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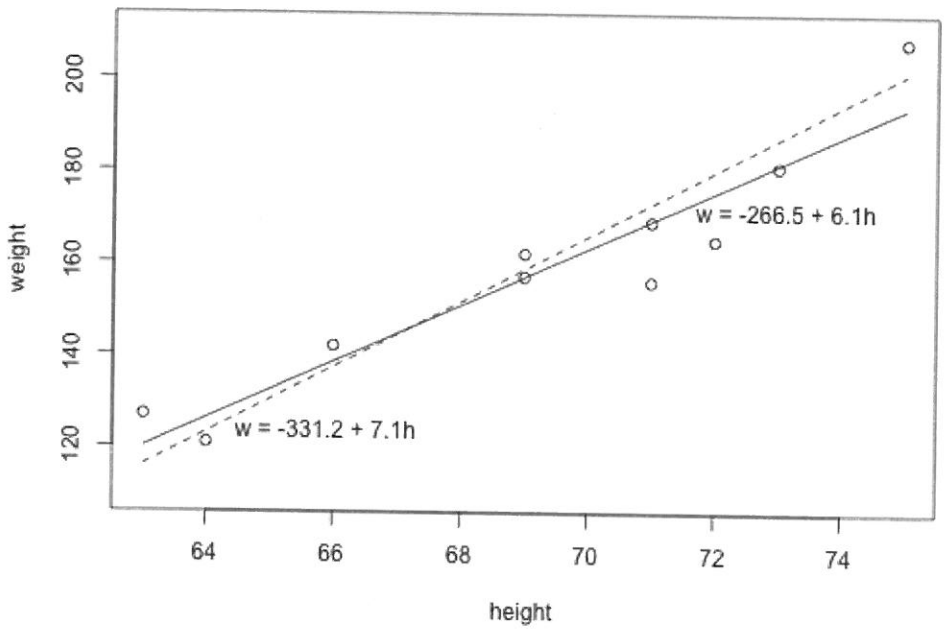
1.2 - What is the "Best Fitting Line"?

Since we are interested in summarizing the trend between two quantitative variables, the natural question arises — "what is the best fitting line?" At some point in your education, you were probably shown a scatter plot of (*x*, *y*) data and were asked to draw the "most appropriate" line through the data. Even if you weren't, you can try it now on a set of heights (*x*) and weights (*y*) of 10 students, (student_height_weight.txt) [1]. Looking at the plot below, which line — the solid line or the dashed line — do you think best summarizes the trend between height and weight?



Hold on to your answer! In order to examine which of the two lines is a better fit, we first need to introduce some common notation:

- y_i denotes the observed response for experimental unit *i*
- x_i denotes the predictor value for experimental unit *i*
- $\hat{y}_i$ is the predicted response (or fitted value) for experimental unit *i*

Then, the equation for the best fitting line is:

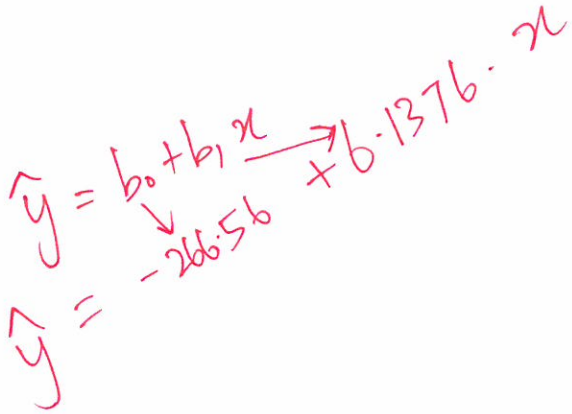
$$\hat{y}_i = b_0 + b_1 x_i$$

Incidentally, recall that an "**experimental unit**" is the object or person on which the measurement is made. In our height and weight example, the experimental units are students.

Let's try out the notation on our example with the trend summarized by the line w = -266.53 + 6.1376 h. (Note that this line is just a more precise version of the above solid line, w = -266.5 + 6.1 h.) The first data point in the list indicates that student 1 is 63 inches tall and weighs 127 pounds. That is, x_1 = 63 and y_1 = 127 . Do you see this point on the plot? If we know this student's height but not his or her weight, we could use the equation of the line to predict his or her weight. We'd predict the student's weight to be -266.53 + 6.1376(63) or 120.1 pounds. That is, $\hat{y}_1$ = 120.1. Clearly, our prediction wouldn't be perfectly correct — it has some "**prediction error**" (or "**residual error**"). In fact, the size of its prediction error is 127-120.1 or 6.9 pounds.

You might want to roll your cursor over each of the 10 data points to make sure you understand the notation used to keep track of the predictor values, the observed responses and the predicted responses:

i	x_i	y_i	$\hat{y}_i$
1	63	127	120.1
2	64	121	126.3
3	66	142	138.5
4	69	157	157.0
5	69	162	157.0
6	71	156	169.2
7	71	169	169.2
8	72	165	175.4
9	73	181	181.5
10	75	208	193.8



As you can see, the size of the prediction error depends on the data point. If we didn't know the weight of student 5, the equation of the line would predict his or her weight to be -266.53 + 6.1376(69) or 157 pounds. The size of the prediction error here is 162-157, or 5 pounds.

In general, when we use $\hat{y}_i = b_0 + b_1 x_i$ to predict the actual response y_i, we make a prediction error (or residual error) of size:

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

A line that fits the data "**best**" will be one for which the ***n* prediction errors** — one for each observed data point — **are as small as possible in some overall sense**. One way to achieve this goal is to invoke the "**least squares criterion**," which says to "minimize the sum of the squared prediction errors." That is:

- The equation of the best fitting line is: $\hat{y}_i = b_0 + b_1 x_i$
- We just need to find the values b_0 and b_1 that make the sum of the squared prediction errors the smallest it can be.
- That is, we need to find the values b_0 and b_1 that minimize:

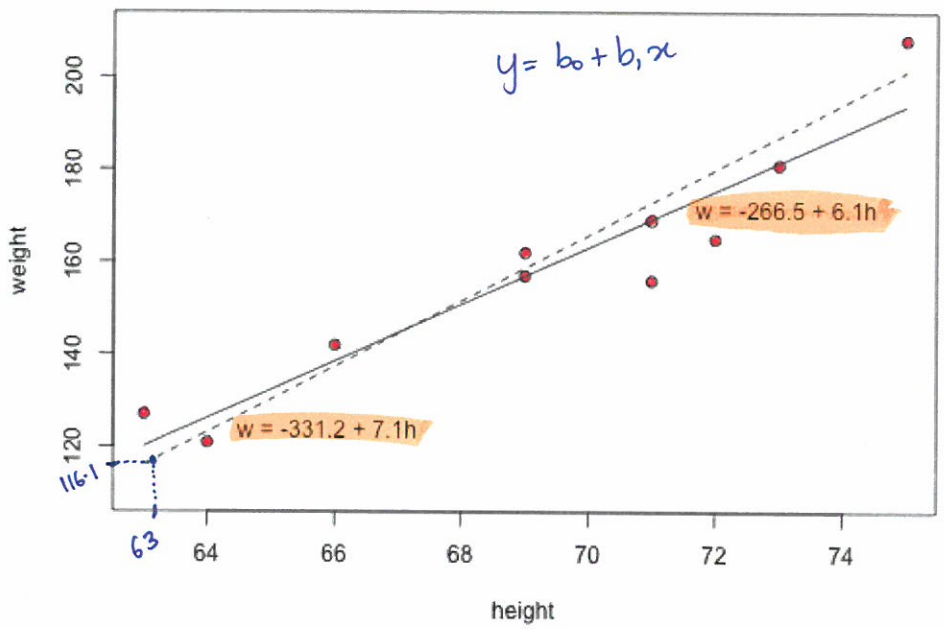
$$Q = \sum_{i=1}^{n} (y_i - \hat{y}_i)^2$$

Here's how you might think about this quantity *Q*:

- The quantity $e_i = y_i - \hat{y}_i$ is the prediction error for data point *i*.
- The quantity $e_i^2 = (y_i - \hat{y}_i)^2$ is the squared prediction error for data point *i*.
- And, the symbol $\sum_{i=1}^{n}$ tells us to add up the squared prediction errors for all *n* data points.

Incidentally, if we didn't square the prediction error $e_i = y_i - \hat{y}_i$ to get $e_i^2 = (y_i - \hat{y}_i)^2$, the positive and negative prediction errors would cancel each other out when summed, always yielding 0.

Now, being familiar with the least squares criterion, let's take a fresh look at our plot again. In light of the least squares criterion, which line do you now think is the best fitting line?



Let's see how you did! The following two side-by-side tables illustrate the implementation of the least squares criterion for the two lines up for consideration — the dashed line and the solid line.

w = -331.2 + 7.1 h (the dashed line)

i	x_i	y_i	$\hat{y}_i$	$(y_i - \hat{y}_i)$	$(y_i - \hat{y}_i)^2$
1	63	127	116.1	10.9	118.81
2	64	121	123.2	-2.2	4.84
3	66	142	137.4	4.6	21.16
4	69	157	158.7	-1.7	2.89
5	69	162	158.7	3.3	10.89
6	71	156	172.9	-16.9	285.61
7	71	169	172.9	-3.9	15.21
8	72	165	180.0	-15.0	225.00
9	73	181	187.1	-6.1	37.21
10	75	208	201.3	6.7	44.89
					766.5

w = -266.53 + 6.1376 h (the solid line)

i	x_i	y_i	$\hat{y}_i$	$(y_i - \hat{y}_i)$	$(y_i - \hat{y}_i)^2$
1	63	127	120.139	6.8612	47.076
2	64	121	126.276	-5.2764	27.840
3	66	142	138.552	3.4484	11.891
4	69	157	156.964	0.0356	0.001
5	69	162	156.964	5.0356	25.357
6	71	156	169.240	-13.2396	175.287
7	71	169	169.240	-0.2396	0.057
8	72	165	175.377	-10.3772	107.686
9	73	181	181.515	-0.5148	0.265
10	75	208	193.790	14.2100	201.924
					597.4

Based on the least squares criterion, which equation best summarizes the data? The sum of the squared prediction errors is 766.5 for the dashed line, while it is only 597.4 for the solid line. Therefore, of the two lines, the solid line, w = -266.53 + 6.1376h, best summarizes the data. But, is this equation guaranteed to be the best fitting line of all of the possible lines we didn't even consider? Of course not!

If we used the above approach for finding the equation of the line that minimizes the sum of the squared prediction errors, we'd have our work cut out for us. We'd have to implement the above procedure for an infinite number of possible lines — clearly, an impossible task! Fortunately,

somebody has done some dirty work for us by figuring out formulas for the **intercept** b_0 and the **slope** b_1 for the equation of the line that minimizes the sum of the squared prediction errors.

The formulas are determined using methods of calculus. We minimize the equation for the sum of the squared prediction errors:

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

(that is, take the derivative with respect to b_0 and b_1, set to 0, and solve for b_0 and b_1) and get the "**least squares estimates**" for b_0 and b_1:

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

and:

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

Because the formulas for b_0 and b_1 are derived using the least squares criterion, the resulting equation — $\hat{y}_i = b_0 + b_1 x_i$— is often referred to as the "**least squares regression line**," or simply the "**least squares line**." It is also sometimes called the "**estimated regression equation**." Incidentally, note that in deriving the above formulas, we made no assumptions about the data other than that they follow some sort of linear trend.

We can see from these formulas that the least squares line passes through the point $(\bar{x}, \bar{y})$, since when $x = \bar{x}$, then $y = b_0 + b_1\bar{x} = \bar{y} - b_1\bar{x} + b_1\bar{x} = \bar{y}$.

In practice, you won't really need to worry about the formulas for b_0 and b_1. Instead, you are are going to let statistical software, such as Minitab, find least squares lines for you. But, we can still learn something from the formulas — for b_1 in particular.

If you study the formula for the slope b_1:

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

you see that the denominator is necessarily positive since it only involves summing positive terms. Therefore, the sign of the slope b_1 is solely determined by the numerator. The numerator tells us, for each data point, to sum up the product of two distances — the distance of the *x*-value from the mean of all of the *x*-values and the distance of the *y*-value from the mean of all of the *y*-values. Let's see how this determines the sign of the slope b_1 by studying the following two plots.

When is the slope $b_1 > 0$? Do you agree that the trend in the following plot is positive — that is, as *x* increases, *y* tends to increase? If the trend is positive, then the slope b_1 must be positive. Let's see how!

- Click on the blue data point in the upper right quadrant..... Note that the product of the two distances for this data point is positive. In fact, the product of the two distances is positive for *any* data point in the upper right quadrant.
- Now, select clear and then click on the blue data point in the lower left quadrant..... Note that the product of the two distances for this data point is also positive. In fact, the product of the two distances is positive for *any* data point in the lower left quadrant.

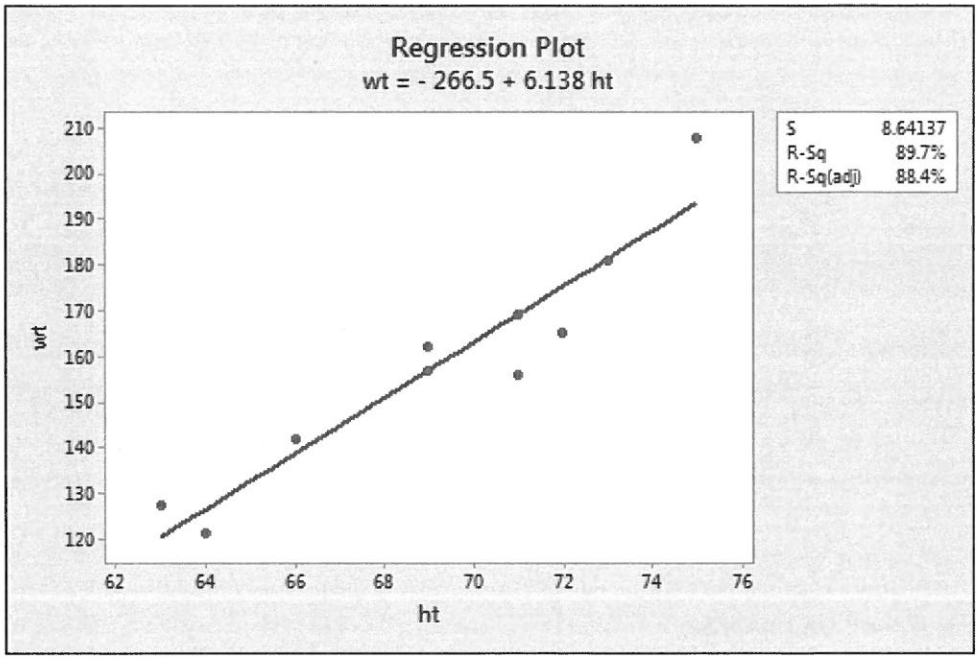
Adding up all of these positive products must necessarily yield a positive number, and hence the slope of the line b_1 will be positive.

When is the slope $b_1 < 0$? Now, do you agree that the trend in the following plot is negative — that is, as x increases, y tends to decrease? If the trend is negative, then the slope b_1 must be negative. Let's see how!

- Click on the blue data point in the upper left quadrant..... Note that the product of the two distances for this data point is negative. In fact, the product of the two distances is negative for *any* data point in the upper left quadrant.
- Now, select clear and then click on the blue data point in the lower right quadrant..... Note that the product of the two distances for this data point is also negative. In fact, the product of the two distances is negative for *any* data point in the lower right quadrant.

Adding up all of these negative products must necessarily yield a negative number, and hence the slope of the line b_1 will be negative.

Now that we finished that investigation, you can just set aside the formulas for b_0 and b_1. Again, in practice, you are going to let statistical software, such as Minitab, find least squares lines for you. We can obtain the estimated regression equation in two different places in Minitab. The following plot illustrates where you can find the least squares line (in box) on Minitab's "**fitted line plot**."



The following Minitab output illustrates where you can find the least squares line (in box) in Minitab's "**standard regression analysis**" output.

```
The regression equation is
weight = - 267 + 6.14 height

Predictor        Coef    SE Coef        T        P
Constant      -266.53      51.03    -5.22    0.001
height         6.1376     0.7353     8.35    0.000

S = 8.641       R-Sq = 89.7%     R-Sq(adj) = 88.4%

Analysis of Variance

Source     DF        SS      MS        F        P
Regression  1    5202.2  5202.2     69.67    0.000
Residual Error  8  597.4    74.7
Total       9    5799.6
```

Note that the estimated values b_0 and b_1 also appear in a table under the columns labeled "**Predictor**" (the intercept b_0 is always referred to as the "**Constant**" in Minitab) and "**Coef**" (for "Coefficients"). Also, note that the value we obtained by minimizing the sum of the squared prediction errors, 597.4, appears in the "**Analysis of Variance**" table appropriately in a row labeled "**Residual Error**" and under a column labeled "**SS**" (for "Sum of Squares").

Although we've learned how to obtain the "**estimated regression coefficients**" b_0 and b_1, we've not yet discussed what we learn from them. One thing they allow us to do is to predict future responses — one of the most common uses of an estimated regression line. This use is rather straightforward:

A common use of the estimated regression line.	$\hat{y}_{i,wt} = -267 + 6.14x_{i,ht}$
Predict (mean) weight of 66"-inch tall people.	$\hat{y}_{i,wt} = -267 + 6.14(66) = 138.24$
Predict (mean) weight of 67"-inch tall people.	$\hat{y}_{i,wt} = -267 + 6.14(67) = 144.38$

Now, what does b_0 tell us? The answer is obvious when you evaluate the estimated regression equation at $x = 0$. Here, it tells us that a person who is 0 inches tall is predicted to weigh -267 pounds! Clearly, this prediction is nonsense. This happened because we "**extrapolated**" beyond the

"scope of the model" (the range of the x values). It is not meaningful to have a height of 0 inches, that is, the scope of the model does not include $x = 0$. So, here the intercept b_0 is not meaningful. In general, if the "scope of the model" includes $x = 0$, then b_0 is the predicted mean response when $x = 0$. Otherwise, b_0 is not meaningful. There is more information on this here [2].

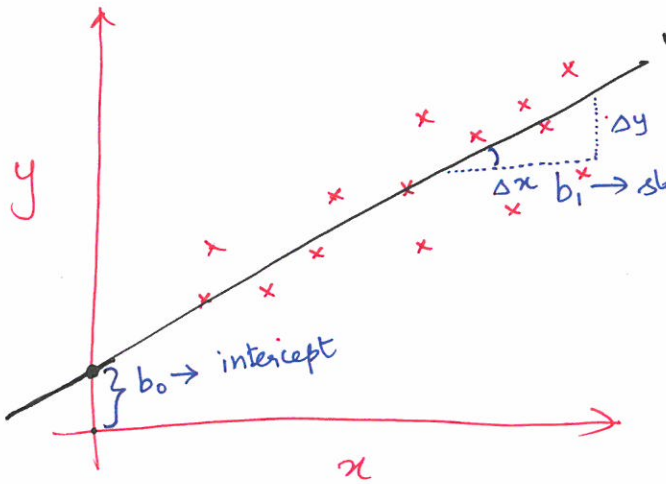
And, what does b_1 tell us? The answer is obvious when you subtract the predicted weight of 66"-inch tall people from the predicted weight of 67"-inch tall people. We obtain 144.38 - 138.24 = 6.14 pounds -- the value of b_1. Here, it tells us that we predict the mean weight to increase by 6.14 pounds for every additional one-inch increase in height. In general, we can expect the mean response to increase or decrease by b_1 units for every one unit increase in x.

Source URL: https://onlinecourses.science.psu.edu/stat501/node/252

Links:
[1] https://onlinecourses.science.psu.edu/stat501/sites/onlinecourses.science.psu.edu.stat501/files/data/student_height_weight.txt
[2] http://blog.minitab.com/blog/adventures-in-statistics/regression-analysis-how-to-interpret-the-constant-y-intercept

Best-fit line for Linear Regression:

Line



slope, intercept

$y = mx + c$ (or)

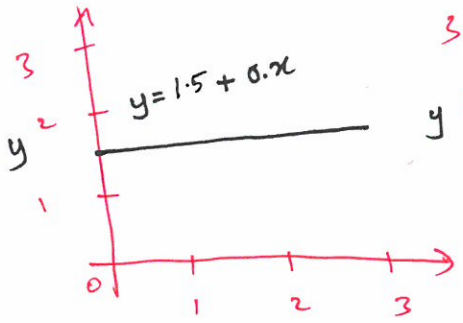
$y = b_1 x + b_0$

Sup. learning

↙ regression (prediction)

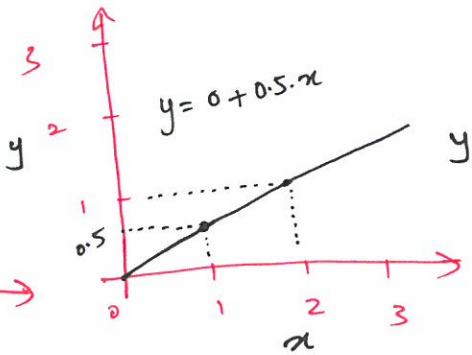
↘ classification

$y = b_0 + b_1 x$



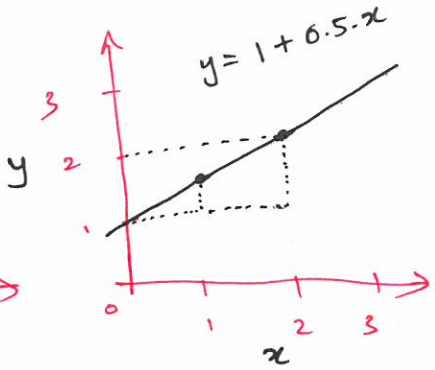
$b_0 = 1.5$

$b_1 = 0$



$b_0 = 0$

$b_1 = 0.5$



$b_0 = 1$

$b_1 = 0.5$

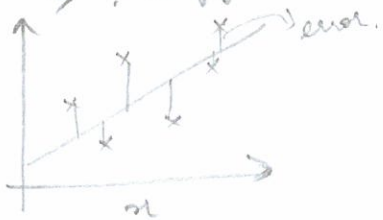
SSE

Which line ?

↓

line that $\min_{b_0, b_1}$ (SSE)

↳ ? in figure



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

Data

x	y

sq ft. cost