Monotonic? If you said yes to monotonic, compute the Spearman correlation coefficient and compare to the Pearson correlation coefficient found in the previous question.

Question 37: The correlation between Calories and Carbohydrates is positive. However, a scatterplot shows two distinct clusters. These are inidicated by the indicator variable defined as

> low.carb = Carbohydrates < 15

Find the correlation for just the low-carbohydrate data and compare to that for the non-low-carbohydrate data. Then compare to the value of 0.867 to the two just found. This is an example of data with two clusters throwing off the interpretation of correlation.

(This can be done with syntax like Calories [low.carb] or Calories [!low.carb].)

4.3 Simple linear regression

Simple linear regression attempts to model a response variable by a independent (predictor) variable using a straight line. Rather than try to model each data point, the simple regression model attempts to describe the mean value of the response variable as a linear function of the predictor variable. For a given data point, (x_i, y_i) , the regression line predicts the mean value of the y with \hat{y}_i . The residual amount is $y_i - \hat{y}_i$

The method of least squares chooses such a line by minimizing the sum of the squared residuals. Formulas for the slope and intercept are used by the lm() function to compute the line. If x and y store the data for the predictor and response variable, then the coefficients are returned by

When only a portion of the data is to be considered, the argument subset= can be added. This argument accepts a vector of indices, or a logical expression of the correct length.

For example, in a model of Calories modeled by Carbohydrates we have the regression coefficients

The output shows an intercept of 14.80 and a slope of 5.77.

Looking just at the low-carbohydrate data could be done with

In each case, the output is stored in a variable. This allows one to reuse the output of lm() which stores much more than is shown. For example, to add the just-found regression line to a scatterplot could be down using abline() with:

```
> plot(Calories ~ Carbohydrates)
> abline(res)
```

Question 38: Make a scatterplot of Fat. Grams predicting the number of calories per serving. Add a regression line to the graphic.

Question 39: Let low.cal be the indicator variable defined by

> low.cal = Calories < 100

Compare the slope of the regression line for low calorie crackers and those that aren't low calorie. Are the slopes similar?

Question 40: Make a plot of Calories due to fat (Fat.Calories) and grams of fat (Fat.Grams). Not suprisingly, the number of calories is linearly related to the amount of fat. What is the slope of the regression line?

Diagnostic plots for regression

The residuals are the key to assessing whether a given set of data is appropriate for modeling with a linear regression model. The residuals are silently returned by the lm() function. If we store the output, then we can access the residuals using the residuals() function.

For instance, to plot the residuals (Figure 7) of the model of Calories by Carbohydrates, we could do this:

```
> res = lm(Calories ~ Carbohydrates)
> plot(residuals(res))
```

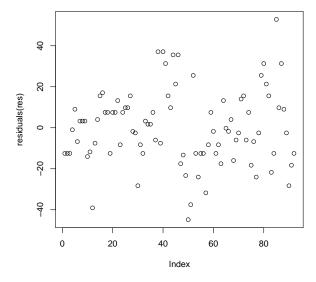


Figure 7: Residuals of model of Calories modeled by Carbohydrates.

This type of plot shows a problem with the modeling, if the data appears to have some structure, or trend. Figure 7 does not show any, although there is some indication that the standard deviation of the residuals grows as the indices get larger.

It is actually preferable to plot the fitted values against the residuals, and not the residuals against their indices. This plot is produced with:

> plot(fitted(res), residuals(res))

Question 41: Produce the plot of fitted values versus the residual values. Is there some structure evident in this plot? Explain.

Question 42: Make a linear model of Calories modeled by Crackers. Then produce the residual plot against the fitted values as above. Does this graph show any structure or trend? Explain.

Question 43: The residuals should be bell-shaped in their distribution. Make a histogram of the residuals from the previous exercise. Does their distribution appear to be bell-shaped?

4.4 Multiple regression models

Calories in food follow this chemical equation:

```
calories = 4 \cdot \text{grams} of carbohydrates + 4 \cdot \text{grams} of protein + 9 \cdot \text{grams} of fat.
```

We can perform a "multiple regression" to see if the data is consistent with this model. As we don't have protein data, we would like to see what the data predicts for values in an equation for the mean number of calories given the amount of carbohydrates and fat:

mean number of calories = $b_0 + b_1 \cdot \text{grams}$ of carbohydrates + $b_2 \cdot \text{grams}$ of fat.

To fit this in R we have

```
> lm(Calories ~ Carbohydrates + Fat.Grams)
```

Call:

lm(formula = Calories ~ Carbohydrates + Fat.Grams)

Coefficients:

```
(Intercept) Carbohydrates Fat.Grams
3.39 4.26 9.33
```

The data yields vales of 4.26 and 9.33 instead of the theoretical 4 and 9. A natural question would be to ask if these values are somehow consistent with the theoretical ones. This is the realm of statistical inference.

Question 44: Repeat the modeling above replacing Fat.Grams by Saturated.Fat.Grams. Compare the coefficients found.