Least Squares Fitting
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Overview

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In this document, you'll learn:

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- how to determine the slope and y-intercept from straight line data

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- how to determine the slope and y-intercept from straight line data
- how to determine standard errors in the slope and y-intercept

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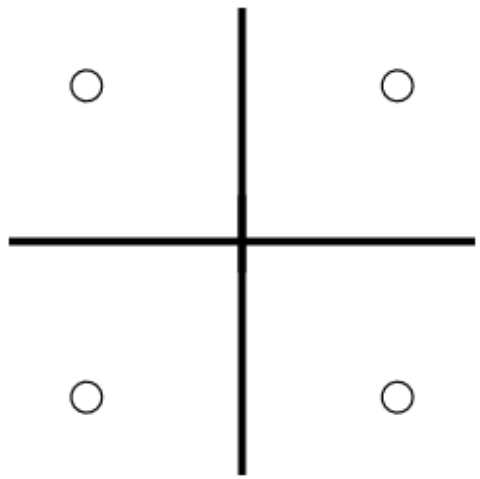
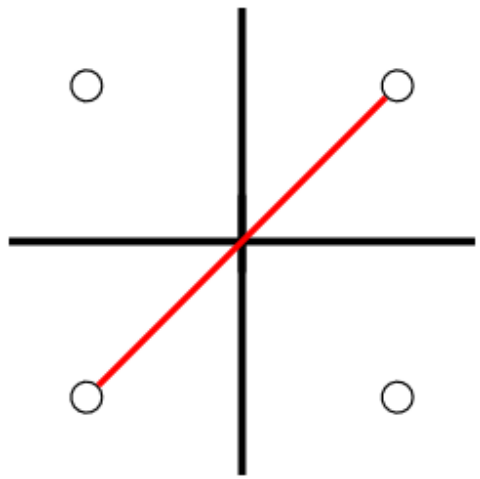
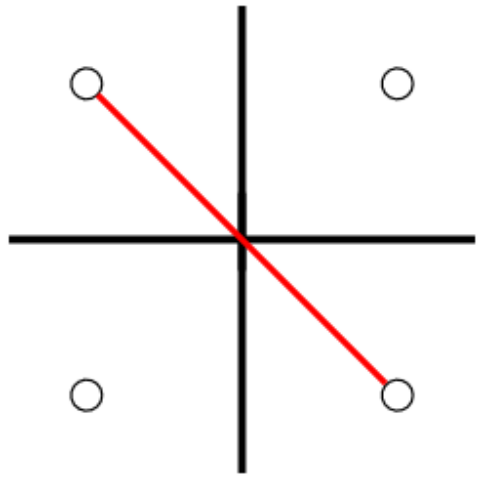
Unless a set of data *exactly* fits a curve, choosing *a* curve of "best fit" is somewhat arbitrary. (For example, consider 4 data points at (-1,1), (1,1), (1,-1) and (-1,-1). What line fits these points best?)



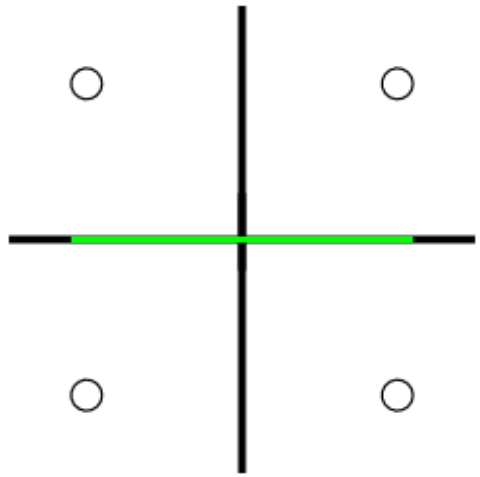
What line best fits these points?



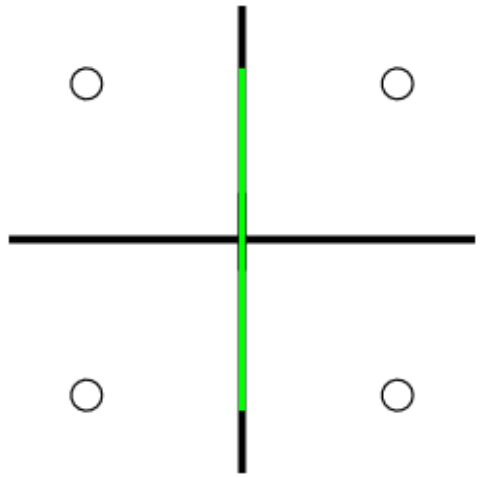
This line goes through two points exactly, and is equidistant from the others.



But then so does this one....



This line is equidistant from all of the points.



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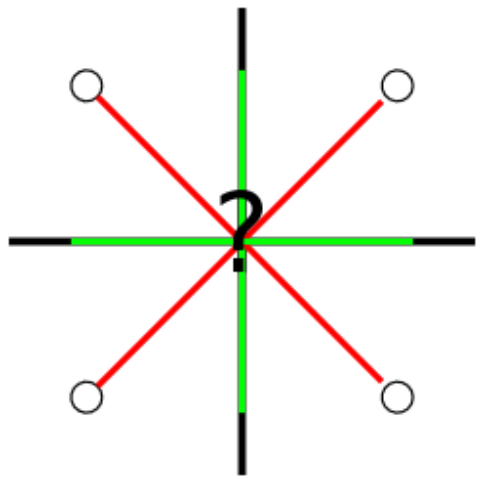

There is no clear "best" line through these four points.

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- it always produces a solution
- it can be updated for additional data points without complete recalculation

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Least **S**quares **F**itting is a procedure for numerically determining the equation of a curve which "best approximates" the data being plotted. If we wish to fit a straight line to data in the form

$$y = mx + b$$

then the least squares fit gives values for b, the y-intercept, and m, the slope, as follows:

$$b = \frac{\left(\sum y_i\right)\left(\sum x_i^2\right) - \left(\sum x_i\right)\left(\sum x_i y_i\right)}{N\left(\sum x_i^2\right) - \left(\sum x_i\right)^2}$$

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and

$$m = \frac{N\left(\sum x_i y_i\right) - \left(\sum x_i\right)\left(\sum y_i\right)}{N\left(\sum x_i^2\right) - \left(\sum x_i\right)^2}$$

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It only takes a couple of lines of algebra to show that this equals

$$N\left(N-1\right){\sigma_x}^2$$

where ${\sigma_x}^2$ is the sample standard deviation of the x values.

(Note: You do not need to calculate uncertainties for m and b during least squares fit calculations like this.

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$$\nu = N - 2$$

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$$R^2 = \frac{(N\sum x_i y_i - (\sum x_i)(\sum y_i))^2}{(N\sum {x_i}^2 - (\sum x_i)^2)\left(N\sum {y_i}^2 - (\sum y_i)^2\right)}$$

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As long as we're dealing with a *linear* fit, this is the quantity that would commonly be used.

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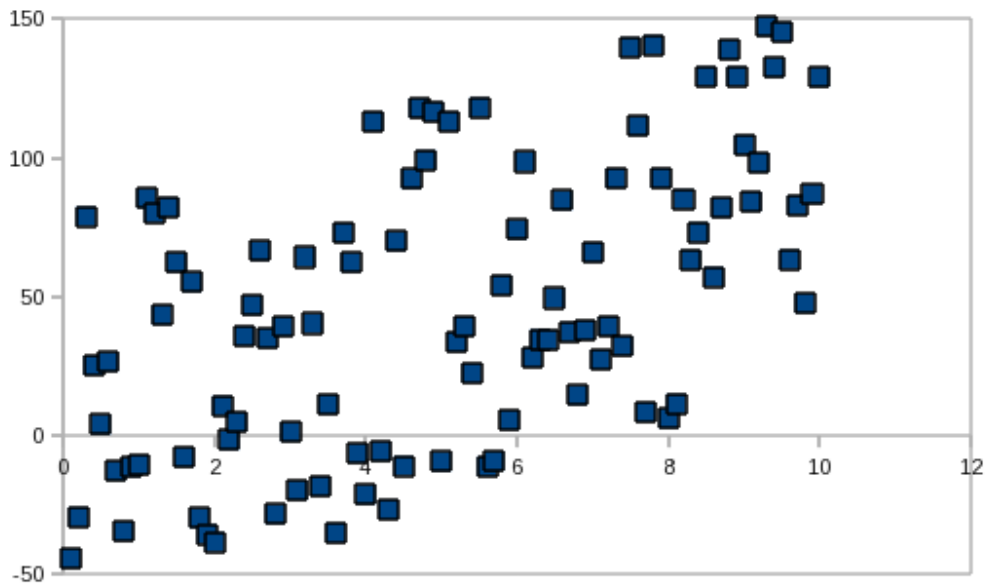
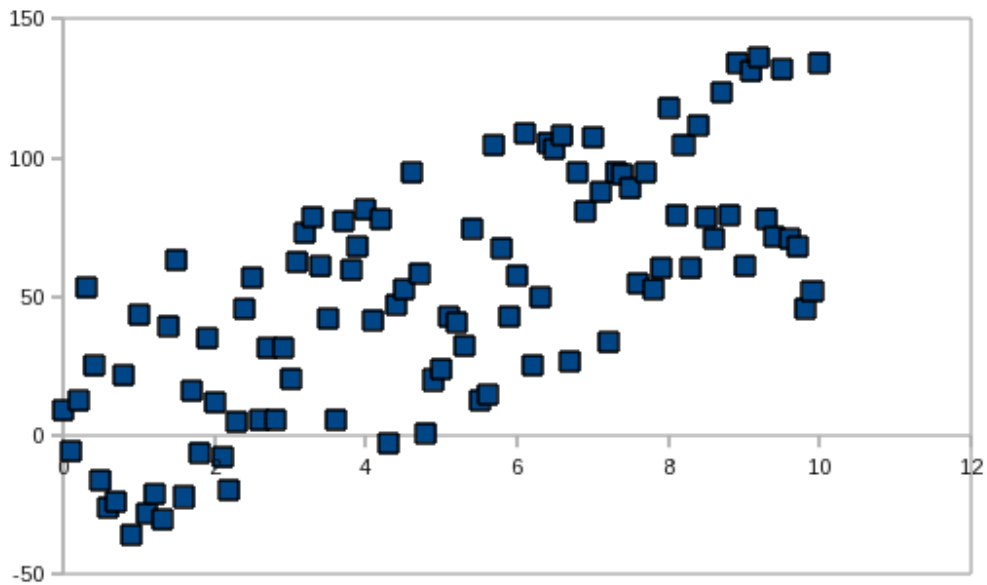
Thus R^2 is a value between zero and 1 indicating just the *strength* of a correlation. The closer R^2 is to one, the stronger the correlation between two variables. To put it another way, the closer it is to one the better one variable can be used as a *predictor* of the other.

Visualization of R^2



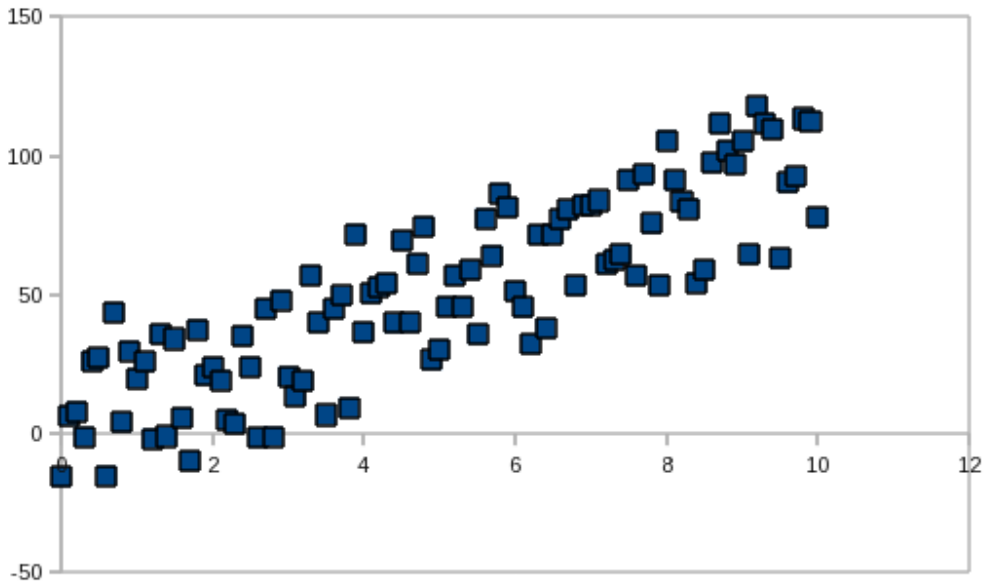
$R^2 \approx 0.3$

Visualization of R^2



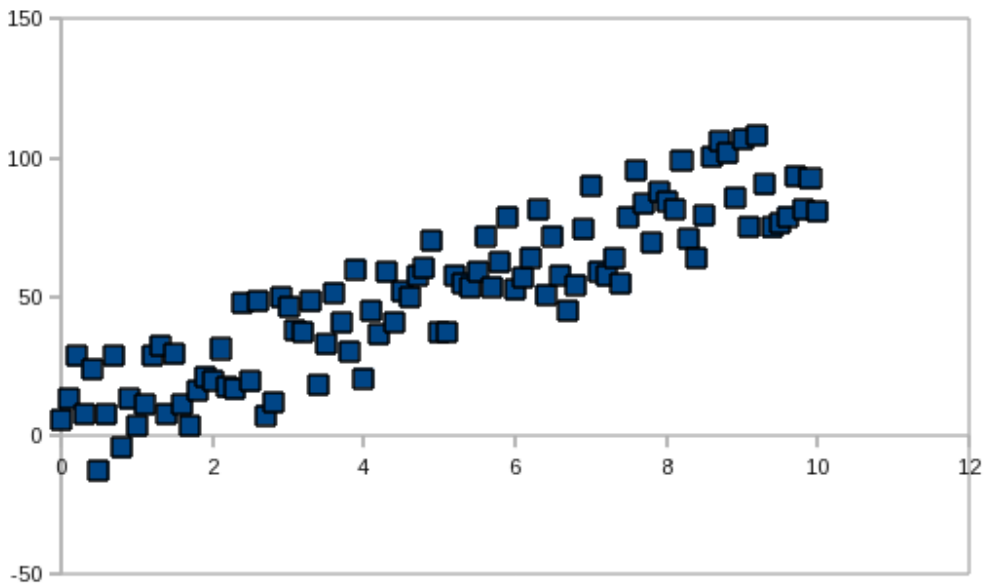
$R^2 \approx 0.5$

Visualization of R^2



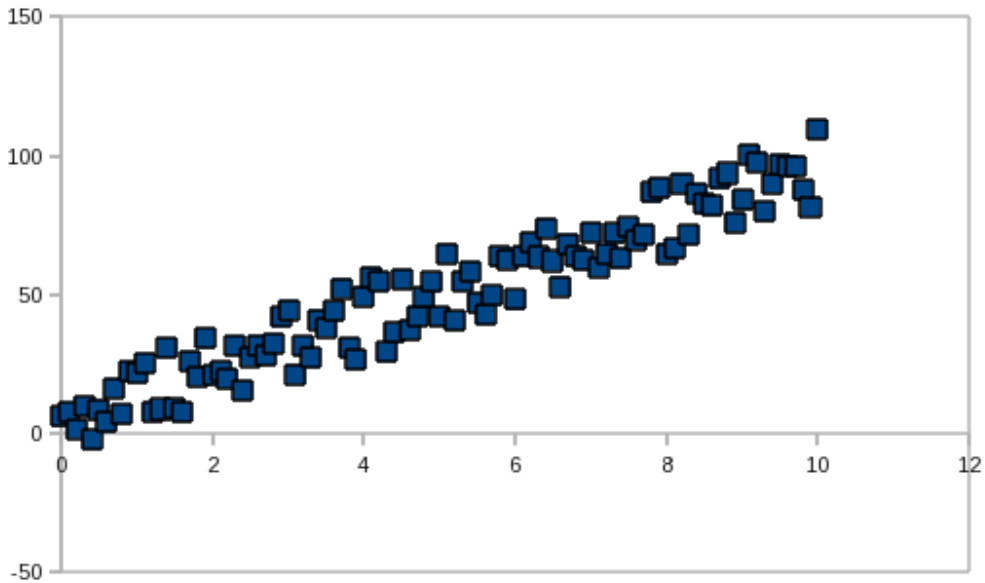
$R^2 \approx 0.7$

Visualization of R^2



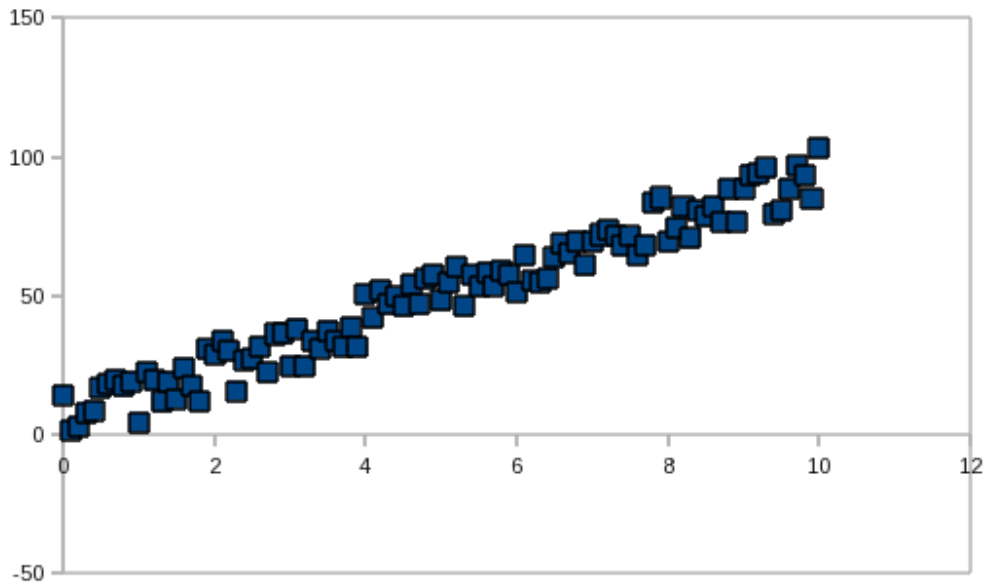
$R^2 \approx 0.8$

Visualization of R^2



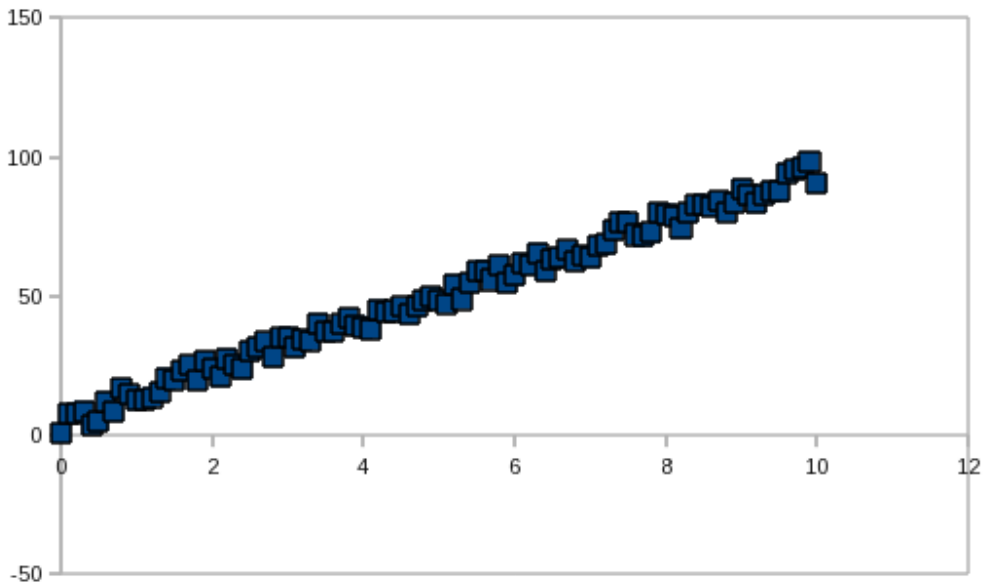
$R^2 \approx 0.9$

Visualization of R^2



$R^2 \approx 0.95$

Visualization of R^2



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and the standard error in the slope is

$$\sigma_m = \sigma \sqrt{\frac{N}{N\left(\sum x_i^2\right) - \left(\sum x_i\right)^2}}$$

Following is a calculation of the least squares fit and the standard error of the slope and intercept for some test data.

i	x_i	x_i^2	$x_i y_i$	y_i	y_i^2
1	0.1			3	
N	$\sum x_i$	$\sum x_i^2$	$\sum x_i y_i$	$\sum y_i$	$\sum y_i^2$
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Sample Least Squares Fit Data

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1	0.1	0.01		3	
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1	0.1	0.01	0.3	3	9
N	$\sum x_i$	$\sum x_i^2$	$\sum x_i y_i$	$\sum y_i$	$\sum y_i^2$
1	0.1	0.01	0.3	3	9

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1	0.1	0.01	0.3	3	9
2	0.2	0.04	0.8	4	16
N	$\sum x_i$	$\sum x_i^2$	$\sum x_i y_i$	$\sum y_i$	$\sum y_i^2$
2	0.3	0.05	1.1	7	25

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2	0.2	0.04	0.8	4	16
3	0.3	0.09	1.2	4	16
N	$\sum x_i$	$\sum x_i^2$	$\sum x_i y_i$	$\sum y_i$	$\sum y_i^2$
3	0.6	0.14	2.3	11	41

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1	0.1	0.01	0.3	3	9
2	0.2	0.04	0.8	4	16
3	0.3	0.09	1.2	4	16
4	0.4	0.16	2.0	5	25
N	$\sum x_i$	$\sum x_i^2$	$\sum x_i y_i$	$\sum y_i$	$\sum y_i^2$
4	1.0	0.3	4.3	16	66

Sample Least Squares Fit Data

Calculation of b and m

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$$N\left(\sum x_i^2\right) - \left(\sum x_i\right)^2$$

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$$b = \frac{\left(\sum y_i\right)\left(\sum x_i^2\right) - \left(\sum x_i\right)\left(\sum x_i y_i\right)}{N\left(\sum x_i^2\right) - \left(\sum x_i\right)^2}$$

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$$= \frac{(16)(0.3) - (1)(4.3)}{0.2}$$

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Calculation of b and m

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$$= \frac{(16)(0.3) - (1)(4.3)}{0.2} = 2.5$$

$$m = \frac{N\left(\sum x_i y_i\right) - \left(\sum x_i\right)\left(\sum y_i\right)}{N\left(\sum x_i^2\right) - \left(\sum x_i\right)^2}$$

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$$= (66) - (6)(4.3) - (2.5)(16)$$

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$$= (66) - (6)(4.3) - (2.5)(16) = 0.2$$

$$\sigma = \sqrt{\frac{S}{N-2}} = \sqrt{\frac{0.2}{4-2}} = 0.316228$$

Calculation of σ_b and σ_m

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   the closer R^2 is to 1, the better the fit.