Linear Regression Basics Notes

09 November, 2020

Objectives

- 1) Obtain parameter estimates of a simple linear regression model given a sample of data.
- 2) Interpret the coefficients of a simple linear regression.
- 3) Create a scatterplot with a regression line.
- 4) Explain and check the assumptions of linear regression.
- 5) Use and be able to explain all new terms.

Linear regression models

The rest of this block will serve as a brief introduction to linear models. In general, a model estimates the relationship between one variable (a **response**) and one or more other variables (**predictors**). Models typically serve two purposes: *prediction* and *inference*. A model allows us to predict the value of a response given particular values of predictors. Also, a model allows us to make inferences about the relationship between the response and the predictors.

Not all models are used or built on the same principles. Some models are better for inference and others are better for prediction. Some models are better for qualitative responses and others are better for quantitative responses. Also, many models require making assumptions about the nature of the relationship between variables. If these assumptions are violated, the model loses usefulness. In Math 378, we will cover a wide array of models, most of which we will explore for the purpose of prediction.

In this block, we will focus on *linear models* and the use of linear regression to produce and evaluate the model. Linear regression is a very powerful statistical technique. Many people have some familiarity with regression just from reading the news, where graphs with straight lines are overlaid on scatterplots, much like we did in the last lesson. Linear models can be used for prediction or to evaluate whether there is a linear relationship between two numerical variables.

Suppose we were interested in exploring the relationship between one response variable (Y) and one predictor variable (X). We can postulate a linear relationship between the two:

$$Y = \beta_0 + \beta_1 X$$

A linear model can be expanded to include multiple predictor variables:

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \dots + \beta_p X_p$$

This model is often referred to as a linear regression model. (When there is only one predictor variable, we often refer to it as a simple linear regression model.) The β_j terms are referred to as coefficients.

Note that the coefficients are **parameters** and thus represented as Greek letters. We typically don't know the true values of β_j , so we have to estimate them with samples from the population of X and Y, our data. Estimating these parameters and using them for prediction and inference will be the majority of the work of this last block.

We consider the models above to be linear models because they are linear in the **parameters**. This means that the following model is also a linear model:

$$Y = \beta_0 + \beta_1 X^2$$

Technically, we can write the parameters as a vector and the explanatory variables as a matrix. The response will then be an inner product of this vector and matrix and thus a linear combination.

Even if we expect two random variables X and Y to share a linear relationship, we don't expect it to be perfect. There will be some scatter around the estimated line. For example, consider the head length and total length of 104 brushtail possums from Australia. The data is in the file possum.csv in the data folder.

Exercise:

Read in the data from data/possum.csv and look at the first few rows of data.

```
possum<-read_csv("data/possum.csv")
```

glimpse(possum)

head(possum)

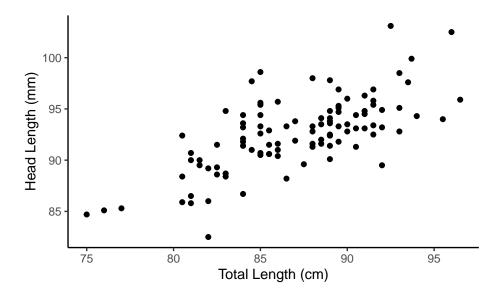
```
## # A tibble: 6 x 8
##
                            age head_l skull_w total_l tail_l
      site pop
                   sex
##
     <dbl> <chr> <chr> <dbl>
                                 <dbl>
                                           <dbl>
                                                    <dbl>
                                                            <dbl>
## 1
                                   94.1
                                            60.4
                                                     89
                                                             36
          1 Vic
                              8
                   m
## 2
          1 Vic
                                   92.5
                                            57.6
                                                     91.5
                                                             36.5
                                                             39
## 3
          1 Vic
                   f
                              6
                                   94
                                            60
                                                     95.5
## 4
          1 Vic
                   f
                              6
                                   93.2
                                            57.1
                                                     92
                                                             38
## 5
                              2
                                            56.3
                                                             36
          1 Vic
                   f
                                   91.5
                                                     85.5
## 6
          1 Vic
                   f
                                   93.1
                                            54.8
                                                     90.5
                                                             35.5
```

We think the head and total length variables are linearly associated. Possums with an above average total length also tend to have above average head lengths. To visual this data, we will use a scatterplot, we have used these multiple times this semester. Scatterplots are a graphical technique to present two numerical variables simultaneously. Such plots permit the relationship between the variables to be examined with ease. The following figure shows a scatterplot for the head length and total length of the possums. Each point represents a single possum from the data.

Exercise:

Create a scatterplot of head length and total length.

```
possum %>%
  gf_point(head_l~total_l) %>%
  gf_labs(x="Total Length (cm)",y="Head Length (mm)") %>%
  gf_theme(theme_classic())
```



While the relationship is not perfectly linear, it could be helpful to partially explain the connection between these variables with a straight line. However, this relationship will not be deterministic. Some longer possums will have shorter heads and some shorter possums will have longer heads. Thus, there is no straight line that can go through all these point. We expect some deviation from the linear fit. This deviation is represented by random variable e, which we refer to as an error term:

$$Y = \beta_0 + \beta_1 X + e$$

For our problem, Y is head length and X is total length.

In general we have:

$$Data = Fit + Residual$$

and what will change in our modeling process is how we specify the Fit.

The error term is assumed to follow a normal distribution with mean 0 and constant standard deviation σ . Note: the assumption of normality is only for inference using the t and F distributions and we can relax this assumption with using a bootstrap. Among other things, these assumptions imply that a linear model should only be used when the response variable is continuous in nature. There are other approaches for non-continuous response variables (discriminant analysis, logistic regression, etc.).

Estimation

We want to describe the relationship between the head length and total length variables in the possum data set using a line. In this example, we will use the total length as the predictor variable, x, to predict a

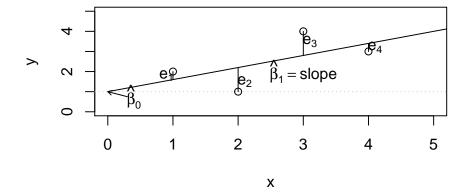
possum's head length, y. Just as a side note, the choice of the predictor and response are not arbitrary. The response is typically what we want to predict or in the case of experiments is the casual result of the predictor(s).

In the possum data we have n = 104 observations: $(x_1, y_1), (x_2, y_2), ..., (x_n, y_n)$. Then for each observation the implied linear model is:

$$y_i = \beta_0 + \beta x_i + e_i$$

We could fit the linear relationship by eye like we did in the case study and obtain estimates of the slope and intercept but this is too ad hoc. So, given a set of data like the **possum**, how do we actually obtain estimates of β_0 and β_1 ? What is the **best** fit line?

We begin by thinking about what we mean by "best". Mathematically, we want a line that has small residuals. There are multiple methods, but the most common is *method of least squares*. In this method, our goal is to find the values of β_0 and β_1 that minimize the squared vertical distance between the points and the resulting line, the **residuals**. See the plot for a visual representation involving only four observations from *made up* data.



Our criterion for best is the estimates of slope and intercept that minimize the sum of the squared residuals:

$$e_1^2 + e_2^2 + \cdots + e_n^2$$

The following are three possible reasons to choose the least squares criterion over other criteria such as the sum of the absolute value of residuals:

- 1. It is the most commonly used method.
- 2. Computing a line based on least squares was much easier by hand when computers were not available.
- 3. In many applications, a residual twice as large as another residual is more than twice as bad. For example, being off by 4 is usually more than twice as bad as being off by 2. Squaring the residuals accounts for this discrepancy.

¹If you want to do try this again use the plot_ss() from the last lesson.

The first two reasons are largely for tradition and convenience; the last reason explains why least squares is typically helpful.²

So, we need to find β_0 and β_1 that minimize the expression, observed minus expected:

$$\sum_{i=1}^{n} (y_i - \beta_0 - \beta_1 x_i)^2$$

Using calculus-based optimization yields the following estimates of β_0 and β_1 :

$$\hat{\beta}_0 = \bar{y} - \hat{\beta}_1 \bar{x}$$

Notice that this implies that the line will always go through the point (\bar{x}, \bar{y}) .

And

$$\hat{\beta}_1 = \frac{\sum x_i y_i - n\bar{x}\bar{y}}{\sum x_i^2 - n\bar{x}^2}$$

A more intuitive formula for the slope and one that links **correlation** to linear regression is:

$$\hat{\beta}_1 = \frac{s_y}{s_x} R$$

where R is the correlation between the two variables, and s_x and s_y are the sample standard deviations of the explanatory variable and response, respectively. Thus the slope is proportional to the correlation.

You may also be interested in estimating σ , the standard deviation of the error:

$$\hat{\sigma} = \sqrt{\frac{1}{n-2} \sum_{i=1}^{n} \hat{e}_i^2}$$

where \hat{e}_i is the observed *i*th **residual** ($\hat{e}_i = y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i$). This estimate is based only on the assumption of constant variance.

Possum example

We will let R do the heavy work of minimizing the sum of squares. The function is lm() as we learned in the case study. This function needs a formula and data for input. The formula notation should be easy for us since we have worked with formulas so much in the mosaic package.

First create the model:

The output of the model object is minimal with just the estimated slope and intercept.

poss_mod

²There are applications where least absolute deviation may be more useful, and there are plenty of other criteria we might consider. However, this course only applies the least squares criterion. Math 378 will look at other criteria such as a shrinkage method called the lasso.

```
##
## Call:
## lm(formula = head_1 ~ total_1, data = possum)
##
## Coefficients:
## (Intercept) total_1
## 42.7098 0.5729
```

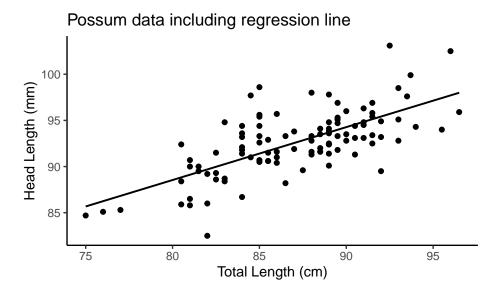
We can get more information using the summary() function:

```
summary(poss_mod)
```

```
##
## Call:
## lm(formula = head_l ~ total_l, data = possum)
##
## Residuals:
               1Q Median
                               3Q
## -7.1877 -1.5340 -0.3345 1.2788 7.3968
##
## Coefficients:
##
              Estimate Std. Error t value Pr(>|t|)
## (Intercept) 42.70979
                          5.17281
                                    8.257 5.66e-13 ***
## total_1
              0.57290
                          0.05933
                                    9.657 4.68e-16 ***
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 2.595 on 102 degrees of freedom
## Multiple R-squared: 0.4776, Adjusted R-squared: 0.4725
## F-statistic: 93.26 on 1 and 102 DF, p-value: 4.681e-16
```

We can plot the data points and least squares line together.

```
possum %>%
  gf_point( head_l ~ total_l) %>%
  gf_lm(color="black") %>%
  gf_labs(x="Total Length (cm)",y="Head Length (mm)") %>%
  gf_labs(x="Total Length (cm)",y="Head Length (mm)") %>%
  gf_labs(title="Possum data including regression line") %>%
  gf_theme(theme_classic())
```



Interpretation

Interpreting parameters in a regression model is often one of the most important steps in the analysis. The intercept term, β_0 , is usually uninteresting. It represents the **average** value of the response when the predictor is 0. Unless we center our predictor variable around 0, the actual value of the intercept is usually not important; it typically just gives the slope more flexibility to fit the data. The slope term, β_1 represents the **average** increase in the response variable per unit increase in the predictor variable. We keep using the word **average** in our discussion. With the assumption of a mean of 0 for the residuals, which least squares ensures with a line going through the point (\bar{x}, \bar{y}) , the output of the model is the expected or average response for the given input. Mathematically we have:

$$E(Y) = E(\beta_0 + \beta_1 X + e) = E(\beta_0 + \beta_1 X) + E(e) = \beta_0 + \beta_1 X$$

Predicting a value of the response variable simply becomes a matter of substituting the value of the predictor variable into the estimated regression equation. Again, it is important to note that for a given value of x, the predicted response, \hat{y} is what we expect the average value of y to be given that specific value of the predictor.

Exercise: The slope and intercept estimates for the possum data are 0.5729 and 42.7098. What do these numbers really mean, interpret them?

Interpreting the slope parameter is helpful in almost any application. For each additional 1 cm of total length of a possum, we would expect the possum's head to be 0.5729 mm longer on average. Note that a longer total length corresponds to longer head because the slope coefficient is positive. We must be cautious in this interpretation: while there is a real association, we cannot interpret a causal connection between the variables because these data are observational. That is, increasing a possum's total length may not cause the possum's head to be longer.

The estimated intercept $b_0 = 42.7$ describes the average head length of a possum with zero total length! The meaning of the intercept is irrelevant to this application since a possum can not practically have a total length of 0.

Earlier we noted a relationship between the slope estimate and the correlation coefficient estimate.

Exercise Find the slope from the correlation and standard deviations.

```
## # A tibble: 1 x 4
## correlation sd_head sd_total slope
## <dbl> <dbl> <dbl> <dbl> <dbl> ## 1 0.691 3.57 4.31 0.573
```

Extrapolation is dangerous

"When those blizzards hit the East Coast this winter, it proved to my satisfaction that global warming was a fraud. That snow was freezing cold. But in an alarming trend, temperatures this spring have risen. Consider this: On February 6^{th} it was 10 degrees. Today it hit almost 80. At this rate, by August it will be 220 degrees. So clearly folks the climate debate rages on." Stephen Colbert April 6th, 2010^3

Linear models can be used to approximate the relationship between two variables and is built on an observed random sample. These models have real limitations as linear regression is simply a modeling framework. The truth is almost always much more complex than our simple line. *Extrapolation* occurs when one tries to make a prediction of a response given a value of the predictor that is outside the range of values used to build the model. We only have information about the relationship between two variables in the region around our observed data. We do not know how the data outside of our limited window will behave. Be careful about extrapolating.

Reading computer output

We stored the results of our linear regression model for the possum data in the object poss_mod but it provided only the bare minimum of information. We can get more information using the function summary().

```
summary(poss_mod)
```

```
##
## Call:
## lm(formula = head 1 ~ total 1, data = possum)
##
## Residuals:
##
       Min
                1Q Median
                                3Q
                                        Max
  -7.1877 -1.5340 -0.3345
                            1.2788
                                    7.3968
##
## Coefficients:
##
               Estimate Std. Error t value Pr(>|t|)
                                     8.257 5.66e-13 ***
## (Intercept) 42.70979
                           5.17281
## total_1
                0.57290
                           0.05933
                                     9.657 4.68e-16 ***
## ---
## Signif. codes:
                   0 '*** 0.001 '** 0.01 '* 0.05 '. ' 0.1 ' ' 1
## Residual standard error: 2.595 on 102 degrees of freedom
## Multiple R-squared: 0.4776, Adjusted R-squared: 0.4725
## F-statistic: 93.26 on 1 and 102 DF, p-value: 4.681e-16
```

³http://www.colbertnation.com/the-colbert-report-videos/269929/

The first line repeats the model formula. The second line is a descriptive summary of the residuals, plots of the residuals are more useful than this summary. We then have a table of the model fit. The first column of numbers provides estimates for b_0 and b_1 , respectively. For the next columns, we'll describe the meaning of the columns using the second row, which corresponds to β_1 . Again, the first column provides the point estimate for β_1 . The second column is a standard error for this point estimate. The third column is a t test statistic for the null hypothesis that $\beta_1 = 0$: T = 9.657. The last column is the p-value for the t test statistic for the null hypothesis $\beta_1 = 0$ and a two-sided alternative hypothesis. We will get into more of these details in the next lessons.

The row with the residual standard error is an estimate of the unexplained variance. The next rows give a summary of the model fit and we will discuss in the next lessons.

In the tidyverse we may want to have the table above in a tibble. The broom package, which we have seen before, helps with this effort.

library(broom)

tidy(poss_mod)

```
## # A tibble: 2 x 5
##
     term
                  estimate std.error statistic p.value
     <chr>>
                     <dbl>
                               <dbl>
                                          <dbl>
                                                    <dbl>
                                           8.26 5.66e-13
## 1 (Intercept)
                    42.7
                              5.17
## 2 total 1
                              0.0593
                                           9.66 4.68e-16
                     0.573
```

Exercise:

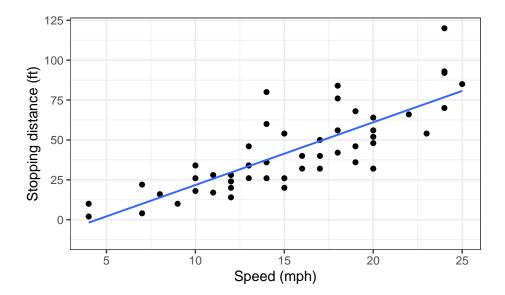
The cars dataset (built-in to R) contains 50 observations of 2 variables. The data give the speed of cars (in mph) and the corresponding distance (in feet) that it took to stop. Attempt to answer the following questions.

a) Build a simple linear regression model fitting distance against speed.

```
cars_mod <- lm(dist~speed,data=cars)
summary(cars_mod)</pre>
```

```
##
## lm(formula = dist ~ speed, data = cars)
##
## Residuals:
                                3Q
                                       Max
      Min
                1Q
                   Median
                   -2.272
## -29.069 -9.525
                             9.215
                                   43.201
##
## Coefficients:
               Estimate Std. Error t value Pr(>|t|)
##
## (Intercept) -17.5791
                            6.7584
                                    -2.601
                                             0.0123 *
                            0.4155
                                     9.464 1.49e-12 ***
## speed
                 3.9324
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
## Residual standard error: 15.38 on 48 degrees of freedom
## Multiple R-squared: 0.6511, Adjusted R-squared: 0.6438
## F-statistic: 89.57 on 1 and 48 DF, p-value: 1.49e-12
```

```
cars %>%
  gf_point(dist~speed) %>%
  gf_lm() %>%
  gf_labs(x="Speed (mph)",y="Stopping distance (ft)") %>%
  gf_theme(theme_bw())
```



As expected, it appears that for larger speeds, stopping distance is greater.

b) Report and interpret the estimated model coefficients.

The estimated intercept term, $\hat{\beta}_0$ is equal to -17.6. This estimate doesn't have a helpful interpretation. Technically, it is the estimated average stopping distance for speed 0. However, "stopping distance" doesn't make sense when a car has no speed. Also, a negative stopping distance doesn't make sense. Furthermore, a speed of 0 is outside of the observed speeds in the data set, so even if a speed of 0 made sense, it is outside the scope of this data and thus an extrapolation.

The estimated slope term, $\hat{\beta}_1$ is equal to 3.9. This means that for an increase of one mph, we expect stopping distance to increase by 3.9 feet, on average.

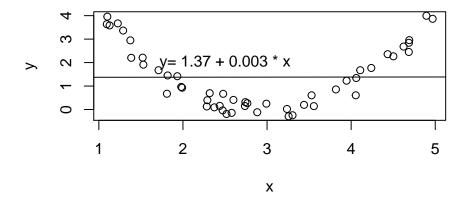
c) Report the estimated common standard deviation of the residuals.

The estimated error variance, $\hat{\sigma}$ is equal to 15.4.

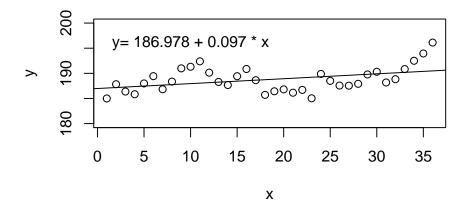
Assumptions

Anytime we build a model, there are assumptions behind it that, if violated, could invalidate the conclusions of the model. In the description of simple linear regression, we briefly mentioned these assumptions. Next lesson, we will discuss how to validate these assumptions.

Linearity. When we build a simple linear regression, we assume that the relationship between the response and the predictor is roughly linear. Suppose two variables are non-linearly related (see plot). While we could build a linear regression model between the two, the resulting model would not be very useful.



Independent Observations. Another assumption is that all observations in a data set are independent of one another. A common way this assumption is violated is by using time as the predictor variable. For example, suppose we were interested in how an individual's weight changes over time. While it may be tempting to plot this and fit a regression line through the data, the resulting model is inappropriate, as simple linear regression assumes that each observation is independent.



Constant Error Variance. In simple linear regression, we assume that the residuals come from a normal distribution with mean 0 and constant standard deviation σ . Violation of this assumption is usually manifested as a "megaphone" pattern in the scatterplot. Specifically, as the value of the predictor increases, the variance in the response also increases, resulting in greater spread for larger values of the predictor.

Normality of Errors. Again, we assume that the residuals are normally distributed. Normality of residuals is not easy to see graphically, so we have to use other diagnostics to check this assumption.

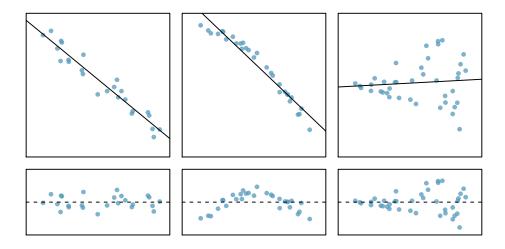
The last three assumptions are important not necessarily for estimating the relationship, but for *inferring* about the relationship. In future lessons, we will discuss how to use a model for prediction, and how to build a confidence/prediction interval around a prediction. Also, we will discuss inference about the coefficient

estimates in a model. Violation of one of the last three assumptions will impact how we can make estimate variability around an estimate.

Residual plots

One purpose of residual plots is to identify characteristics or patterns still apparent in data after fitting a model. These can help to evaluate the assumptions.

The following figure shows three scatterplots with linear models in the first row and residual plots in the second row.



In the first data set (first column), the residuals show no obvious patterns. The residuals appear to be scattered randomly around the dashed line that represents 0.

The second data set shows a pattern in the residuals. There is some curvature in the scatterplot, which is more obvious in the residual plot. We should not use a straight line to model these data. Instead, a more advanced technique should be used.

In the last plot the spread, variance of the data, seems to increase as the explanatory variable increases. We can see this clearly in the residual plot. To make inference using the t or F distribution would require a transformation to equalize the variance.

Summary

We have introduced the ideas of linear regression in this lesson. There are many new terms as well as new R functions to learn. We will continue to use these ideas in the remainder of this block of material. Next we will learn about inference and prediction.

File Creation Information

• File creation date: 2020-11-09

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