Linear regression

By Dominic Waithe

"You can regress that out"
Sorcha 2018. former CGAT fellow.

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Today’s talk and presentation.

- Talk
  - What is linear regression.
  - How do we do it. Little bit of maths here.
  - Simple Vs multiple linear regression.
  - Error and other things.

- Practical content (after the lecture).
  - Download ‘jupyter notebook’.
  - Work through the notebook.

Sources:

Introduction

- Simple linear regression is a statistical method that allows us to summarise and study relationships between two continuous (quantitative variables)

  - One variable often denoted (x), is regarded as the predictor, explanatory or independent variable.

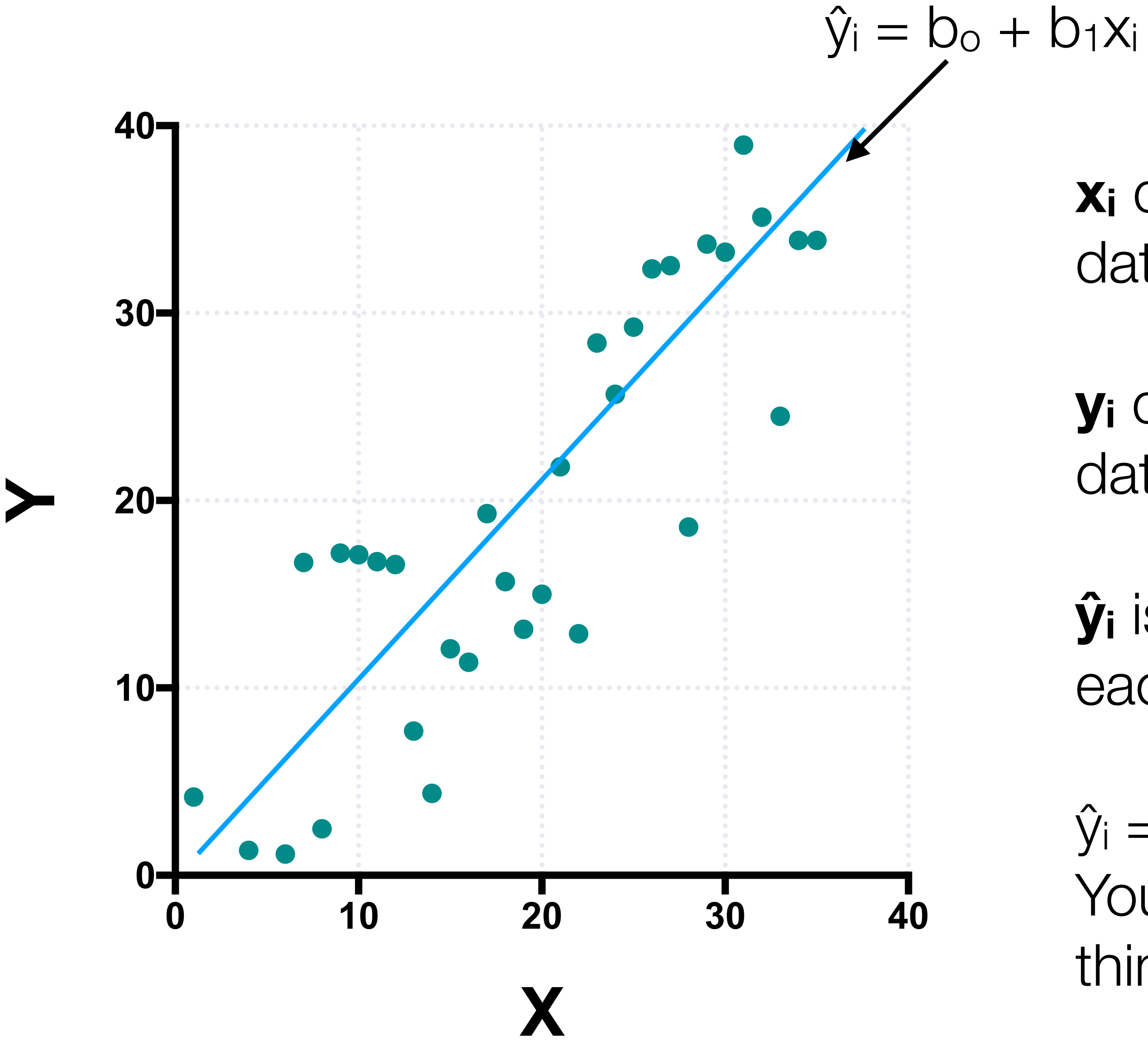
  - The other variable, called (y) is regarded as the target, response, outcome or dependent variable

- Why do we fit? We fit data so we can make inferences (conclusions) about that data. Also we can make predictions for data for which we don't have the output.

Sources: https://onlinecourses.science.psu.edu/stat501/node/251

Introduction

- Common nomenclature



$\mathbf{x_i}$ denotes the independent variable for each datapoint **i**

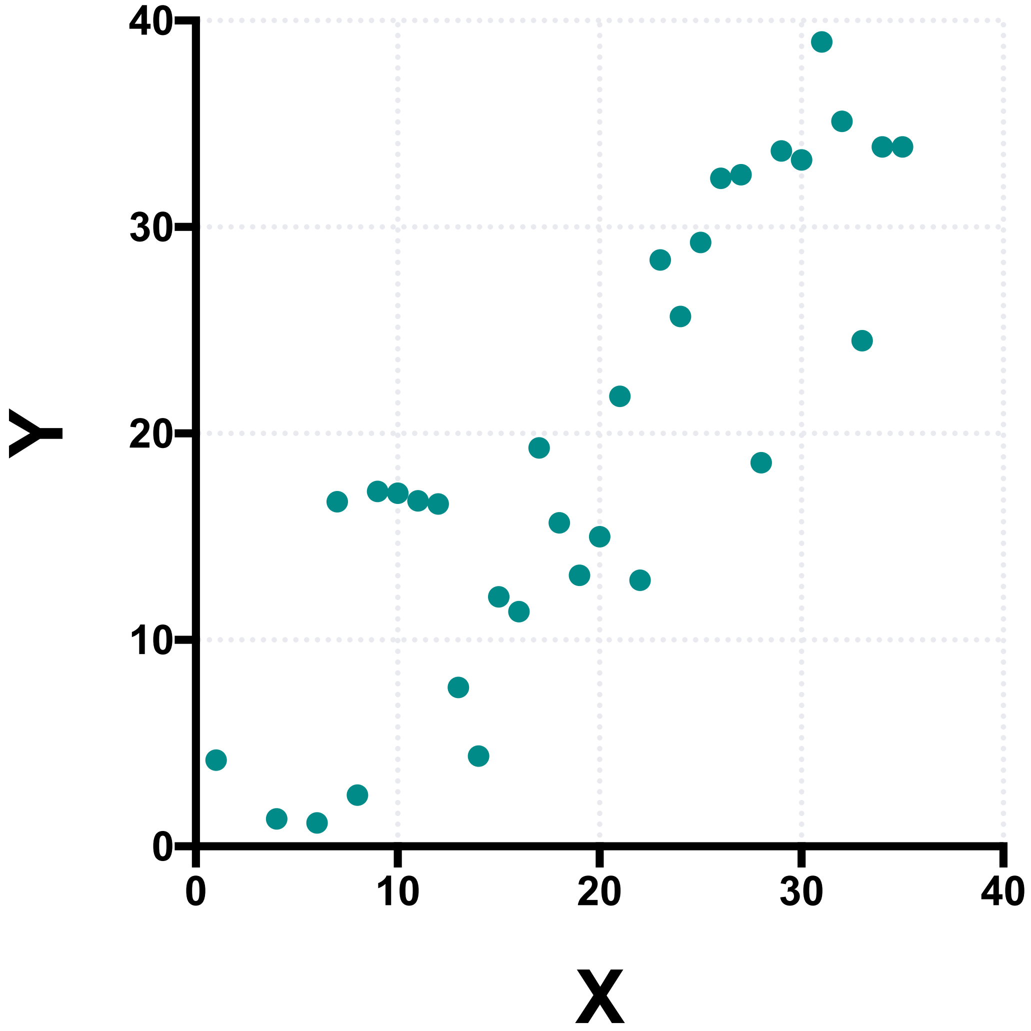
$\mathbf{y_i}$ denotes the dependent variable for each datapoint **i**

$\mathbf{\hat{y}_i}$ is the predicted dependent variable for each datapoint **i**

$\hat{y}_i = b_o + b_1 x_i$ The equation of a straight-line. You most likely know y=Mx+c (its the same thing).

Linear Regression

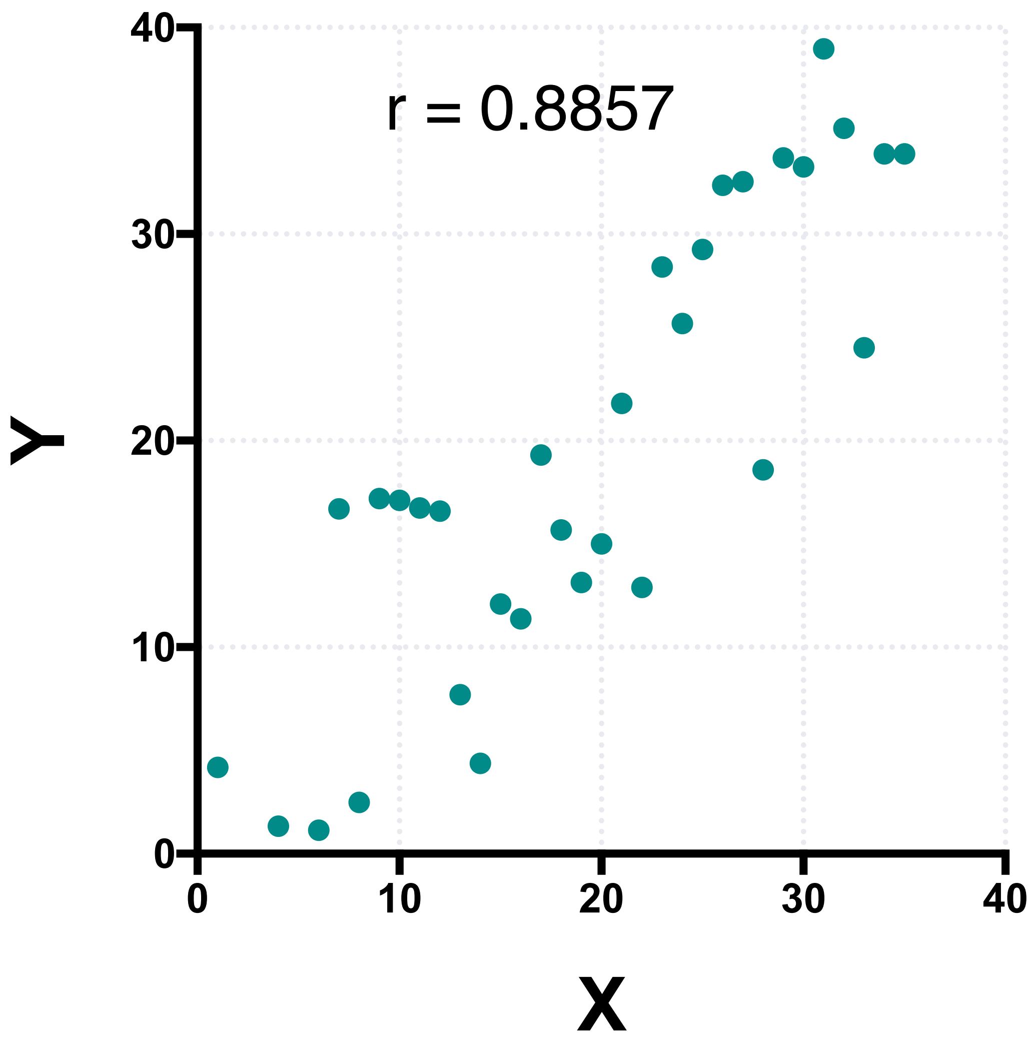
- An example of “simple linear regression”.
- It is called simple when there is only one independent variable (x).
- When there is more than one independent variable then it is called ‘multiple linear regression’.



Sources:

Should I fit a line to my data?

- We should first establish whether the data should be fit or not. A good metric through which to decide to this is through correlation.
- Correlation measures the linear relationship between x and y, and is expressed through the coefficient **ρ** (rho) for a population or **r** for sample.



$$r = \frac{1}{n-1} \sum \left(\frac{x - \bar{x}}{s_x} \right) \left(\frac{y - \bar{y}}{s_y} \right)$$

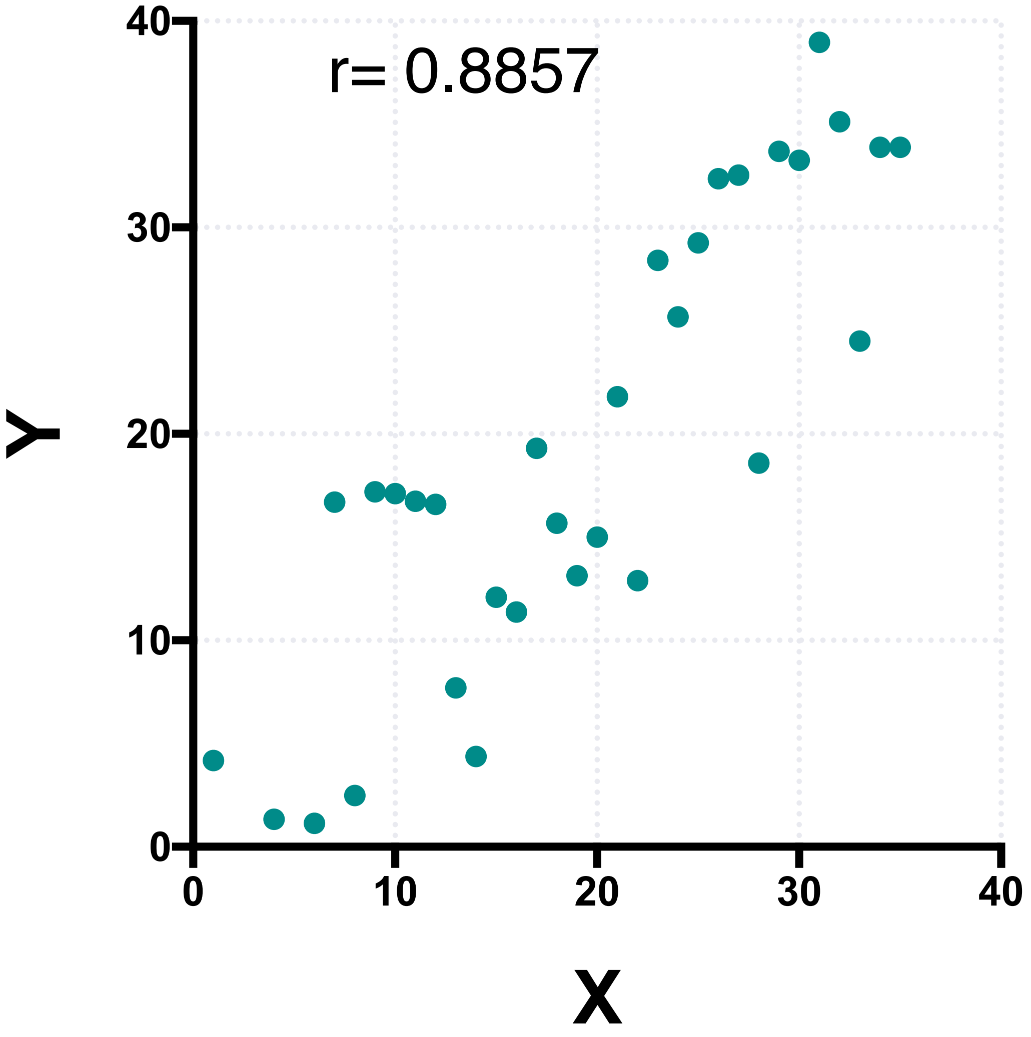
S_x, S_y = standard deviation of x, y$\bar{x}$,$\bar{y}$, = mean of x, y

- A correlation value of zero, means no relationship between x and y.
- -1 or 1 means a perfect negative or positive relationship (i.e a straight line).

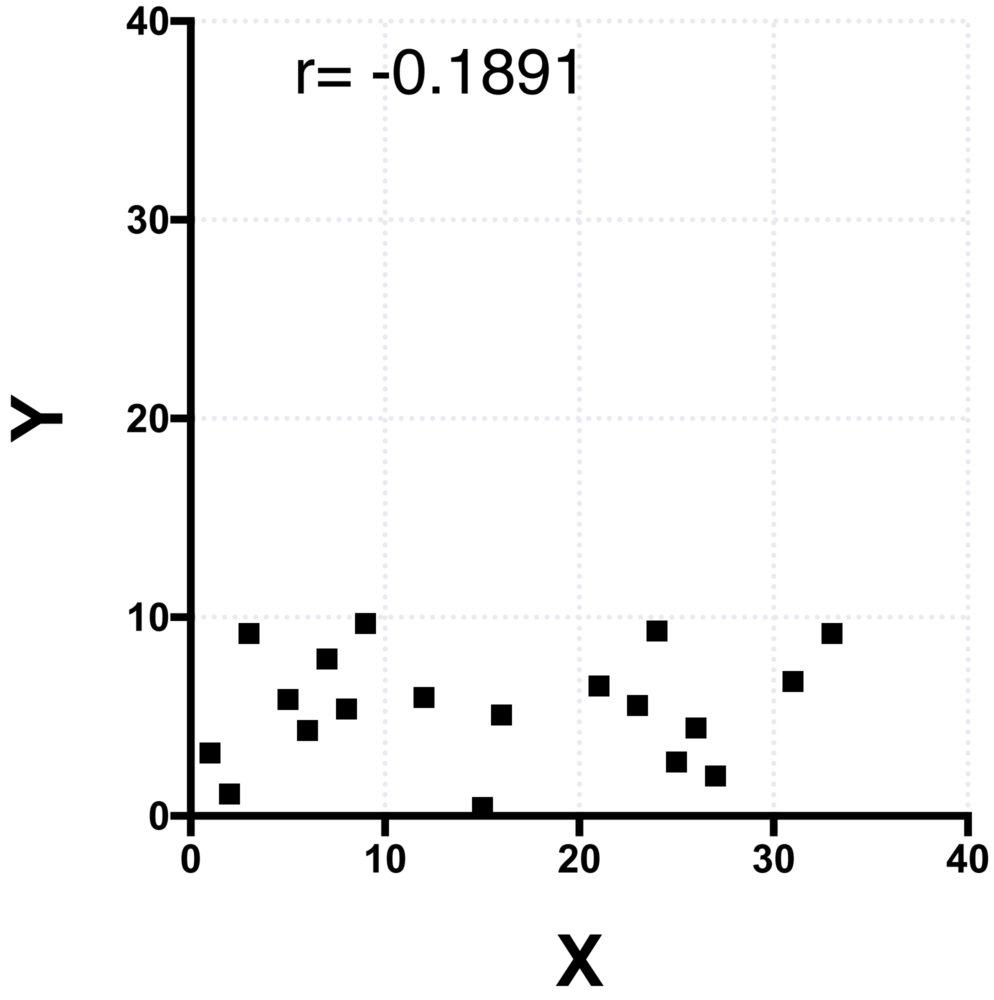
Sources:

Weakly correlated data

- If the relationship is weak, then x won’t tell you about y, they are independent, no need to fit.



Statistical relationship

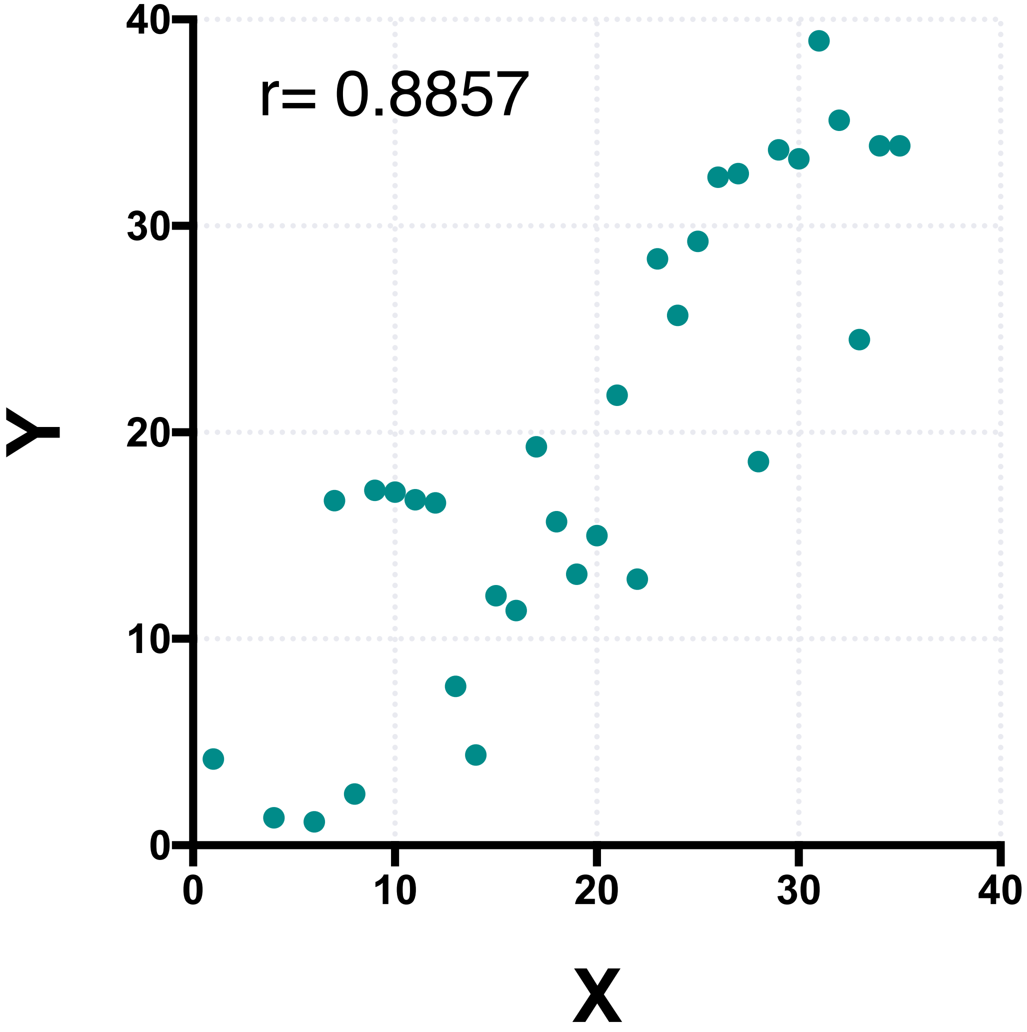


Statistical relationship

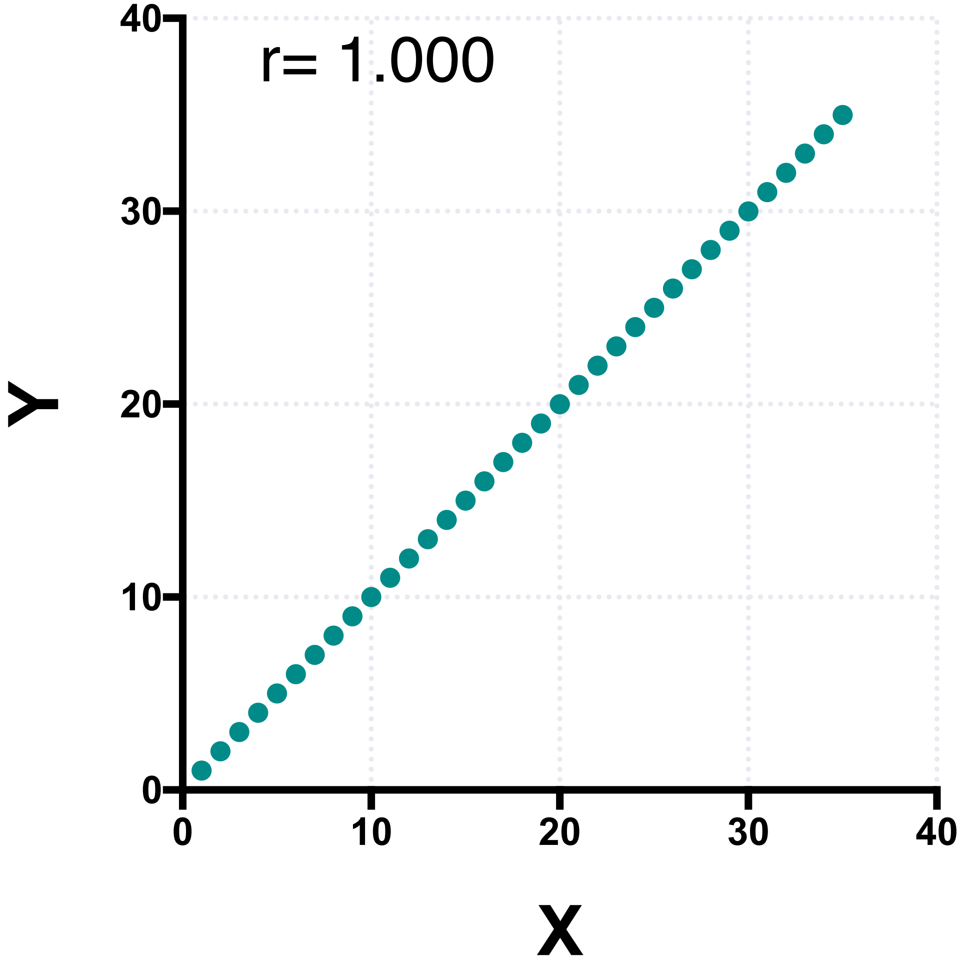
Sources:

Deterministic and Statistical data.

- Statistical relationships (e.g. x: latitude, y:skin cancer mortality, x:height, y:weight), non-perfect relationships.
- Deterministic relationship (e.g. x: x, y: pi*r^2, Ohm's law, Boyles law), perfect relationships. We don't need to fit these either.



Statistical relationship

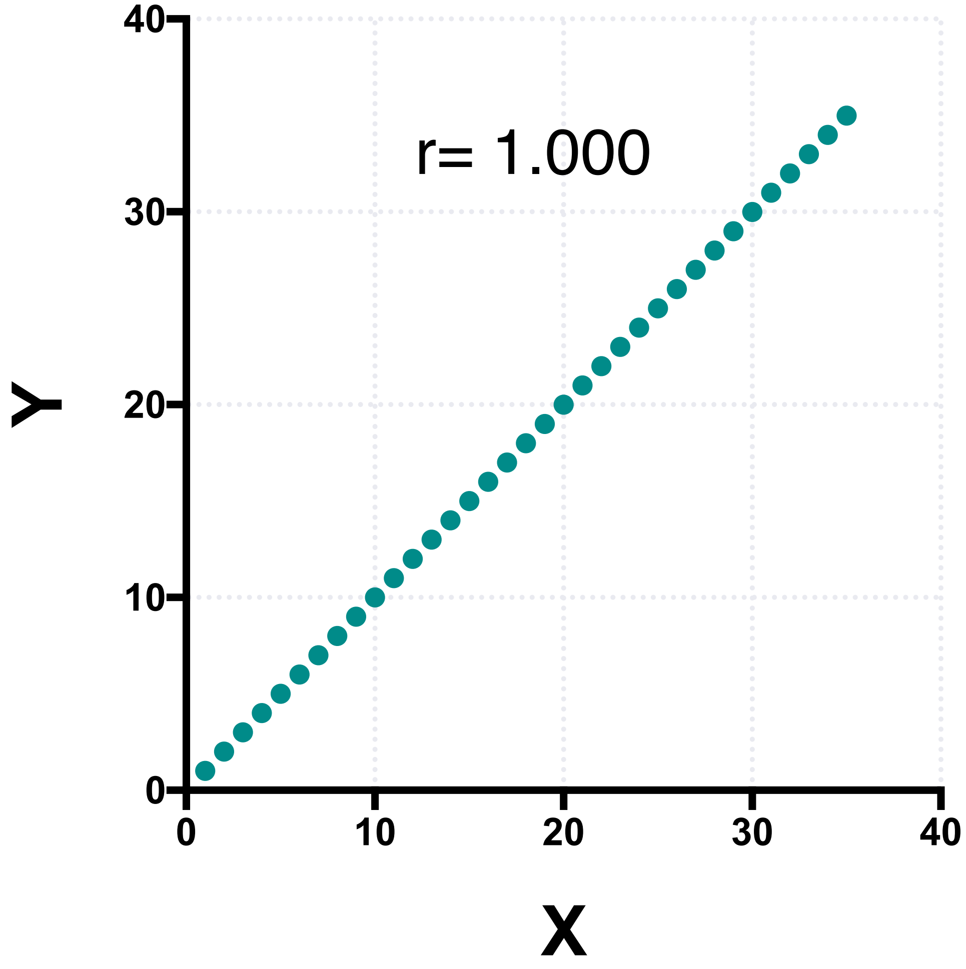


Deterministic relationship

Sources:

Deterministic data.

- With deterministic data we can directly calculate the gradient of the line so there is no need to fit the data. Linear regression is not required.



Deterministic relationship

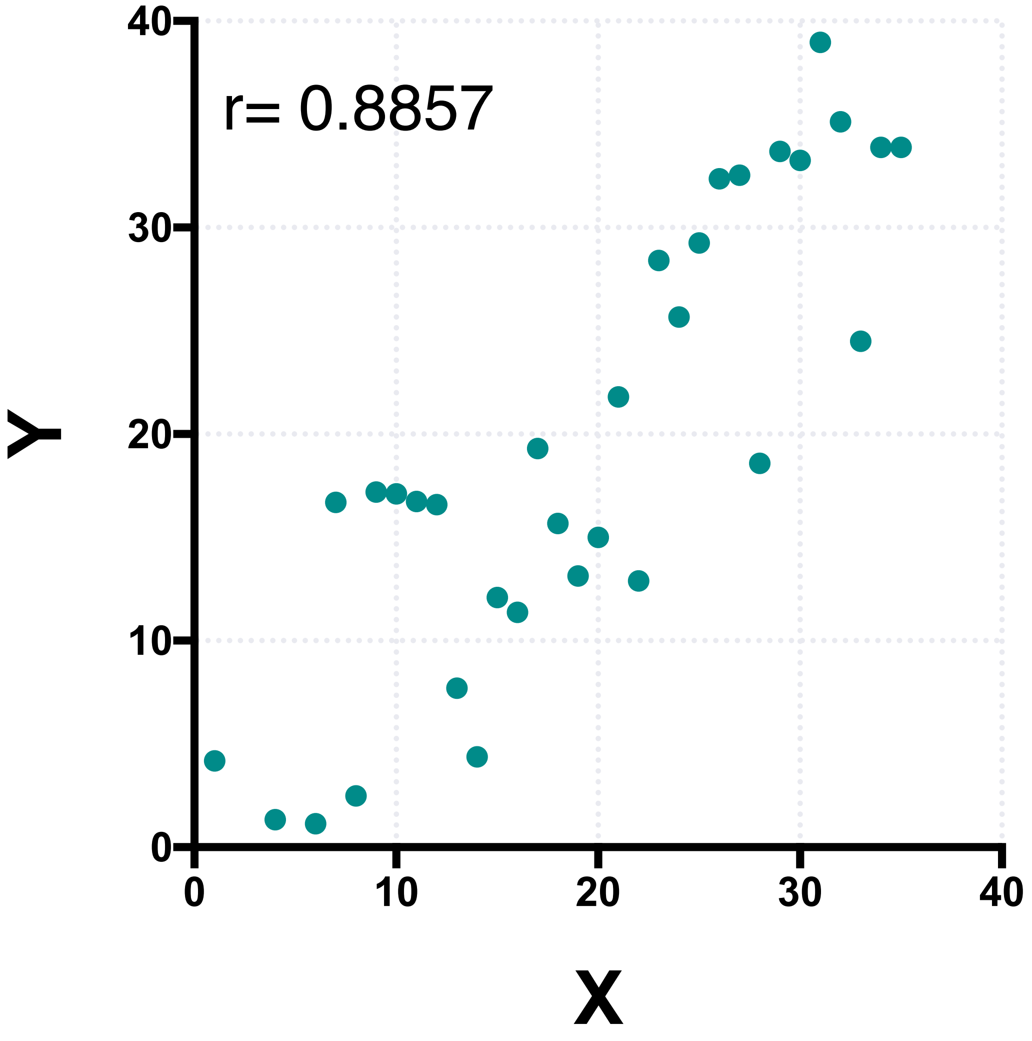
$y_i = b_o + b_1 x_i$

y_i is the dependent (not predicted) variable for each datapoint **i**

Sources:

Correlation has another purpose

- The square of the correlation coefficient, r^2, is indicative of the relation of x and y in our model.



Statistical relationship

r= 0.8857, r^2 = 0.7845 = R^2 ("R squared”)

- R^2 (or r^2), The coefficient of determination, tells us that 78 % of the variability (variance) in y can be explained by x, the remainder comes from other influences.

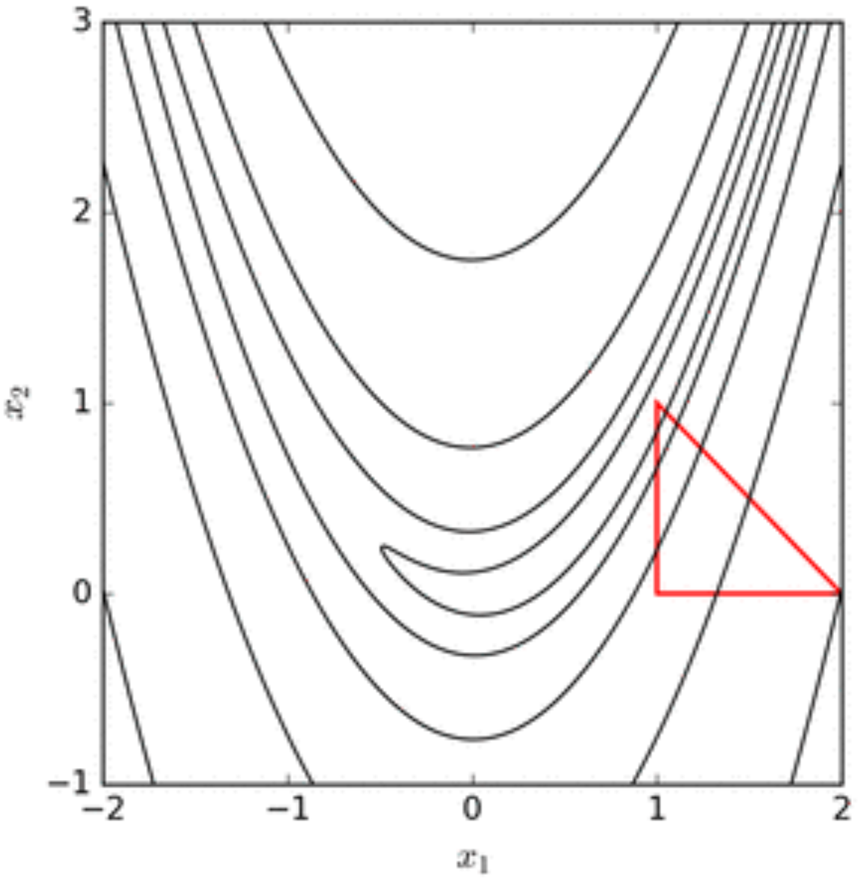
Sources:

So how do we fit?

Manually

http://userweb.molbiol.ox.ac.uk/dwaithe/WIMM_Advanced_Imaging/linearRegressionOpt.html

Using numerical optimisation



Sources:https://upload.wikimedia.org/wikipedia/commons/thumb/e/e4/Nelder-Mead_Rosenbrock.gif/320px-

The basis of the analytical solution

- The most common method for linear regression is the method of "linear least squares" which is analytically derived…
- I.e. the method is 'closed form' and 'convex', meaning it can be solved without iteration and there is only one global solution.
- The only constraints are that x and y must be real numbers and also there must be more equations (data pairs) than parameters (b_0, b_1).

Lets take the following equations

$b_0 + 1*b_1 = 6$
$b_0 + 2*b_1 = 5$
$b_0 + 3*b_1 = 7$
$b_0 + 4*b_1 = 10$

$b_0 + b_1x_i = y_i$

The goal is to minimise the sum of error produced by choice of b_0 and b_1 for all the equations
That is when we know we have the best fitting line.

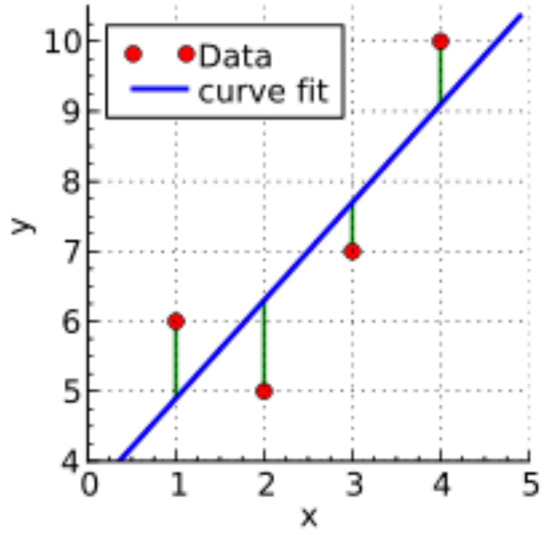
Sources:

The basis of the analytical solution

Let us take the following equations. The error for each equation is:

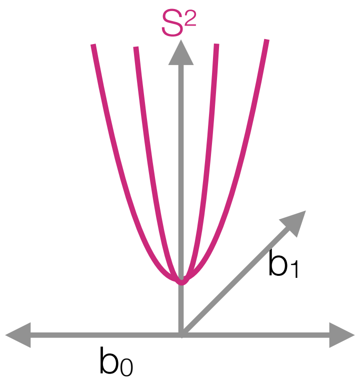
$b_0 + 1*b_1 = 6$ the error is $6-(b_0 + 1*b_1)$
$b_0 + 2*b_1 = 5$ the error is $5-(b_0 + 2*b_1)$
$b_0 + 3*b_1 = 7$ the error is $7-(b_0 + 3*b_1)$
$b_0 + 4*b_1 = 10$ the error is $10-(b_0 + 4*b_1)$

Parameterised as $y_i - (b_0 + x_1*b_1)$



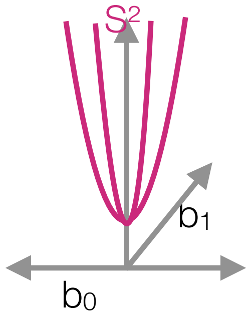
The sum of differences. We want to minimise this, that is the optimum.

$S^2(b_0,b_1) = (6-(b_0 + 1*b_1))^2 + (5-(b_0 + 2*b_1))^2 + (7-(b_0 + 3*b_1))^2 + (10-(b_0 + 4*b_1))^2$



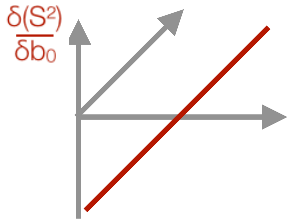
The basis of the analytical solution

- To find the minima analytically we calculate the partial derivatives of the function with respect to each parameter.

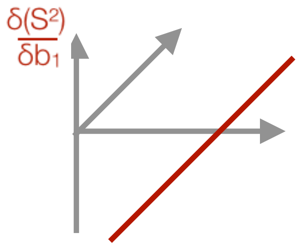


$$S^2(b_0,b_1) = \sum(yi-(b_0 + 1*b_1))^2$$

$$\frac{\delta(S^2)}{\delta b_0} = -\,2\sum[y_i - (b_0 + b_1.x_i)]$$



$$\frac{\delta(S^2)}{\delta b_1} = -\,2\sum[y_i - (b_0 + b_1.x_i)].x_i$$



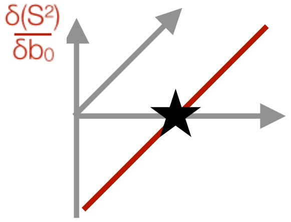
- We calculate the derivatives, because we know that the derivative will equal zero when you are in the global minimum of the cost function. (remember our function is convex, there is only one minima).

Sources:

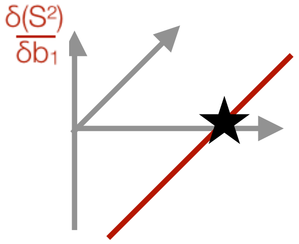
The basis of the analytical solution

- We then evaluate where the derivative is zero. This is the minimum of the sum of differences function. Our optimum solution.

$$\frac{\delta(S^2)}{\delta b_0} = -\,2\sum_{i=1}^{n}[y_i - (b_0 + b_1.x_i)] \quad = \quad 0$$



$$\frac{\delta(S^2)}{\delta b_1} = -\,2\sum_{i=1}^{n}[y_i - (b_0 + b_1.x_i)].x_i \quad = \quad 0$$



- When we do this, we have two linear equations

Sources:

Then some algebra

$$nb_0 + b_1 \sum_{i=1}^{n} x_i = \sum_{i=1}^{n} y_i$$ Rearrange $\frac{\delta(S^2)}{\delta b_0}$ $$\frac{\delta(S^2)}{\delta b_0} = -2\sum[y_i - (b_0 + b_1.x_i)] \quad = \quad 0$$

$$b_0\sum_{i=1}^{n} x_i + b_1\sum_{i=1}^{n} x_i x_i = \sum_{i=1}^{n} x_i y_i$$ Rearrange $\frac{\delta(S^2)}{\delta b_1}$ $$\frac{\delta(S^2)}{\delta b_1} = -2\sum[y_i - (b_0 + b_1.x_i)].x_i \quad = \quad 0$$

$$b_0 = \frac{\sum y_i - b_1 \sum x_i}{n}$$

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

$$b_1 = \frac{\sum x_i y_i - b_0 \sum x_i}{\sum x^2}$$

$$b_0 = \bar{y} - \left[\frac{\sum x_i y_i - b_0 \sum x_i}{\sum x^2}\right]\bar{x}$$

$$b_0 = \bar{y} - \left[\frac{\sum x_i y_i \bar{x}}{\sum x^2}\right] + \left[\frac{b_0 \sum x_i \bar{x}}{\sum x^2}\right]$$

$$b_0 - \left[\frac{b_0 \sum x_i \bar{x}}{\sum x^2}\right] = \bar{y} - \left[\frac{\sum x_i y_i \bar{x}}{\sum x^2}\right]$$

$$\left[\frac{b_0 \sum x^2}{\sum x^2}\right] - \left[\frac{b_0 \sum x_i \bar{x}}{\sum x^2}\right] = \bar{y} - \left[\frac{\sum x_i y_i \bar{x}}{\sum x^2}\right]$$

$$\frac{b_0 \left[\sum x^2 - \sum x_i \bar{x}\right]}{\sum x^2} = \bar{y} - \left[\frac{\sum x_i y_i \bar{x}}{\sum x^2}\right]$$

$$\frac{b_0 \left[\sum x^2 - \sum x_i \bar{x}\right]}{\sum x^2} = \bar{y} - \left[\frac{\sum x_i y_i \bar{x}}{\sum x^2}\right]$$

$$\frac{b_0 \left[\sum x^2 - \sum x_i \bar{x}\right]}{\sum x^2} = \frac{\sum x^2 \bar{y}}{\sum x^2} - \frac{\sum x_i y_i \bar{x}}{\sum x^2}$$

$$b_0 = \frac{\sum x^2 \bar{y} - \sum x_i y_i \bar{x}}{\sum x^2 - \sum x_i \bar{x}}$$

$$b_0 = \frac{\bar{y}\sum x^2 - \bar{x}\sum x_i y_i}{\sum x^2 - n\bar{x}^2} \qquad (1)$$

I skipped a bit for b1

$$b_1 = \frac{n\sum x_i y_i - \sum x_i \sum y_i}{n\sum x^2 - \left(\sum x_i\right)^2}$$

$$b_1 = \frac{\sum x_i y_i - n\bar{x}\bar{y}}{\sum x^2 - n\bar{x}^2} \qquad (2)$$

Finally we have the solutions. These are neat, but require some processing.

Sources: https://en.wikipedia.org/wiki/Linear_least_squares_(mathematics)

The same but expressed through linear algebra

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

Rearrange $\frac{\delta(S^2)}{\delta b_0}$

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

Rearrange $\frac{\delta(S^2)}{\delta b_1}$

$$\overset{X'X}{\begin{bmatrix} n & \sum_{i=1}^{n} x_i \\ \sum_{i=1}^{n} x_i & \sum_{i=1}^{n} x_i^2 \end{bmatrix}} \overset{\beta}{\begin{bmatrix} b_0 \\ b_1 \end{bmatrix}} = \overset{X'Y}{\begin{bmatrix} \sum_{i=1}^{n} y_i \\ \sum_{i=1}^{n} x_i \, y_i \end{bmatrix}},$$

Arrange as a matrix (3)

$$\begin{bmatrix} b_0 \\ b_1 \end{bmatrix} = \frac{1}{n \sum_{i=1}^{n} x_i^2 - (\sum_{i=1}^{n} x_i)^2} \begin{bmatrix} \sum_{i=1}^{n} y_i \sum_{i=1}^{n} x_i^2 - \sum_{i=1}^{n} x_i \sum_{i=1}^{n} x_i \, y_i \\ n \sum_{i=1}^{n} x_i \, y_i - \sum_{i=1}^{n} x_i \sum_{i=1}^{n} y_i \end{bmatrix},$$

invert matrix $\beta = (X'X)^{-1} X'Y$ (4)

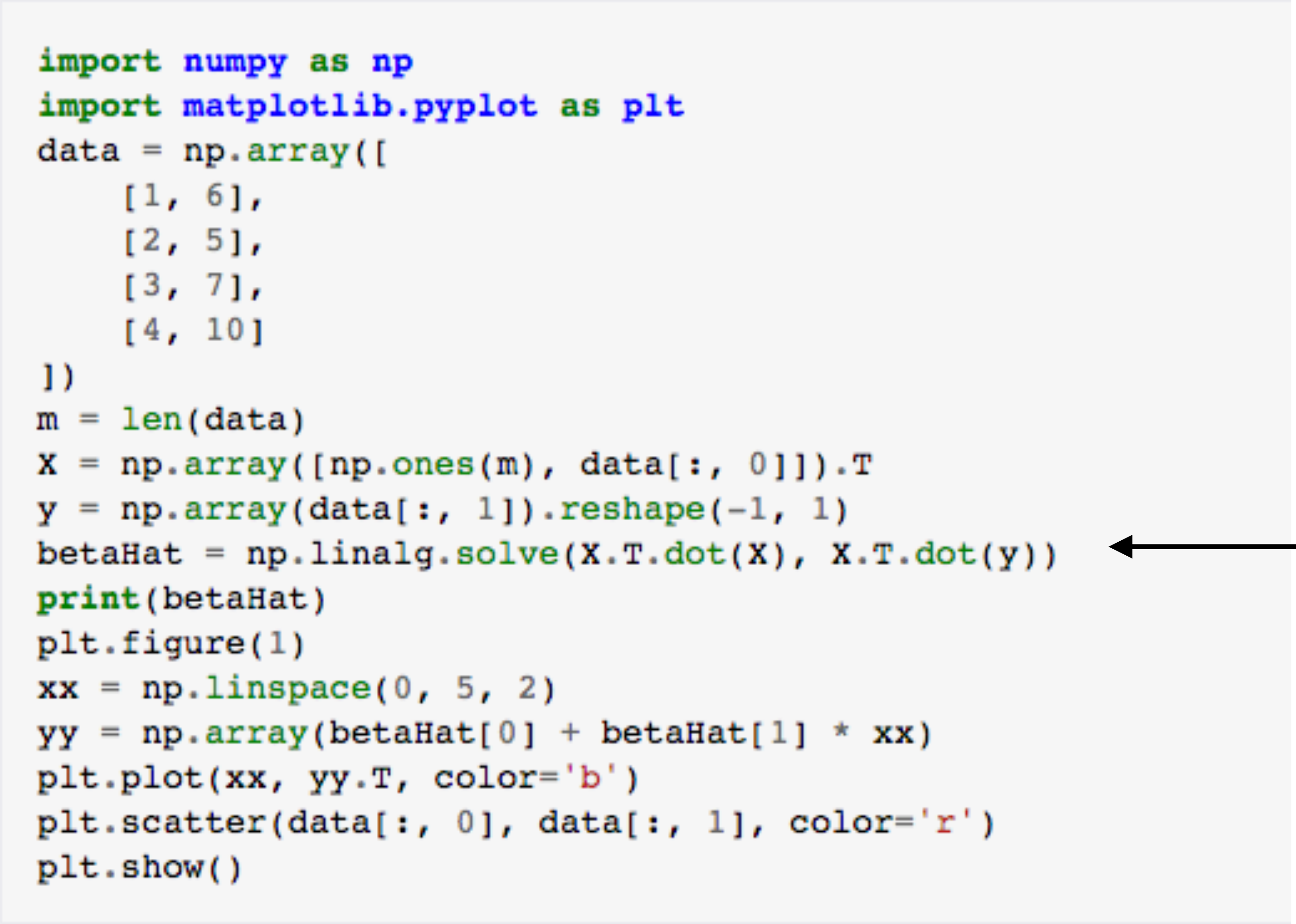
This can be easily generalised to higher dimensions (e.g. more independent variables).

If you want to get good at linear algebra (who wouldn't) I highly recommend the Strang lectures on linear algebra: https://www.youtube.com/watch?v=ZK3O402wf1c

Sources: https://en.wikipedia.org/wiki/Linear_least_squares_(mathematics)

Don’t worry python code is simple.

Some python code for simple linear regression.



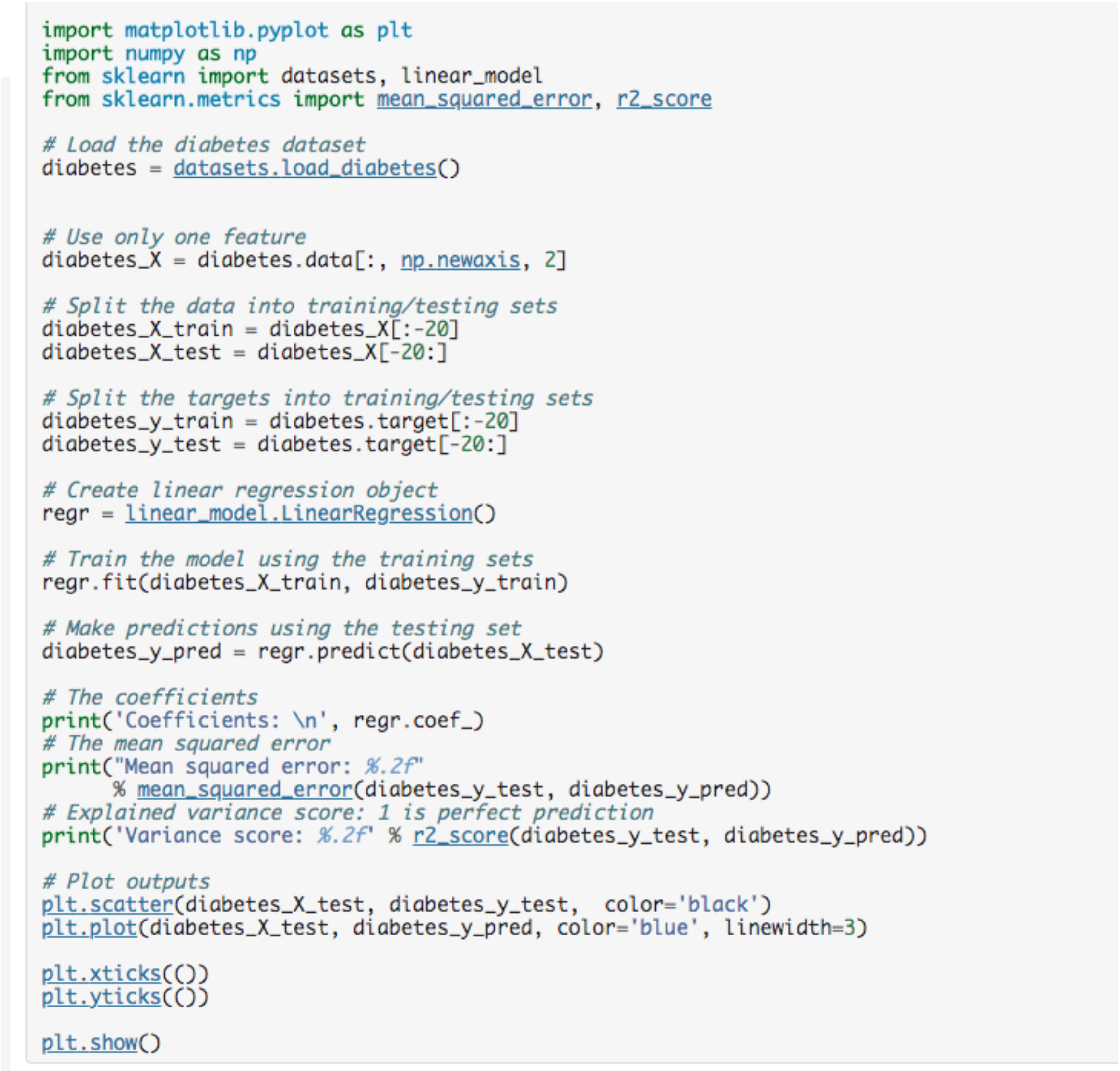
```python
import numpy as np
import matplotlib.pyplot as plt
data = np.array([
    [1, 6],
    [2, 5],
    [3, 7],
    [4, 10]
])
m = len(data)
X = np.array([np.ones(m), data[:, 0]]).T
y = np.array(data[:, 1]).reshape(-1, 1)
betaHat = np.linalg.solve(X.T.dot(X), X.T.dot(y))
print(betaHat)
plt.figure(1)
xx = np.linspace(0, 5, 2)
yy = np.array(betaHat[0] + betaHat[1] * xx)
plt.plot(xx, yy.T, color='b')
plt.scatter(data[:, 0], data[:, 1], color='r')
plt.show()
```

invert matrix

$$\beta = (X'X)^{-1}X'Y$$

Sources: https://en.wikipedia.org/wiki/Linear_least_squares_(mathematics)

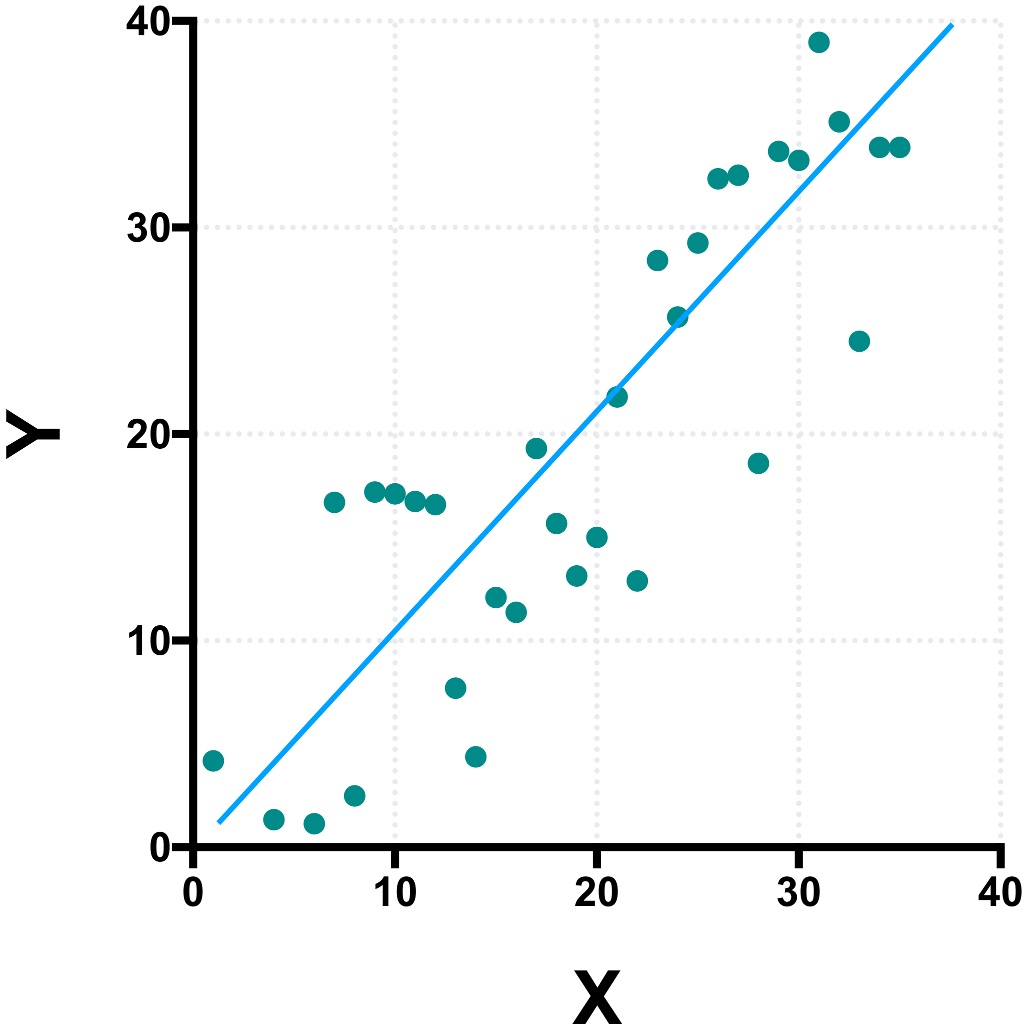
Scikit-learn regression example (no math)



```python
import matplotlib.pyplot as plt
import numpy as np
from sklearn import datasets, linear_model
from sklearn.metrics import mean_squared_error, r2_score

# Load the diabetes dataset
diabetes = datasets.load_diabetes()


# Use only one feature
diabetes_X = diabetes.data[:, np.newaxis, 2]

# Split the data into training/testing sets
diabetes_X_train = diabetes_X[:-20]
diabetes_X_test = diabetes_X[-20:]

# Split the targets into training/testing sets
diabetes_y_train = diabetes.target[:-20]
diabetes_y_test = diabetes.target[-20:]

# Create linear regression object
regr = linear_model.LinearRegression()

# Train the model using the training sets
regr.fit(diabetes_X_train, diabetes_y_train)

# Make predictions using the testing set
diabetes_y_pred = regr.predict(diabetes_X_test)

# The coefficients
print('Coefficients: \n', regr.coef_)
# The mean squared error
print("Mean squared error: %.2f"
      % mean_squared_error(diabetes_y_test, diabetes_y_pred))
# Explained variance score: 1 is perfect prediction
print('Variance score: %.2f' % r2_score(diabetes_y_test, diabetes_y_pred))

# Plot outputs
plt.scatter(diabetes_X_test, diabetes_y_test,  color='black')
plt.plot(diabetes_X_test, diabetes_y_pred, color='blue', linewidth=3)

plt.xticks(())
plt.yticks(())

plt.show()
```

Sources: http://scikit-learn.org/stable/auto_examples/linear_model/plot_ols.html

What we get. Coefficients



We get b0 and b1. We have to make the line.

```
xx = np.linspace(0,40,2)
yy = np.array(b0+ b1* xx)
plot(xx,yy, color='b')
```

$\hat{y}_i = b_o + b_1x_i$ The equation of a straight-line.

Sources: https://en.wikipedia.org/wiki/Linear_least_squares_(mathematics)

What we get. Residuals

- Residuals measure the error between our data and our predicted line.

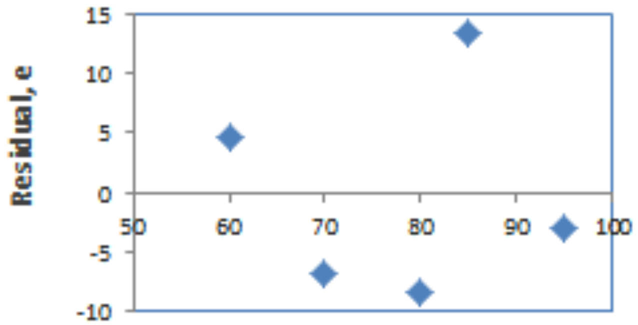
Residual = Observed value - Predicted value

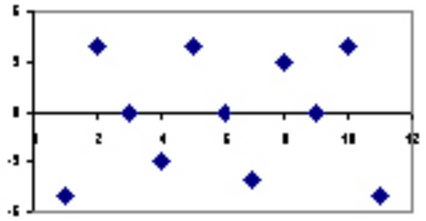
$$e = y - \hat{y}$$

Residual Sum of Squares (RSS)

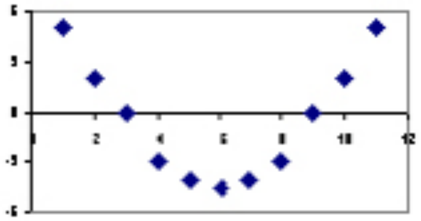
$$RSS = \sum_{i=1}^{n} e^2$$

- A residual plot, shows this error for each datapoint x.

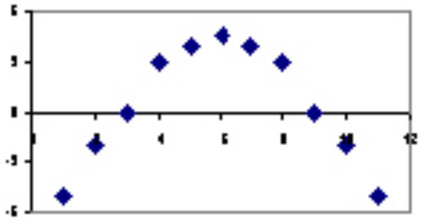




Random pattern



Non-random: U-shaped



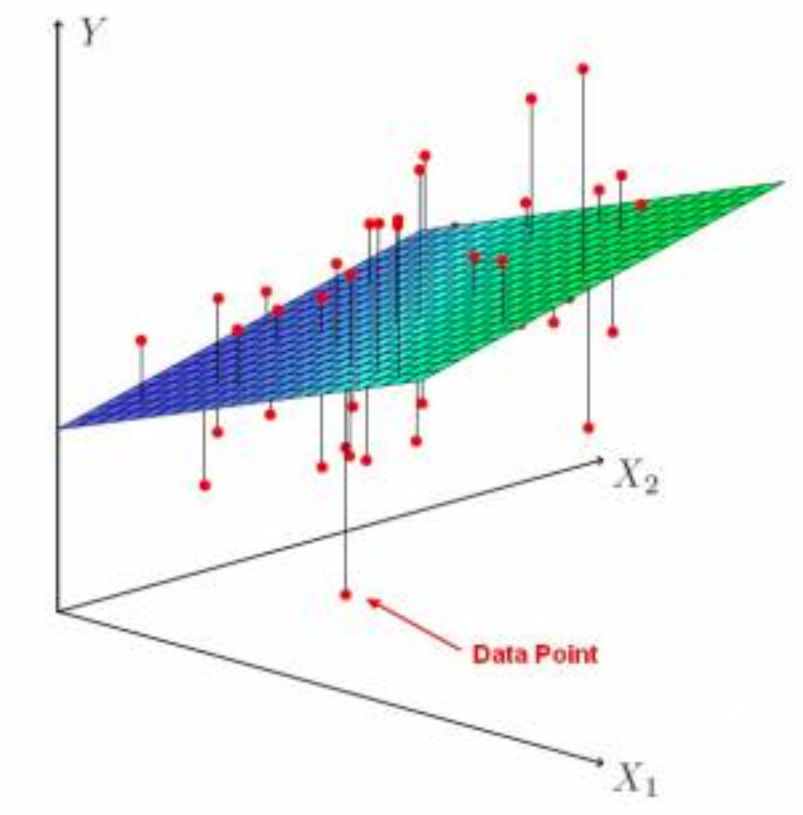
Non-random: Inverted U

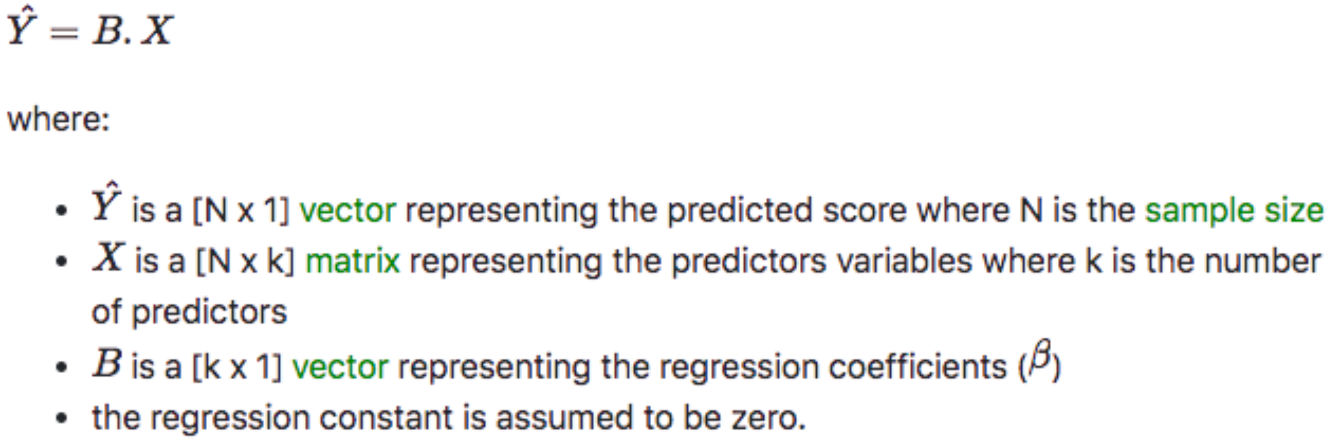
If your data, doesn't look randomly distributed, rethink your model. Maybe straight-line is not enough this time.

Sources: http://stattrek.com/regression/residual-analysis.aspx?Tutorial=AP

simple linear regression to multiple linear regression

- Simple linear regression involves one independent variable
- Multiple linear regression can involve > 1 independent variables (predictors)





$\hat{Y} = B.X$

where:

- $\hat{Y}$ is a [N x 1] vector representing the predicted score where N is the sample size
- X is a [N x k] matrix representing the predictors variables where k is the number of predictors
- B is a [k x 1] vector representing the regression coefficients (β)
- the regression constant is assumed to be zero.

$$\beta = (X'X)^{-1}X'Y$$

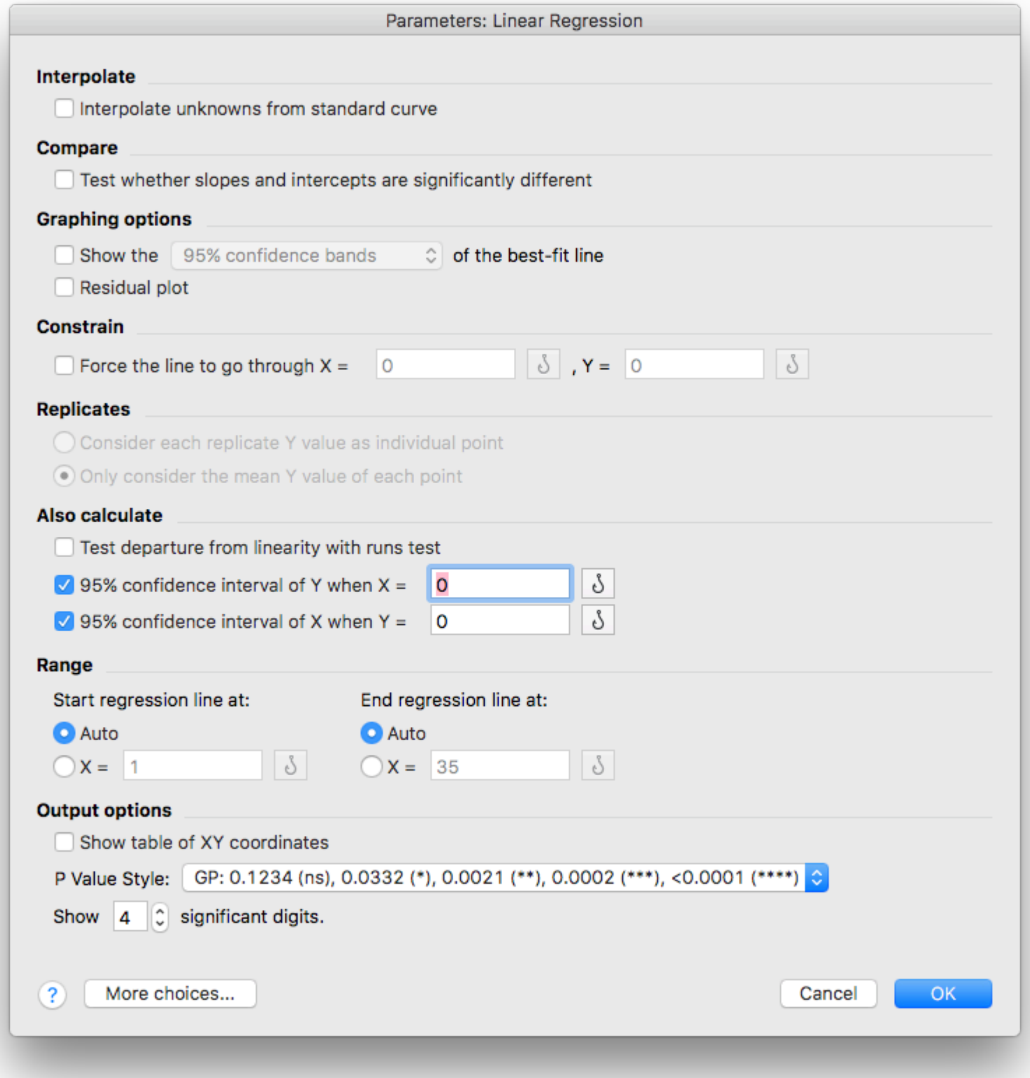
e.g. two independent variables.

- Good news is we can solve with the same approach, just add more x columns (independent variables).

Sources: https://gerardnico.com/data_mining/multiple_regression

Its easy-peasy to do regression with Graphpad Prism.

- Good for checking your methods :-). But only if simple case.



Parameters: Linear Regression

Interpolate

□ Interpolate unknowns from standard curve

Compare

□ Test whether slopes and intercepts are significantly different

Graphing options

□ Show the 95% confidence bands of the best-fit line

□ Residual plot

Constrain

□ Force the line to go through X = 0 , Y = 0

Replicates

○ Consider each replicate Y value as individual point

● Only consider the mean Y value of each point

Also calculate

□ Test departure from linearity with runs test

☑ 95% confidence interval of Y when X = 0

☑ 95% confidence interval of X when Y = 0

Range

Start regression line at: ● Auto ○ X = 1

End regression line at: ● Auto ○ X = 35

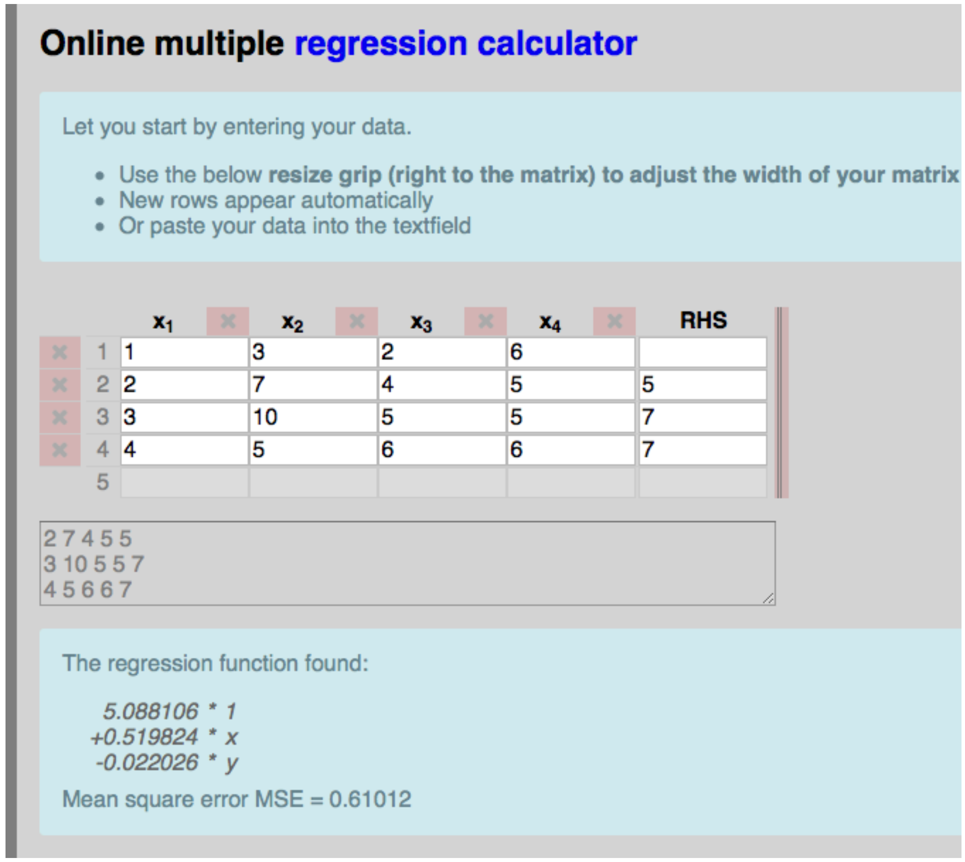
Output options

□ Show table of XY coordinates

P Value Style: GP: 0.1234 (ns), 0.0332 (*), 0.0021 (**), 0.0002 (***), <0.0001 (****)

Show 4 significant digits.

- Also online methods for doing multiple linear regression
- http://regression.structural-analyser.com



Online multiple regression calculator

Let you start by entering your data.

- Use the below **resize grip (right to the matrix) to adjust the width of your matrix**
- New rows appear automatically
- Or paste your data into the textfield

	x_1	x_2	x_3	x_4	RHS
1	1	3	2	6	
2	2	7	4	5	5
3	3	10	5	5	7
4	4	5	6	6	7
5					

```
2 7 4 5 5
3 10 5 5 7
4 5 6 6 7
```

The regression function found:

*5.088106 * 1*
*+0.519824 * x*
*-0.022026 * y*

Mean square error MSE = 0.61012

Sources:

Limitations of linear regression

- Only describes linear relationships
- Linear Regression Is Sensitive to Outliers
- Data Must Be Independent (Thats why they are called ‘independent’)

Advantages of linear regression

- Fast.
- Easy to use.
- Easyish to understand.

Conclusion

- Its good to know how things work.
- People take linear regression for granted, it is used a lot.

Sources:

Practicals.

- https://github.com/dwaithe/linear_regression_practical

- clone the repository. download: CGAT_linear_regression_basics.ipynb
- Work through ask questions.

Thanks for your attention

Please follow me on Twitter.
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Sources: