Regression Inference Notes

Lt Col Ken Horton Lt Col Kris Pruitt Professor Bradley Warner

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Objectives

1) Given a simple linear regression model, conduct inference on the coefficients β_0 and β_1.
2) Given a simple linear regression model, calculate the predicted response for a given value of the predictor.
3) Build and interpret confidence and prediction intervals for values of the response variable.

Introduction

In this lesson we discuss uncertainty in the estimates of the slope and y-intercept for a regression line. This will allow us to perform inference and predictions. Just as we identified standard errors for point estimates in previous lessons, we first discuss standard errors for these new estimates. This lesson is a classical lesson in the sense that we will be using the normal distribution. We will assume that the errors are normally distributed with constant variance. Later in the course, we will relax these assumptions.

Regression

Last lesson, we introduced linear models using the simple linear regression model:

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

where here we assume the error term follows a normal distribution with mean 0 and constant standard deviation σ. Using the method of least squares, which does not require the assumption of normality, we obtain estimates of β_0 and β_1:

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

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

Using these estimates, for a given value of the predictor, x_*, we can obtain a prediction of the response variable. The resulting prediction, which we will denote $\hat{Y}_*$, is the **average** or **expected value** of the response given predictor value x_*:

$$\hat{Y}_* = \hat{\beta}_0 + \hat{\beta}_1 x_*$$

The reason this model returns the expected value of the response at the given value of the predictor is because the error term has an expected value of zero. As a review of the properties of expectation:

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

because β_0, β_1, and X are constants.

It should be abundantly clear by now that $\hat{Y}_*$, $\hat{\beta}_0$, and $\hat{\beta}_1$ are ***estimates***. Being estimates, they are dependent on our random sample, our data. If we collect a new random sample from the same population, we will get new estimates. Thus, we can think of $\hat{Y}_*$, $\hat{\beta}_0$, and $\hat{\beta}_1$ as **random variables**. Like all random variables, they have distributions. We can use the distribution of an estimate to build confidence intervals and conduct hypothesis tests about the true values of the parameter it is intended to estimate. These estimates are unbiased, they are centered around the actual values of Y, β_0 and β_1, respectively.

Review of assumptions

We will review the assumptions of the least squares model because they are important for inference. Refer to the figure below which plots the linear regression in the top row and the residuals in the second row. We generally assume the following:

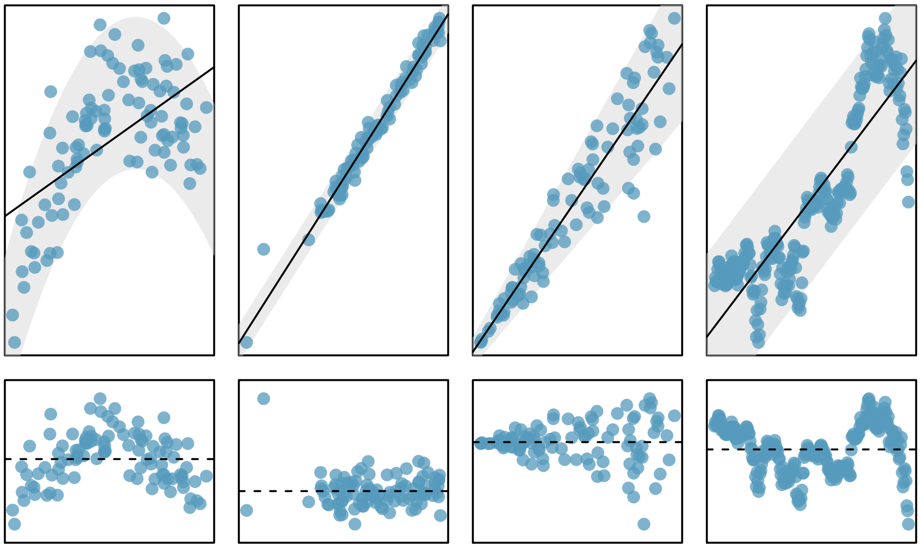
1. **Linearity**. The data should show a linear trend. If there is a nonlinear trend, a transformation of the explanatory variable or an advanced regression method from Math 378 should be applied. When looking at the residual plot, if the trend is linear, we should see a spread of points that are flat. The left column is an example of a nonlinear relationship. The top plot is the regression plot and we can see what looks like a quadratic relationship instead of a linear one. The residual plot, the plot in the lower left corner, also exhibits this non-linear trend.

2. **Nearly normal residuals**. Generally the residuals must be nearly normal to use a t or F for inference. When this assumption is found to be unreasonable, it is usually because of **outliers** or concerns about **influential** points. An example of non-normal residuals is shown in the second column of the figure. A **qq** plot is also useful as a diagnostic tool as we have seen. We can still use the **bootstrap** as an inference tool if the normality assumption is unreasonable.

3. **Constant variability**. The variability of points around the least squares line remains roughly constant. An example of non-constant variability is shown in the third panel of the figure. The constant variability assumption is needed for the t and F distributions. It is not required for the bootstrap method.

4. **Independent observations**. Be cautious about applying regression to data collected sequentially in what is called a **time series**. Such data may have an underlying structure that should be considered in a model and analysis. An example of a time series where independence is violated is shown in the fourth panel of the figure. More advanced methods are required for time series data even including using a bootstrap.

In a future lesson we will explore more regression diagnostics.



Estimates' probability distributions

With the assumption that the error term is normally distributed, we can find the distributions of our estimates, which turn out to be normal:

$$\hat{\beta}_0 \sim N\left(\beta_0, \sigma\sqrt{\frac{1}{n} + \frac{\bar{x}^2}{\sum(x_i - \bar{x})^2}}\right)$$

$$\hat{\beta}_1 \sim N\left(\beta_1, \frac{\sigma}{\sqrt{\sum(x_i - \bar{x})^2}}\right)$$

$$\hat{Y}_* \sim N\left(\beta_0 + \beta_1 x_*, \sigma\sqrt{\frac{1}{n} + \frac{(x_* - \bar{x})^2}{\sum(x_i - \bar{x})^2}}\right)$$

Notice that all three of these are unbiased, the expected value is equal to the parameter being estimated. Looking at the variance of the slope estimate we can see that is a function of the underlying unexplained variance, σ^2 and the data. The denominator is increased by having a larger spread in the explanatory variable. The slope of the estimated line is more stable, less variable, if the independent variables has high variance. That is interesting. If you are designing an experiment, this gives you insight in how to select the range of values for your explanatory variable. Math 359 is a course that discusses this point in detail.

Inference

Now that we know how the coefficient estimates and the average predicted values behave, we can perform inference on their true values. Let's take $\hat{\beta}_1$ for demonstration:

$$\hat{\beta}_1 \sim N\left(\beta_1, \frac{\sigma}{\sqrt{\sum(x_i - \bar{x})^2}}\right)$$

Thus,

$$\frac{\hat{\beta}_1 - \beta_1}{\frac{\sigma}{\sqrt{\sum(x_i - \bar{x})^2}}} \sim N(0, 1)$$

However, note that the expression on the left depends on error standard deviation, σ. In reality, we will not know this value and will have to estimate it with

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

where $\hat{e}_i$ is the observed ith **residual** ($\hat{e}_i = y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i$).

As we learned in the last block, if we replace population standard deviation (σ) with an estimation, the resulting random variable no longer has the standard normal distribution. In fact, it can be shown that

$$\frac{\hat{\beta}_1 - \beta_1}{\frac{\hat{\sigma}}{\sqrt{\sum(x_i-\bar{x})^2}}} \sim \mathsf{t}\left(n-2\right)$$

We can use this information to build a $(1-\alpha)*100\%$ confidence interval for β_1. First, we recognize that

$$\mathrm{P}\left(-t_{\alpha/2,n-2} \leq \frac{\hat{\beta}_1 - \beta_1}{\frac{\hat{\sigma}}{\sqrt{\sum(x_i-\bar{x})^2}}} \leq t_{\alpha/2,n-2}\right) = \alpha$$

Solving the expression inside the probability statement for β_1 yields a confidence interval of

$$\beta_1 \in \left(\hat{\beta}_1 \pm t_{\alpha/2,n-2}\frac{\hat{\sigma}}{\sqrt{\sum(x_i-\bar{x})^2}}\right)$$

We can also evaluate the null hypothesis $H_0: \beta_1 = \beta_1^*$. If the true value of β_1 were β_1^*, then the estimated $\hat{\beta}_1$ should be around that value. In fact, if H_0 were true, the value

$$\frac{\hat{\beta}_1 - \beta_1^*}{\frac{\hat{\sigma}}{\sqrt{\sum(x_i-\bar{x})^2}}}$$

has the t distribution with $n-2$ degrees of freedom. Thus, once we collect a sample and obtain the observed $\hat{\beta}_1$ and $\hat{\sigma}$, we can calculate this quantity and determine whether it is far enough from zero to reject H_0.

Similarly, we can use the distribution of $\hat{\beta}_0$ to build a confidence interval or conduct a hypothesis test on β_0, but we usually don't. This has to do with the interpretation of β_0.

Starbucks

That was a great deal of mathematics and theory. Let's put it to use on the example from Starbucks. In the file `data/starbucks.csv` we have nutritional facts for several Starbucks food items. We used this data in the homework for last lesson. We will use this data again to illustrate the ideas we have introduced in this section.

Read in the data.

```
starbucks <- read_csv("data/starbucks.csv")  %>%
  mutate(type=factor(type))
```

Exercise
Summarize and explore the data.

Let's look at a summary of the data.

```
glimpse(starbucks)
```

```
## Rows: 77
## Columns: 7
## $ item     <chr> "8-Grain Roll", "Apple Bran Muffin", "Apple Fritter", "Ban...
## $ calories <dbl> 350, 350, 420, 490, 130, 370, 460, 370, 310, 420, 380, 320...
## $ fat      <dbl> 8, 9, 20, 19, 6, 14, 22, 14, 18, 25, 17, 12, 17, 21, 5, 18...
## $ carb     <dbl> 67, 64, 59, 75, 17, 47, 61, 55, 32, 39, 51, 53, 34, 57, 52...
## $ fiber    <dbl> 5, 7, 0, 4, 0, 5, 2, 0, 0, 0, 2, 3, 2, 2, 3, 3, 2, 3, 0, 2...
## $ protein  <dbl> 10, 6, 5, 7, 0, 6, 7, 6, 5, 7, 4, 6, 5, 5, 12, 7, 8, 6, 0,...
## $ type     <fct> bakery, bakery, bakery, bakery, bakery, bakery, bakery, ba...
```

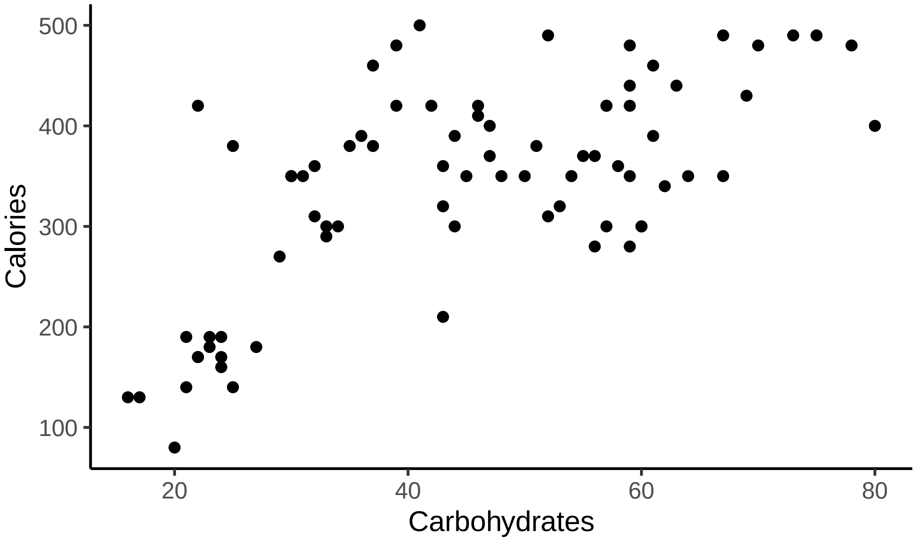
```
inspect(starbucks)
```

```
## 
## categorical variables:  
##   name     class levels  n missing
## 1 item character     77 77       0
## 2 type    factor      7 77       0
##                                     distribution
## 1 8-Grain Roll (1.3%) ...                       
## 2 bakery (53.2%), petite (11.7%) ...            
## 
## quantitative variables:  
##          name   class min  Q1 median  Q3 max       mean         sd  n missing
## ...1 calories numeric  80 300    350 420 500 338.831169 105.368701 77       0
## ...2      fat numeric   0   9     13  18  28  13.766234   7.095488 77       0
## ...3     carb numeric  16  31     45  59  80  44.870130  16.551634 77       0
## ...4    fiber numeric   0   0      2   4   7   2.220779   2.112764 77       0
## ...5  protein numeric   0   5      7  15  34   9.480519   8.079556 77       0
```

> **Exercise**
> Create a scatterplot of calories and carbohydrate, carbs, content.

Let's predict calories from the carbohydrate content. Let's use a scatterplot to examine the relationship.

```
starbucks %>%
  gf_point(calories~carb) %>%
  gf_labs(x="Carbohydrates",y="Calories") %>%
  gf_theme(theme_classic())
```



Exercise Use `R` to fit a linear regression model by regressing `calories` on `carb`.

The results of fitting a linear least squares model is stored in the `star_mod` object.

```
star_mod <- lm(formula = calories ~ carb, data = starbucks)
```

```
summary(star_mod)
```

```
##
## Call:
## lm(formula = calories ~ carb, data = starbucks)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -151.962  -70.556   -0.636   54.908  179.444
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept) 146.0204    25.9186   5.634 2.93e-07 ***
## carb          4.2971     0.5424   7.923 1.67e-11 ***
## ---
## Signif. codes:  0 ’***’ 0.001 ’**’ 0.01 ’*’ 0.05 ’.’ 0.1 ’ ’ 1
##
## Residual standard error: 78.26 on 75 degrees of freedom
## Multiple R-squared:  0.4556, Adjusted R-squared:  0.4484
## F-statistic: 62.77 on 1 and 75 DF,  p-value: 1.673e-11
```

Hypothesis test In the second row of the **Coefficients** table we have our point estimate, standard error, test statistic, and p-value for the slope.

The hypothesis for this output is
H_0: $\beta_1 = 0$. The true linear model has slope zero.
H_A: $\beta_1 \neq 0$. The true linear model has a slope different than zero. The higher the carb content, the greater the average calorie content or vice-versa.

Our estimate of the slope is 4.297 with a standard error of 0.5424. Just for demonstration purposes, we will use `R` to calculate the test statistic and p-value. The test statistic under the null hypothesis is:

$$\frac{\hat{\beta}_1 - 0}{\frac{\hat{\sigma}}{\sqrt{\sum(x_i - \bar{x})^2}}}$$

The denominator is the standard error of the estimate. The estimate of the residual standard deviation is reported in the last line as 78.26. But it is just the square root of the sum of squared residuals divided by the degrees of freedom.

```r
sighat<-sqrt(sum((star_mod$residuals)^2)/75)
sighat
```

```
## [1] 78.25956
```

The standard error of the slope estimate is, and confirmed in the table:

```r
std_er<-sighat/sqrt(sum((starbucks$carb-mean(starbucks$carb))^2))
std_er
```

```
## [1] 0.5423626
```

The test statistic is

```r
(4.2971-0)/std_er
```

```
## [1] 7.922928
```

And the p-value

```r
2*pt((4.2971-0)/std_er,73,lower.tail = FALSE)
```

```
## [1] 1.965319e-11
```

This is slightly different from the table value because of the precision of the computer and the small p-value.

We reject H_0 in favor of H_A because the data provide strong evidence that the true slope parameter is greater than zero.

The computer software uses zero in the null hypothesis, if you wanted to test another value of the slope then you would have to do the calculations step by step like we did above.

By the way, this was not a `tidy` way to do the calculation. The `broom` package makes it easier to use `tidy` ideas on the regression model.

Confidence interval We could calculate the confidence interval from the point estimate, standard error, and critical value but we will let R do it for us.

```
confint(star_mod)
```

```
##                 2.5 %     97.5 %
## (Intercept) 94.387896 197.652967
## carb         3.216643   5.377526
```

This confidence interval does not contain the value 0. This suggests that a value of 0 is not feasible for β_1.

In the end, we would declare that carbohydrate and calorie content of Starbucks menu items are linearly correlated. However, we DID NOT prove causation. We simply showed that the two variables are correlated.

Inference on Predictions

Similarly, we can take advantage of the distribution of $\hat{Y}_*$ to build a confidence interval on Y_* (the average value of Y at some value x_*):

$$Y_* \in \left(\hat{Y}_* \pm t_{\alpha/2,n-2}\hat{\sigma}\sqrt{\frac{1}{n}+\frac{(x_*-\bar{x})^2}{\sum(x_i-\bar{x})^2}}\right)$$

There are a couple of things to point out about the above. First, note that the width of the confidence interval is dependent on how far x_* is from the average value of x. The further we are from the center of the data, the wider the interval will be.

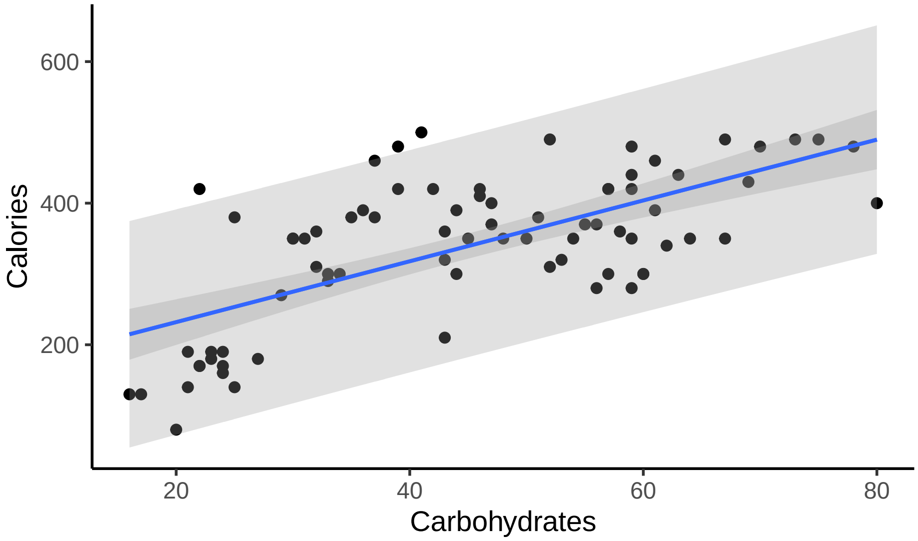
Second, note that this in an interval on Y_* the ***average*** value of Y at x_*. If we want to build an interval for a single observation of Y (Y_{new}), we will need to build a *prediction* interval, which is considerably wider than a confidence interval on Y_*:

$$Y_{new} \in \left(\hat{Y}_* \pm t_{\alpha/2,n-2}\hat{\sigma}\sqrt{1+\frac{1}{n}+\frac{(x_*-\bar{x})^2}{\sum(x_i-\bar{x})^2}}\right)$$

Starbucks

Continuing with the `starbucks` example. In plotting the data, we can have R plot the confidence and prediction bands. We will observe the width of these intervals increase as we move away from the center of the data and also that prediction intervals are wider.

```
starbucks %>%
  gf_point(calories~carb) %>%
  gf_labs(x="Carbohydrates",y="Calories") %>%
  gf_lm(stat="lm",interval="confidence") %>%
  gf_lm(stat="lm",interval="prediction") %>%
  gf_theme(theme_classic())
```



We have not done diagnostics yet and it may be that using a linear regression model for this data may not be appropriate. But for the sake of learning we will continue. To find these confidence intervals we need a value for `carb` so let's use 60 and 70.

We create a dataframe with the values of `carb` in it. Then we will use the `predict` function to find the confidence interval. Using the option `interval` set to `confidence` will return a confidence interval for the average calorie content for each value in the new dataframe.

```
new_carb <- data.frame(carb=c(60,70))
predict(star_mod, newdata = new_carb, interval = 'confidence')
```

```
##        fit      lwr      upr
## 1 403.8455 379.7027 427.9883
## 2 446.8163 414.3687 479.2640
```

As an example, we are 95% confident that the average calories in a Starbuck's menu item with 60 grams of carbs is between 379.7 and 428.0.

Exercise Give the 95% confidence interval of average calories for 70 grams of carbohydrates.

We are 95% confident that the average calories in a Starbuck's menu item with 70 grams carbs is between 414.4 and 479.3.

For the prediction interval, we simply need to change the option in `interval`:

```
new_carb <- data.frame(carb=c(60,70))
predict(star_mod, newdata = new_carb, interval = 'prediction')
```

```
##        fit      lwr      upr
## 1 403.8455 246.0862 561.6048
## 2 446.8163 287.5744 606.0582
```

We are 95% confident the next Starbuck's menu item that has 60 grams of carbs will have a calorie content between 246 and 561. Notice how prediction intervals are wider since they are intervals on individual observations and not an averages.

Summary

This lesson has introduced the process of inference for a simple linear regression model. We tested the slope estimate as well as generated confidence intervals for average and individual predicted values.

File Creation Information

- File creation date: 2020-11-09
- Windows version: Windows 10 x64 (build 18362)
- R version 3.6.3 (2020-02-29)
- `mosaic` package version: 1.7.0
- `tidyverse` package version: 1.3.0