STAT 305: Lecture 5

Amin Shirazi

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Chapter 4: Describing Relationships Between Variables

Introduction to Models

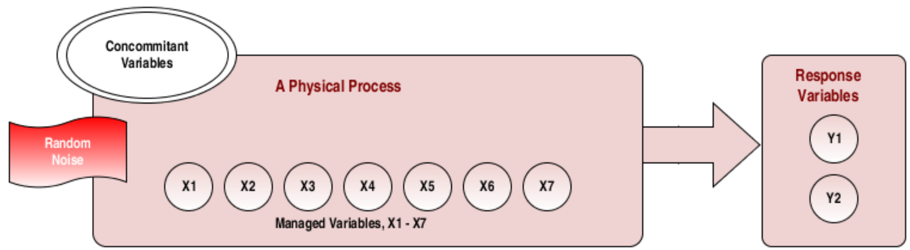
Course page:
ashirazist.github.io/stat305.github.io

Chapter 4, Section 1

Linear Relationships Between Variables

Describing Relationships

We have a standard idea of how our experiment works:



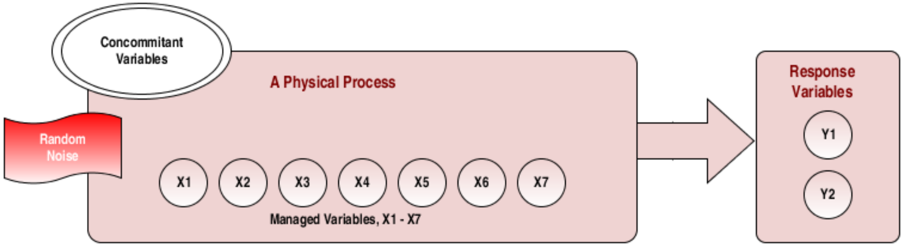
and we know that with an valid experiment, we can say that the changes in our experimental variables actually *cause* changes in our response.

But how do we describe those response when we know that random error would make each result different…

Describing Relationships

The Underlying Idea

Idea



We start with a valid mathematical model, for instance a line:

$$y = \beta_0 + \beta_1 \cdot x$$

In this case,

- β_0 is the intercept - when $x = 0$, $y = \beta_0$.
- β_1 is the slope - when x increase by one unit, y increases by β_1 units.

Example: Stress on Bars

An experiment examining the effects of **stress** on **time until fracture** is performe by taking a sample of 10 stainless steel rods immersed in 40% CaCl solution at 100 degrees Celsius and applying different amounts of uniaxial stress.

The results are recorded below:

stress (kg/mm^2)	2.5	5.0	10.0	15.0	17.5	20.0	25.0	30.0	35.0	40.0
lifetime (hours)	63	58	55	61	62	37	38	45	46	19

A good first place to investigate the relationship between our experimental variables (in this case, stress) and the response (in this case, lifetime) is to use a scatterplot and look to see if there might be any basic mathematical function that could describe the relationship between the variables.

Describing Relationships

Idea

Ex: Bar Stress

Example: Strain on Bars (continued)

Our data:

stress (kg/mm^2)	2.5	5.0	10.0	15.0	17.5	20.0	25.0	30.0	35.0	40.0
lifetime (hours)	63	58	55	61	62	37	38	45	46	19

- Plotting stress along the x-axis and plotting lifetime along the y-axis we get

Describing Relationships

Idea

Ex: Bar Stress

Example: Strain on Bars (continued)

Our data:

stress (kg/mm^2)	2.5	5.0	10.0	15.0	17.5	20.0	25.0	30.0	35.0	40.0
lifetime (hours)	63	58	55	61	62	37	38	45	46	19

- Examining the plot, we might determine that there could be a linear relationship between the two. The red line looks like it fits the data pretty well.

Describing Relationships

Idea

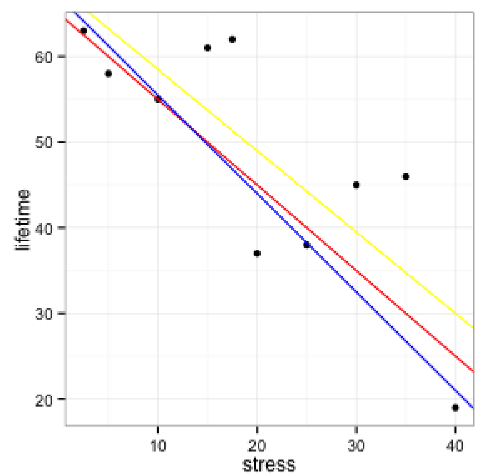
Ex: Bar Stress

Example: Strain on Bars (continued)

Our data:

stress (kg/mm^2)	2.5	5.0	10.0	15.0	17.5	20.0	25.0	30.0	35.0	40.0
lifetime (hours)	63	58	55	61	62	37	38	45	46	19

- But there are several other lines that fit the data pretty well, too.



- How do we decide which is best?

Describing Relationships

Idea

Ex: Bars

Fitting Lines

Where the line comes from

When we are trying to find a line that fits our data what we are *really* doing is saying that there is a true physical relationship between our experimental variable x is related to our response y that has the following form:

Theoretical Relationship

$$y = \beta_0 + \beta_1 \cdot x$$

However, the response we observe is also effected by random noise:

Observed Relationship

$$y = \beta_0 + \beta_1 \cdot x + \text{errors}$$

$$= \text{signal} + \text{noise}$$

If we did a good job, hopefully we will have small enough errors so that we can say

$$y \approx \beta_0 + \beta_1 \cdot x$$

Describing Relationships

Idea

Ex: Bars

Fitting Lines

Where the line comes from

So, if things have gone well, we are attempting to estimate the value of β_0 and β_1 from our observed relationship

$$y \approx \beta_0 + \beta_1 \cdot x$$

Using the following notation:

- b_0 is the estimated value of β_0 and
- b_1 is the estimated value of β_1
- $\hat{y}$ is the estimated response

We can write a **fitted relationship**:

$$\hat{y} = b_0 + b_1 \cdot x$$

The key here is that we are going from the underlying *true, theoretical* relationship to an *estimated* relationship.

In other words, we will never get the true values β_0 and β_1 but we can estimate them.

However, this doesn't tell us *how* to estimate them.

The principle of Least Squares

A good estimte should be based on the data.

Suppose that we have observed responses $y_1, y_2, \ldots, y_n$ for experimental variables set at $x_1, x_2, \ldots, x_n$.

Then the **Principle of Least Squares** says that the best estimate of β_0 and β_1 are values that **minimize**

$$\sum_{i=1}^{n} (y_i - \hat{y}_i)^2$$

In our case, since $\hat{y}_i = b_0 + b_1 \cdot x_i$ we need to choose values for b_0 and b_1 that minimize

$$\sum_{i=1}^{n} (y_i - \hat{y}_i)^2 = \sum_{i=1}^{n} \left(y_i - (b_0 + b_1 \cdot x_i)\right)^2$$

In other words, we need to minimize something with respect to two values we get to choose - we can do this by taking derivatives.

Deriving the Least Squares Estimates

We can rewrite the target we want to minimize so that the variables are less tangled together:

$$\sum \_i = 1^n (y\_i - \hat{y}\_i)^2 = \sum \_i = 1^n (y\_i - (b\_0 + b\_1x\_i))^2$$

$$= \sum \_i = 1^n \left(y\_i^2 - 2y\_i(b\_0 + b\_1x\_i) + (b\_0 + b\_1x\_i)^2\right)$$

$$= \sum \_i = 1^n y\_i^2 - \sum \_i = 1^n 2y\_i(b\_0 + b\_1x\_i) + \sum \_i = 1$$

$$= \sum \_i = 1^n y\_i^2 - \sum \_i = 1^n (2y\_ib\_0 + 2y\_ib\_1x\_i) + \sum \_i$$

$$= \sum \_i = 1^n y\_i^2 - \sum \_i = 1^n 2y\_ib\_0 - \sum \_i = 1^n 2y\_ib\_1x\_$$

$$= \sum \_i = 1^n y\_i^2 - 2b\_0 \sum \_i = 1^n y\_i - 2b\_1 \sum \_i = 1^n y\_ix\_$$

Deriving the Least Squares Estimates (continued)

How do we minimize it?

- Since we have two "variables" we need to take derivates with respect to both.
- Remember we have our data so we know every value of x_i and y_i and can treat those parts as constants.

The derivative with respect to $\mathbf{b_0}$:

$$-2\sum_{i=1}^{n} y_i + 2nb_0 + 2b_1\sum_{i=1}^{n} x_i$$

The derivative with respect to $\mathbf{b_0}$:

$$-2b_0\sum_{i=1}^{n} y_i x_i + 2b_0\sum_{i=1}^{n} x_i + 2b_1\sum_{i=1}^{n} x_i^2$$

Deriving the Least Squares Estimates (continued)

We set both equal to 0 and solve them at the same time:

$$-2\sum\_i = 1^n y\_i + 2nb\_0 + 2b\_1\sum\_i$$

$$-2b\_0\sum\_i = 1^n y\_ix\_i + 2b\_0\sum\_i = 1^n x\_i + 2b\_1\sum\_i =$$

We can rewrite the first equation as:

$$b\_0 = \frac{1}{n}\sum\_i = 1^n y\_i - b\_1\frac{1}{n}\sum\_i = 1^n x\_i$$

$$= \bar{y} - b\_1\bar{x}$$

and then replace all b_0 in the second equation (there is some algebra type stuff along the way, of course)

Deriving the Least Squares Estimates (continued)

After a little simplification we arrive at our estimates:

Least Squares Estimates for Linear Fit

$$b\_0 = \bar{y} - b\_1\bar{x}$$

$$b\_1 = \frac{\sum \_i = 1^n y\_ix\_i - n\bar{x}\bar{y}}{\sum \_i = 1^n x\_i^2 - n\bar{x}^2}$$

$$= \frac{\sum \_i = 1^n (x\_i - \bar{x})(y\_i - \bar{y})}{\sum \_i = 1^n (x\_i - \bar{x})^2}$$

Wrap Up

- Don't try to memorize the derivation. I will never ask you to do that on an exam.
- Try to understand the simplification steps - the ones that moved constants out of summations for example.
- This is one rule - there are others, but **Least Squares Estimates** have some useful properties that will make