

STAT 305: Chapter 4

Part I

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Course page:
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Recap on Numerical Summaries (Chapter 3)

Summaries of Variability (Measures of Spread)

Chapter 4: Describing Relationships Between Variables

Introduction to Models

Recap

Spread

Summaries of Variability (Measures of Spread)

Motivated by asking what kind of *variability is seen in the data* or *how spread out* the data is.

Range: The difference between the highest and lowest values (Range = max - min)

IQR: The Interquartile Range, how spread out is the middle 50% (IQR = Q3 - Q1)

Variance/Standard Deviation: Uses squared distance from the mean.

	Variance	Standard Deviation
Population	$\sigma^2 = \frac{1}{N} \sum_{i=1}^N (x_i - \bar{x})^2$	$\sigma = \sqrt{\frac{1}{N} \sum_{i=1}^N (x_i - \bar{x})^2}$
Sample	$s^2 = \frac{1}{n-1} \sum_{i=1}^n (x_i - \bar{x})^2$	$s = \sqrt{\frac{1}{n-1} \sum_{i=1}^n (x_i - \bar{x})^2}$

Recap

Spread

Summarizing Data Numerically

Example: Taking a sample of size 5 from a population we record the following values:

68, 57, 67, 52, 60

Find the variance and standard deviation of this sample.

Example: Finding the Variance

Since we are told it is a sample, we need to use **sample variance**. The mean of 68, 57, 67, 52, 60 is 60.8

$$\begin{aligned}s^2 &= \frac{1}{n-1} \sum_{i=1}^5 (x_i - \bar{x})^2 \\&= \frac{1}{n-1} ((x_1 - \bar{x})^2 + (x_2 - \bar{x})^2 + (x_3 - \bar{x})^2 + (x_4 - \bar{x})^2 + (x_5 - \bar{x})^2) \\&= \frac{1}{5-1} ((68 - 60.8)^2 + (57 - 60.8)^2 + (67 - 60.8)^2 + (52 - 60.8)^2 + (60 - 60.8)^2) \\&= \frac{1}{4} ((7.2)^2 + (-3.8)^2 + (6.2)^2 + (-8.8)^2 + (-0.8)^2) \\&= \frac{1}{4} (51.84 + 14.44 + 38.44 + 77.44 + 0.64) \\&= 45.7\end{aligned}$$

Example: Finding the Standard Deviation

With s^2 known, finding s is simple:

$$\begin{aligned}s &= \sqrt{s^2} \\ &= \sqrt{45.7} \\ &= 6.7601775\end{aligned}$$

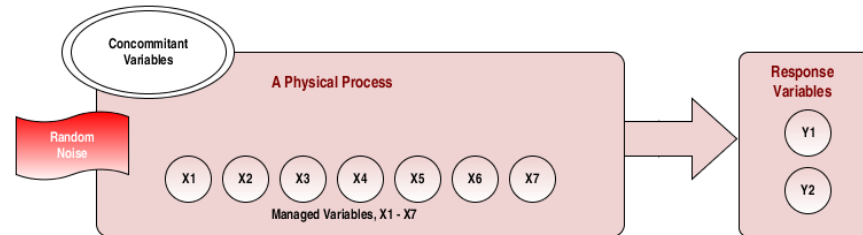
Chapter 4, Section 1

Linear Relationships Between Variables

Describing Relationships

Idea

We have a standard idea of how our experiment works:



Bivariate data often arise because a quantitative experimental variable x has been varied between several different settings (treatment).

It is helpful to have an equation relating y (the response) to x when the purposes are summarization, interpolation, limited extrapolation, and/or process optimization/adjustment.

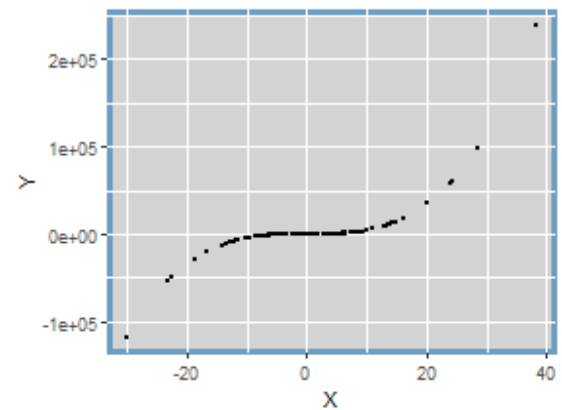
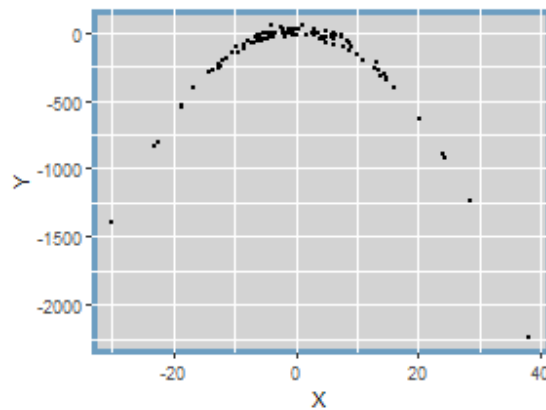
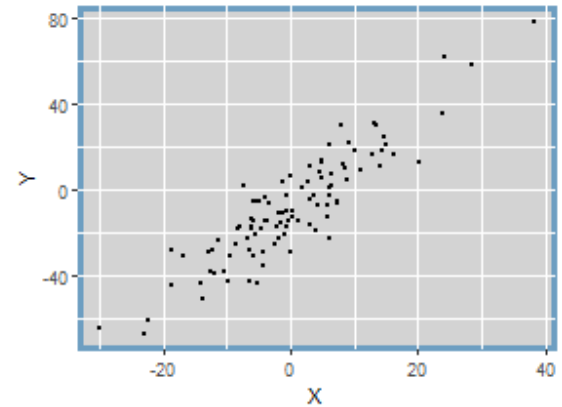
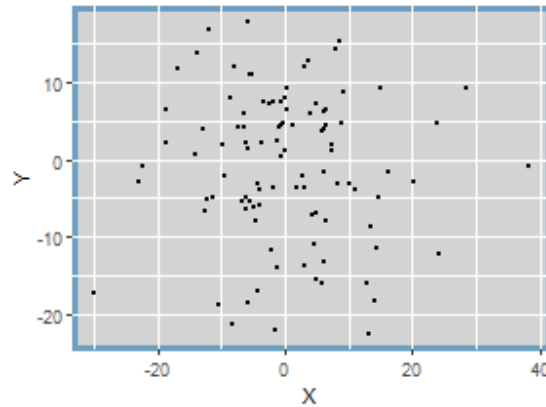
and we know that with a valid experiment, we can say that the changes in our experimental variables actually *cause* changes in our response.

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

Describing Relationships

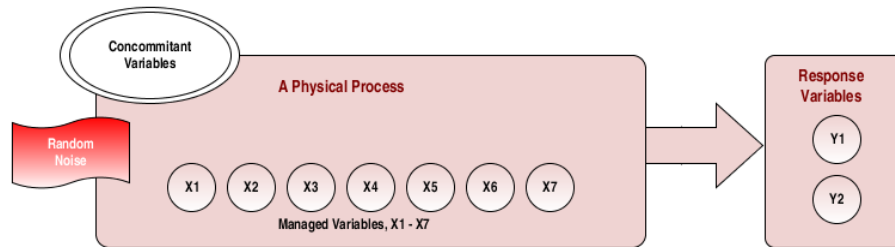
Types of relationships

Idea



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.

Describing Relationships

Example: Stress on Bars

Idea

An experiment examining the effects of **stress** on **time until fracture** is performed 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.

Ex: Bar 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

Example: Strain on Bars (continued)

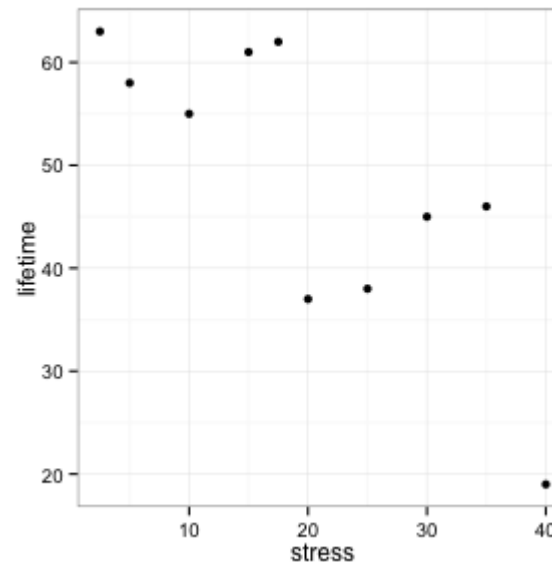
Our data:

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

Idea

Ex: Bar Stress

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



Describing Relationships

Example: Strain on Bars (continued)

Our data:

Idea

Ex: Bar Stress

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

Example: Strain on Bars (continued)

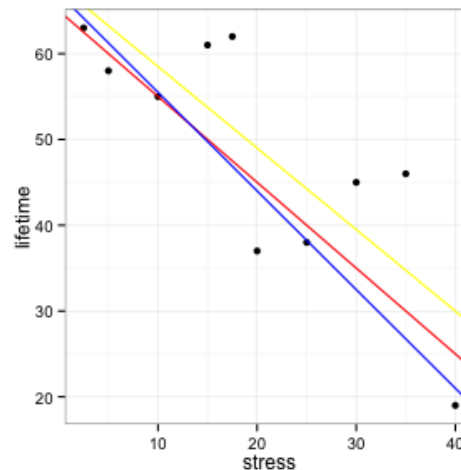
Our data:

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

Idea

Ex: Bar Stress

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



- How do we decide which is best?

Describing Relationships

Where the line comes from

Idea

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:

Ex: Bars

Theoretical Relationship

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

Fitting Lines

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

Where the line comes from

Idea

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

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

Ex: Bars

Using the following notation:

Fitting Lines

- 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.

Describing Relationships

The principle of Least Squares

A good estimate should be based on the data.

Idea

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

Ex: Bars

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

Fitting Lines

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

Best Estimate

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

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

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(Optional reading)

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

Describing Relationships

Deriving the Least Squares Estimates (continued)

How do we minimize it?

Idea

- Since we have two "variables" we need to take derivatives with respect to both.

Ex: Bars

- Remember we have our data so we know every value of x_i and y_i and can treat those parts as constants.

Fitting Lines

The derivative with respect to b_0 :

Best Estimate

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

The derivative with respect to b_1 :

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

Describing Relationships

Deriving the Least Squares Estimates (continued)

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

Idea

$$-2 \sum_{i=1}^n y_i + 2nb_0 + 2b_1 \sum_{i=1}^n x_i = 0$$

Ex: Bars

$$-2b_0 \sum_{i=1}^n y_i x_i + 2b_0 \sum_{i=1}^n x_i + 2b_1 \sum_{i=1}^n x_i^2 = 0$$

Fitting Lines

Best Estimate

We can rewrite the first equation as:

$$\begin{aligned} b_0 &= \frac{1}{n} \sum_{i=1}^n y_i - b_1 \frac{1}{n} \sum_{i=1}^n x_i \\ &= \bar{y} - b_1 \bar{x} \end{aligned}$$

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

Describing Relationships

Deriving the Least Squares Estimates (continued)

After a little simplification we arrive at our estimates:

Idea

Least Squares Estimates for Linear Fit

$$b_0 = \bar{y} - b_1 \bar{x}$$

Ex: Bars

$$b_1 = \frac{\sum_{i=1}^n y_i x_i - n \bar{x} \bar{y}}{\sum_{i=1}^n x_i^2 - n \bar{x}^2}$$

Fitting Lines

$$= \frac{\sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^n (x_i - \bar{x})^2}$$

Best Estimate

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 them the obvious best choice as we continue the course.

Describing Relationships

Example: Strain on Bars

Idea

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

Ex: Bars

Estimating the best slope and intercept using least squares:

Fitting Lines

$$b_0 = \bar{y} - b_1 \bar{x}$$

Best Estimate

$$b_1 = \frac{\sum_{i=1}^n y_i x_i - n \bar{x} \bar{y}}{\sum_{i=1}^n x_i^2 - n \bar{x}^2}$$
$$= \frac{\sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y})}{\sum_{i=1}^n (x_i - \bar{x})^2}$$

In our case we have the following:

$$\sum_{i=1}^{10} y_i = 484, \sum_{i=1}^{10} x_i = 200, \sum_{i=1}^{10} x_i y_i = 8407.5, \sum_{i=1}^{10} x_i^2 = 5412.5,$$

Describing Relationships

Example: Strain on Bars

Idea

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

Ex: Bars

$$\sum_{i=1}^{10} y_i = 484, \sum_{i=1}^{10} x_i = 200, \sum_{i=1}^{10} x_i y_i = 8407.5, \sum_{i=1}^{10} x_i^2 = 5412.5,$$

Fitting Lines

Using this we can estimate b_1 :

Best Estimate

$$\begin{aligned} b_1 &= \frac{\sum_{i=1}^n y_i x_i - n \bar{x} \bar{y}}{\sum_{i=1}^n x_i^2 - n \bar{x}^2} \\ &= \frac{8407.5 - 10 \left(\frac{200}{10} \right) \left(\frac{484}{10} \right)}{5412.5 - 10 \left(\frac{200}{10} \right)^2} \\ &= \frac{-1272.5}{1412.5} \\ &\approx -0.9009 \end{aligned}$$

Describing Relationships

Example: Strain on Bars

Idea

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

Ex: Bars

$$\sum_{i=1}^{10} y_i = 484, \sum_{i=1}^{10} x_i = 200, \sum_{i=1}^{10} x_i y_i = 8407.5, \sum_{i=1}^{10} x_i^2 = 5412.5,$$

Fitting Lines

And using b_1 we can estimate b_0 :

Best Estimate

$$\begin{aligned} b_0 &= \bar{y} - b_1 \bar{x} \\ &= \left(\frac{484}{10} \right) - b_1 \left(\frac{200}{10} \right) \\ &= 48.4 - \left(\frac{-1272.5}{1412.5} \right) 20.0 \\ &= 66.4177 \end{aligned}$$

Which gives us the **Fitted Relationship**:

Describing Relationships

Example: Strain on Bars

Idea

stress
(kg/mm²)

2.5	5.0	10.0	15.0	17.5	20.0	25.0	30.0	35.0	40.0
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lifetime
(hours)

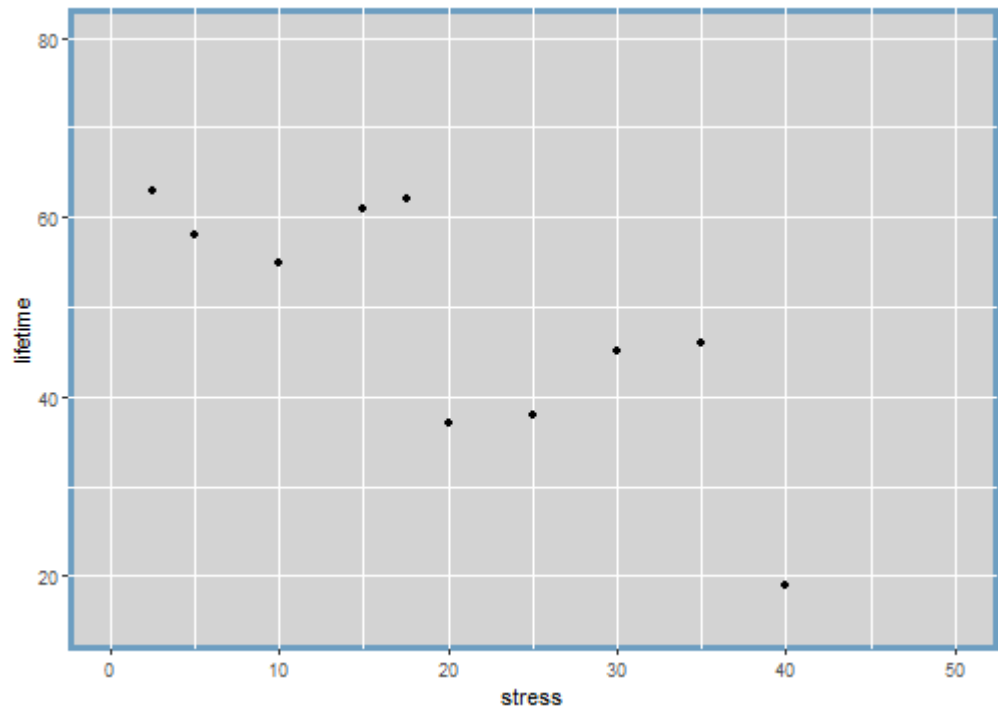
63	58	55	61	62	37	38	45	46	19
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Ex: Bars

$$\hat{y} = 66.4177 - 0.9009x$$

Fitting Lines

Best Estimate



Describing Relationships

Example: Strain on Bars

Idea

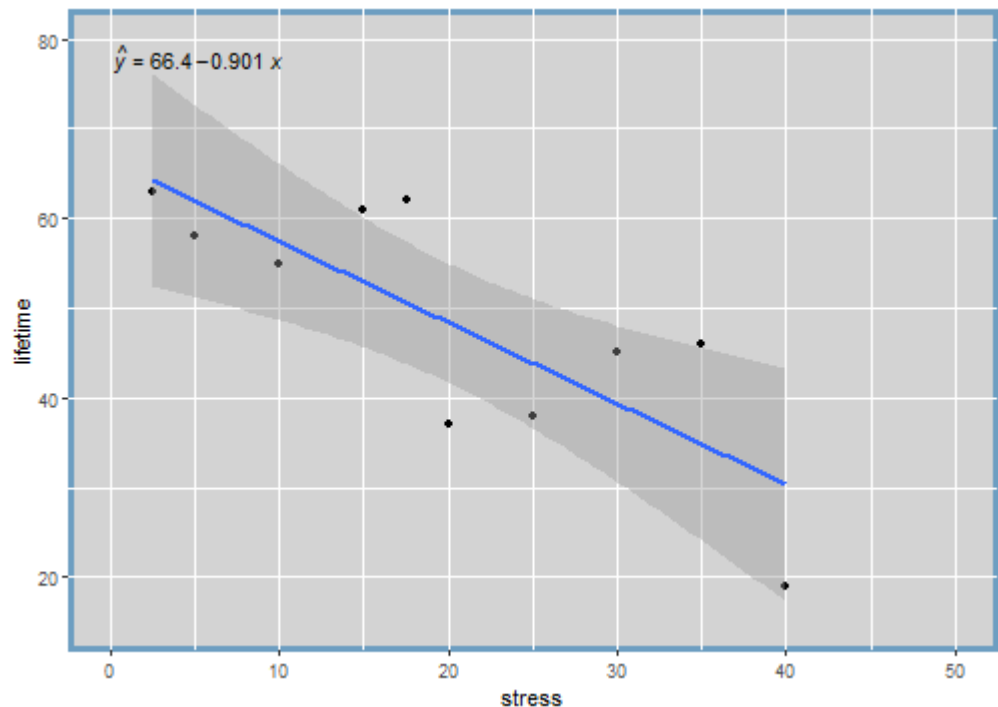
Ex: Bars

Fitting Lines

Best Estimate

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	

Fitted line



JMP

Describing Relationships

Topics to be covered in JMP

Using JMP

- Fitting linear relationships
- Describing quality of fit (correlation, R^2)
- Fitting relationships using multiple variables
- Fitting non-linear relationships

An example

Example: Manufacturing Ball Bearings

Controlling surface roughness is an important part of the manufacture of bearing balls. The key step in this smoothing the balls involves the use of a spinning weighted disc. Two important aspects of this are the rotation speed of the disc and the weight applied to the disc. Since higher weights and higher rotation speed are all known to cause shorter lifetimes for the discs (which requires halts in production, costs of new discs, and so on), a team of engineers are attempting to better understand the relationship between the rotation speed, the weight, and the resulting surface roughness of the balls produced.

Experiment 1: Constant speed, changing applied weight

With the disc rotation speed locked at 50 rotations/second, the team of engineers created 60 batches of balls using differently weighted discs (0.025 g, 0.050 g, 0.075 g, 0.100 g, ..., 0.500 g) and randomly selected one ball from each batch. The results are recorded in the dataset "balls-001.csv" on the course page.

Experiment 2: Changing speed, constant applied weight

With an better understanding of the relationship between weight and surface roughness, the team turned their attention to rotation speed. This time the produced 3 batches for each of 15 rotation speeds (25, 30, 35, 40, 45, 50, 55, 60, 65, 70, 75, 80, 85, 90, and 95 rotations per second). The results are recorded in the dataset "balls-002.csv" on the course page.

Experiment 3: Changing speed changing applied weight

With a better understanding of the relationship between weight and surface roughness, the team turned their attention to rotation speed. This time the produced 3 batches for each combination of 20 weights (0.025 g, 0.050 g, 0.075 g, 0.100 g, ..., 0.500 g) and 15 rotation speeds (25, 30, 35, 40, 45, 50, 55, 60, 65, 70, 75, 80, 85, 90, and 95 rotations per second). The results are recorded in the dataset "balls-003.csv"

Experiment 4: Changing categorical speed changing applied weight

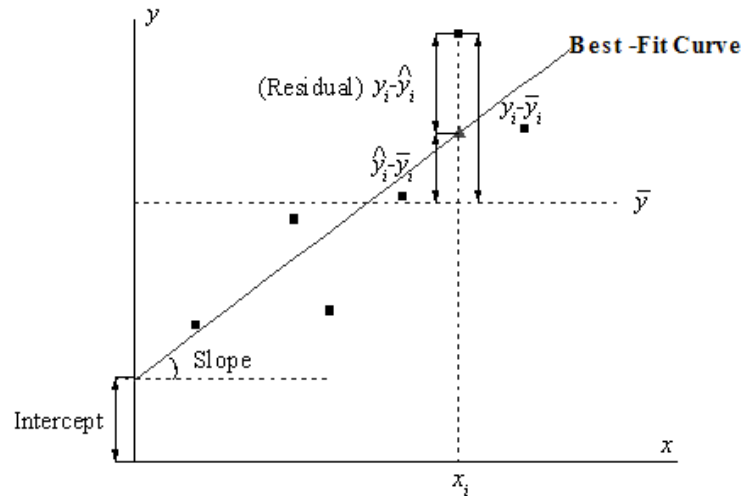
Now that they have a complete model, what if they had attempted this experiment with a machine in which rotation speed only consisted of "low, medium, and high"?

Again, time the produced 3 batches for each combination of 20 weights (0.025 g, 0.050 g, 0.075 g, 0.100 g, ..., 0.500 g) and three rotation speeds: low (encoded as 1), medium (encoded as 2), high (encoded as 3). The results are recorded in the dataset "balls-004.csv"

Residuals

Residuals

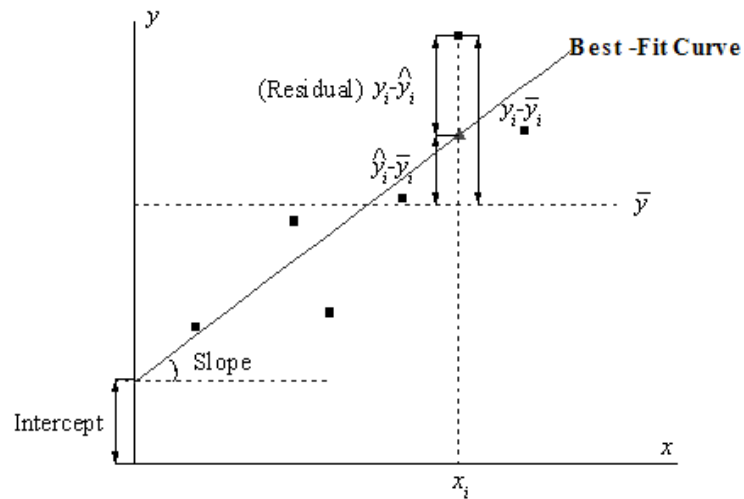
- The "residue" left over from fitting a line



- Each point represents some (x_i, y_i) pair from our data
- We use the Least Squares approach to find the best fit line, $\hat{y} = b_0 + b_1x$
- For any value x_i in our data set, we can get a fitted (or predicted) value $\hat{y}_i = b_0 + b_1x_i$

Residuals

Residuals



- The residual is the difference between the observed data point and the fitted prediction:

$$e_i = y_i - \hat{y}_i$$

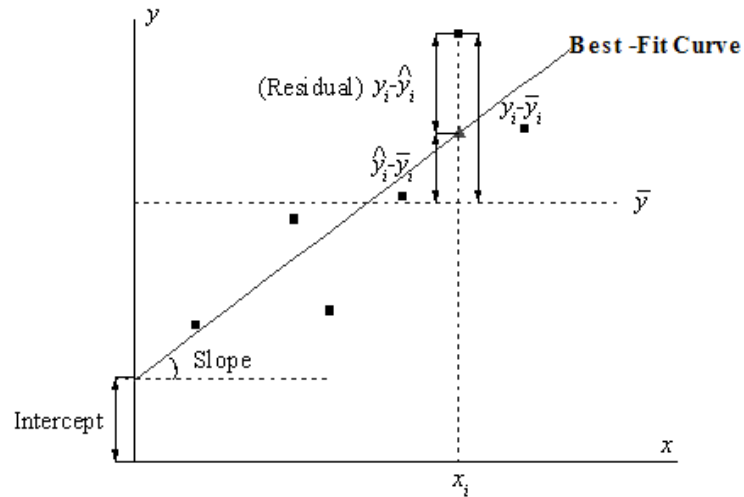
- **In the linear case**, using $\hat{y} = b_0 + b_1x$, we can also write

$$e_i = y_i - \hat{y}_i = y_i - (b_0 + b_1x_i)$$

for each pair (x_i, y_i) .

Residuals

Residuals



ROPe: Residuals = Observed - Predicted (using symbol e_i)

- If $e_i > 0$ then $y_i - \hat{y}_i > 0$ and $y_i > \hat{y}_i$ meaning the observed is larger than the predicted - we are "underpredicting"
- If $e_i < 0$ then $y_i - \hat{y}_i < 0$ and $y_i < \hat{y}_i$ meaning the observed is smaller than the predicted - we are "overpredicting"

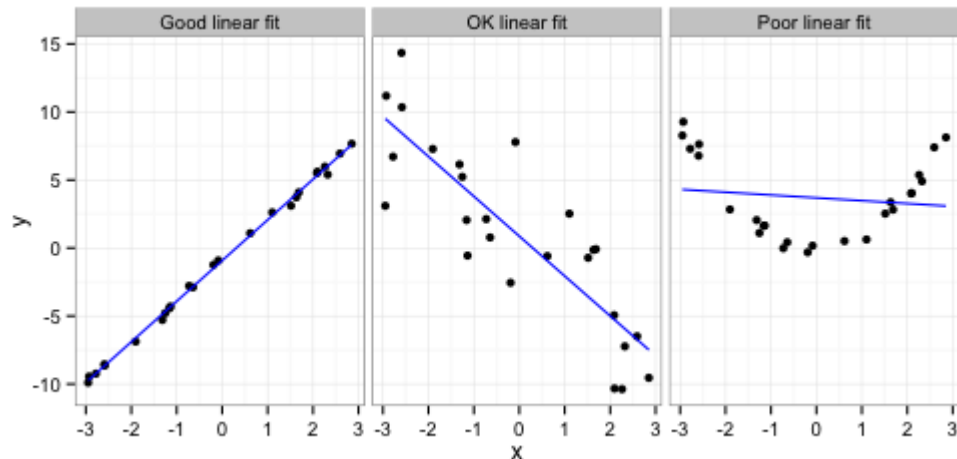
Good Fit

Knowing when a relationship fits the data well

So far we have been fitting lines to describe our data. A first question to ask may be something like:

- **Q:** What kind of situations can a linear fit be used to describe the relationship between an experimental variable and a response?
- **A:** Any time both the experimental variable and the response variable are numeric.

However all fits are not created the same:



Good Fit

Describing Fit Numerically

Numeric Desc.

1. Sample correlation (aka, sample linear correlation)

For a sample consisting of data pairs $(x_1, y_1), (x_2, y_2), (x_3, y_3), \dots (x_n, y_n)$, the sample linear correlation, r , is defined by

$$r = \frac{\sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y})}{\sqrt{(\sum_{i=1}^n (x_i - \bar{x})^2) (\sum_{i=1}^n (y_i - \bar{y})^2)}}$$

which can also be written as

$$r = \frac{\sum_{i=1}^n x_i y_i - n\bar{x}\bar{y}}{\sqrt{(\sum_{i=1}^n x_i^2 - n\bar{x}^2) (\sum_{i=1}^n y_i^2 - n\bar{y}^2)}}$$

Good Fit

Numeric Desc.

1. Sample correlation (aka, sample linear correlation)

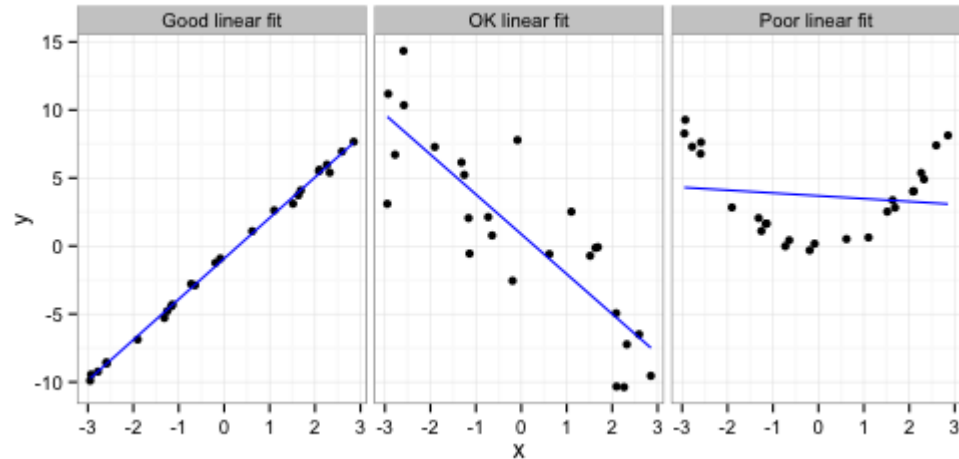
The value of r is always between -1 and +1.

- The closer the value is to -1 or +1 the stronger the linear relationship.
- Negative values of r indicate a negative relationship (as x increases, y decreases).
- Positive values of r indicate a positive relationship (as x increases, y increases).
- One possible rule of thumb:

Range of r	Strength	Direction
0.9 to 1.0	Very Strong	Positive
0.7 to 0.9	Strong	Positive
0.5 to 0.7	Moderate	Positive
0.3 to 0.5	Weak	Positive
-0.3 to 0.3	Very Weak/No Relationship	
-0.5 to -0.3	Weak	Negative

Good Fit

Numeric Desc.



The values of r from left to right are in the plot above are:

$$r=0.9998782$$

$$r=-0.8523543$$

$$r=-0.1347395$$

- In the first case the linear relationship is almost perfect, and we would happily refer to this as a **very strong, positive** relationship between x and y .
- In the second case the linear relationship seems appropriate - we could safely call it a **strong, negative** linear relationship between x and y .
- In the third case the value of r indicates that there is **no linear relationship** between the value of x and the value of y .

Good Fit

Numeric Desc.

1. Sample correlation (aka, sample linear correlation)

Example: Stress and Lifetime of Bars

We can use it to calculate the following values:

$$\sum_{i=1}^{10} x_i = 200, \sum_{i=1}^{10} x_i^2 = 5412.5,$$

$$\sum_{i=1}^{10} y_i = 484, \sum_{i=1}^{10} y_i^2 = 25238, \sum_{i=1}^{10} x_i y_i = 8407.5,$$

and we can write:

$$\begin{aligned} r &= \frac{\sum_{i=1}^n x_i y_i - n\bar{x}\bar{y}}{\sqrt{(\sum_{i=1}^n x_i^2 - n\bar{x}^2)(\sum_{i=1}^n y_i^2 - n\bar{y}^2)}} \\ &= \frac{8407.5 - 10(20)(48.5)}{\sqrt{(5412.5 - 10(20)^2)(25238 - 10(48.4)^2)}} \\ &= -0.795 \end{aligned}$$

So we would say that stress applied and lifetime of the bar have a **strong, negative, linear relationship**.

Good Fit

Numeric Desc.

2. Coefficient of Determination (R^2)

We know that our responses have variability - they are not always the same. We hope that the relationship between our response and our explanatory variables explains some of the variability in our responses.

R^2 is the fraction of the total variability in the response (y) accounted for by the fitted relationship.

- When R^2 is close to 1 we have explained **almost all** of the variability in our response using the fitted relationship (i.e., the fitted relationship is good).
- When R^2 is close to 0 we have explained **almost none** of the variability in our response using the fitted relationship (i.e., the fitted relationship is bad).

There are a number of ways we can calculate R^2 . Some require you to know more than others or do more work by hand.

Good Fit

Numeric Desc.

2. Calculating Coefficient of Determination (R^2)

Method a. Using the data and our fitted relationship:

For an experiment with response values y_1, y_2, \dots, y_n and fitted values $\hat{y}_1, \hat{y}_2, \dots, \hat{y}_n$ we calculate the following:

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

- This is the longest way to calculate R^2 by hand.
- It requires you to know every response value in the data (y_i) and every fitted value (\hat{y}_i)

Good Fit

Numeric Desc.

2. Calculating Coefficient of Determination (R^2)

Method b. Using Sums of Squares

For an experiment with response values y_1, y_2, \dots, y_3 and fitted values $\hat{y}_1, \hat{y}_2, \dots, \hat{y}_3$ we calculate the following:

- Total Sum of Squares (SSTO): a baseline for the variability in our response.

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

- Error Sum of Squares (SSE): The variability in the data after fitting the line

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

- Regression Sum of Squares (SSR): The variability in the data accounted for by the fitted relationship

$$SSR = SSTO - SSE$$

Good Fit

Numeric Desc.

2. Calculating Coefficient of Determination (R^2)

Method b. Using Sums of Squares, continued

We can write the R^2 using these sums of squares:

$$R^2 = \frac{SSR}{SSTO} = \frac{SSTO - SSE}{SSTO} = 1 - \frac{SSE}{SSTO}$$

- **Q:** What's the advantage of using the sums of squares?
- **A:** The values of SSTO, SSE, and SSR are used in many statistical calculations. Because of this, they are commonly reported by statistical software. For instance, fitting a model in JMP produces these as part of the output.

Good Fit

2. Calculating Coefficient of Determination (R^2)

Method c. A special case when the relationship is linear

Numeric Desc.

If the relationship we fit between y and x is linear, then we can use the sample correlation, r to get:

$$R^2 = (r)^2$$

NOTE: Please, please, please, understand that this is only true for linear relationships.

Good Fit

Example: Stress and Lifetime of Bars

The data can be found in Lecture 9.

Numeric Desc.

Earlier, we found $r = -0.795$.

Since we are describing the relationship using a line, then we can use the special case:

$$R^2 = (r)^2 = (-0.795)^2 = 0.633$$

In other words, 63.3% of the variability in the lifetime of the bars can be explained by the stress the bars were placed under.