Simple linear regression

Introduction

Simple linear regression is a statistical method for obtaining a formula to predict values of one variable from another where there is a causal relationship between the two variables.

Straight line formula

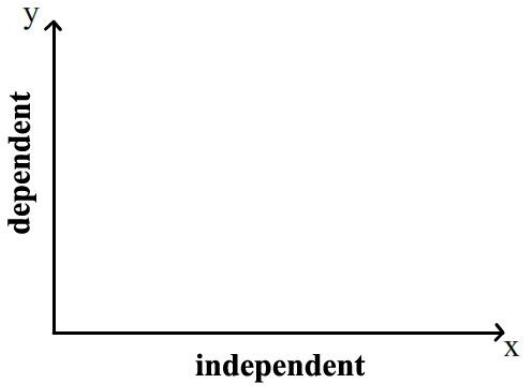
Central to simple linear regression is the formula for a straight line that is most commonly represented as $y = mx + c$ or $y = a + bx$. Statisticians however generally prefer to use the following form involving betas:

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

The variables *y* and *x* are those whose relationship we are studying. We give them the following names:

- *y*: dependent (or response) variable;
- *x*: independent (or predictor or explanatory) variable.

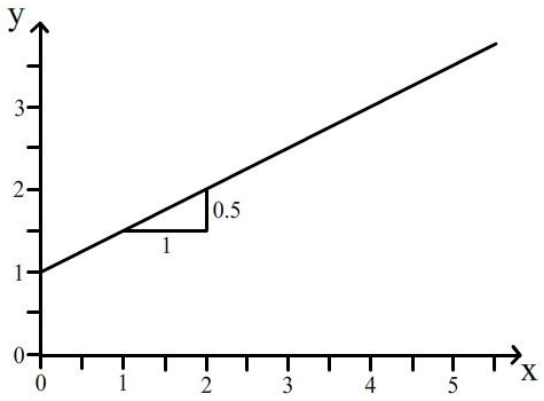
It is convention when plotting data to put the dependent and independent data on the *y* and *x* axis respectively;



β_0 and β_1 are constants and are parameters (or coefficients) that need to be estimated from data. Their roles in the straight line formula are as follows:

- β_0 : intercept;
- β_1 : gradient.

For instance the line $y = 1 + 0.5x$ has an intercept of 1 and a gradient of 0.5. Its graph is as follows:



Model assumptions

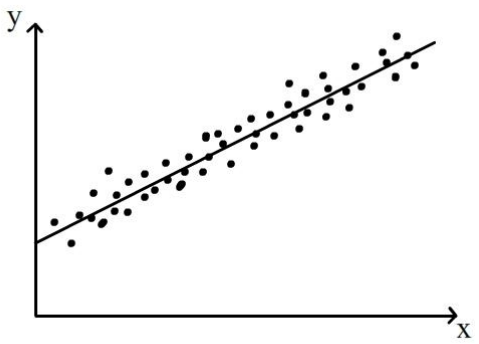
In simple linear regression we aim to predict the response for the *i*th individual, Y_i, using the individual's score of a single predictor variable, X_i. The form of the model is given by:

$$Y_i = \beta_0 + \beta_1 X_i + \varepsilon_i$$

which comprises a deterministic component involving the two *regression coefficients* (β_0 and β_1) and a random component involving the *residual* (error) term (ε_i).

The deterministic component is in the form of a straight line which provides the predicted (mean/expected) response for a given predictor variable value.

The residual terms represent the difference between the predicted value and the observed value of an individual. They are assumed to be independently and identically distributed normally with zero mean and variance σ^2, and account for natural variability as well as maybe measurement error. Our data should thus appear to be a collection of points that are randomly scattered around a straight line with constant variability along the line:



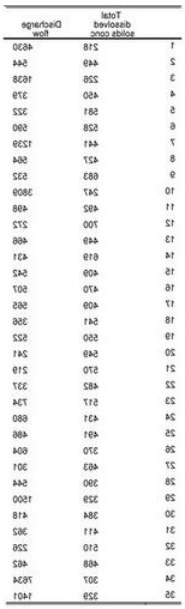
The deterministic component is a linear function of the unknown regression coefficients which need to be estimated so that the model 'best' describes the data. This is achieved mathematically by minimising the sum of the squared residual terms (*least squares*). The fitting also produces an estimate of the error variance which is necessary for things like significance test regarding the regression coefficients and for producing confidence/prediction intervals.

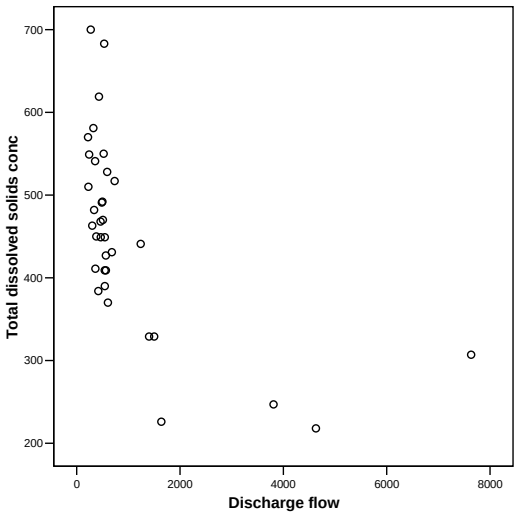
Example

Suppose we are interested in predicting the total dissolved solids (TDS) concentrations (mg/L) in a particular river as a function of the discharge flow (m^3/s). We have collected data that comprise a sample of 35 observations that were collected over the previous year.

The first step is to look carefully at the data:

- Is there an upwards/downwards trend in the data or could a horizontal line be fit though the data?
- Is the trend linear or curvilinear?
- Is there constant variance along the regression line or does it systematically change as the predictor variable changes?





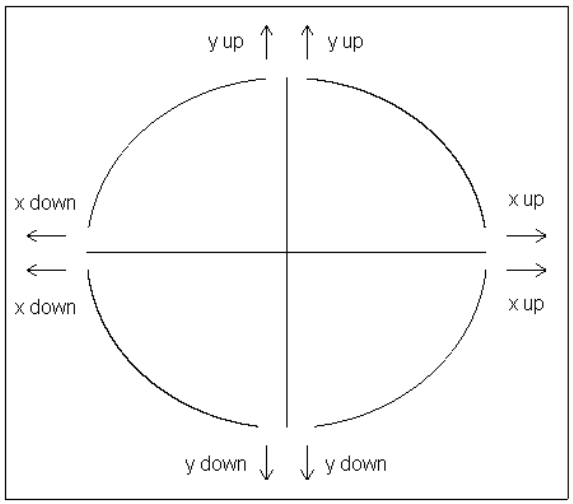
The scatterplot above suggests that there is a downwards trend in the data, however there is a curvilinear relationship. The variance about a hypothetical curve appears fairly constant.

Transformations

Simple linear regression is appropriate for modelling linear trends where the data is uniformly spread around the line. If this is not the case then we should be using other modelling techniques and/or transforming our data to meet the requirements. When considering transformations the following is a guide:

- If the trend is curvilinear consider a transformation of the predictor variable, *x*.
- If constant variance is a problem (and maybe curvilinear as well) consider either a transformation of the response variable, *y*, or a transformation of both the response and the predictor variable, *x* and *y*.

Tukey's "bulging rule" can act as a guide to selecting power transformations.



Compare your data to the above and if it has the shape in any of the quadrants then consider the transformations where:

- up – use powers of the variable greater than 1 (e.g. x^2, etc);
- down - powers of the variable less than 1 (e.g. log(x), 1/x, √x etc).

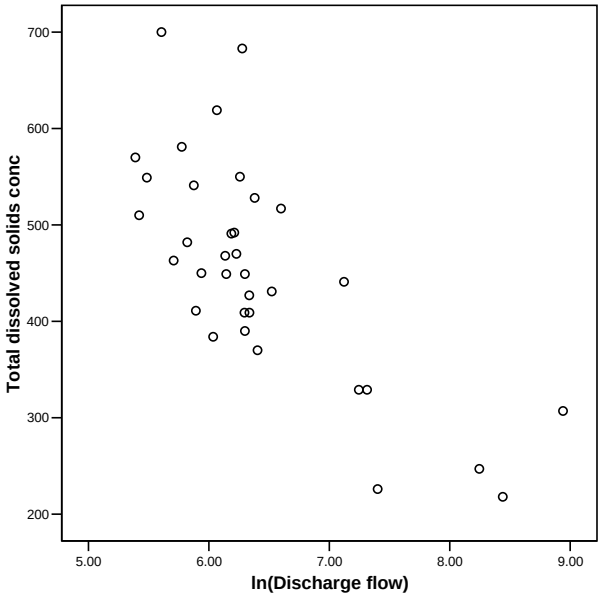
Note, sometimes a second application of Tukey's bulging rule is necessary to gain linearity with constant variability.

Example (revisited)

Returning to our example, the scatterplot reveals the data to belong to the bottom left quadrant of Tukey's bulging rule. Since the variance about a hypothetical curve appears fairly constant, thus we shall try transforming just the predictor variable.
Tukey's bulging rule suggests a "down" power; we shall try the log natural transformation first

The resulting scatterplot of TDS against ln(Discharge) is now far more satisfactory:

	Total dissolved solids conc (mg/L)	Discharge flow (cu m/s)	Ln Discharge
1	218	4630	8.44
2	449	544	6.30
3	226	1638	7.40
4	450	379	5.94
5	581	322	5.77
6	528	590	6.38
7	441	1239	7.12
8	427	564	6.34
9	683	532	6.28
10	247	3809	8.25
11	492	498	6.21
12	700	272	5.61
13	449	466	6.14
14	619	431	6.07
15	409	542	6.30
16	470	507	6.23
17	409	565	6.34
18	541	356	5.87
19	550	522	6.26
20	549	241	5.48
21	570	219	5.39
22	482	337	5.82
23	517	734	6.60
24	431	680	6.52
25	491	486	6.19
26	370	604	6.40
27	463	301	5.71
28	390	544	6.30
29	329	1500	7.31
30	384	418	6.04
31	411	362	5.89
32	510	226	5.42
33	468	462	6.14
34	307	7634	8.94
35	329	1401	7.24



The data now appears to be suitable for simple linear regression and we shall now consider selected output from the statistics package SPSS.

Correlations

		Total dissolved solids conc	ln(Discharge flow)
Pearson Correlation	Total dissolved solids conc	1.000	-.735
	ln(Discharge flow)	-.735	1.000
Sig. (1-tailed)	Total dissolved solids conc	.	.000
	ln(Discharge flow)	.000	.
N	Total dissolved solids conc	35	35
	ln(Discharge flow)	35	35

The correlations table displays Pearson correlation coefficients, significance values, and the number of cases with non-missing values. As expected we see that we have a strong negative correlation (-.735) between the two variables. From the significance test p-value we can see that we have very strong evidence ($p<0.001$) to suggest that there is a linear correlation between the two variables.

Model Summary[b]

Model	R	R Square	Adjusted R Square	Std. Error of the Estimate
1	.735[a]	.540	.526	78.261

a. Predictors: (Constant), ln(Discharge flow)

b. Dependent Variable: Total dissolved solids conc

The model summary table displays:

- R, the multiple correlation coefficient, is a measure of the strength of the linear relationship between the response variable and the set of explanatory variables. It is the highest possible simple correlation between the response variable and any linear combination of the explanatory variables. For simple linear regression where we have just two variables, this is the same as the absolute value of the Pearson's correlation coefficient we have already seen above. However, in multiple regression this allows us to measure the correlation involving the response variable and more than one explanatory variable.
- R squared is the proportion of variation in the response variable explained by the regression model. The values of R squared range from 0 to 1; small values indicate that the model does not fit the data well. From the above we can see that the model fits the data reasonably well; 54% of the variation in the *TDS* values can be explained by the fitted line together with the *lnDischarge* values. R squared is also known as the *coefficient of determination*.
- The R squared value can be over optimistic in its estimate of how well a model fits the population; the adjusted R square value is attempts to correct for this. Here we can see it has slightly reduced the estimated proportion. If you have a small data set it may be worth reporting the adjusted R squared value.
- The standard error of the estimate is the estimate of the standard deviation of the error term of the model, σ. This gives us an idea of the expected variability of predictions and is used in calculation of confidence intervals and significance tests.

Coefficients[a]

Model		Unstandardized Coefficients		Standardized Coefficients	t	Sig.	95% Confidence Interval for B	
		B	Std. Error	Beta			Lower Bound	Upper Bound
1	(Constant)	1103.967	105.320		10.482	.000	889.693	1318.242
	ln(Discharge flow)	-101.275	16.281	-.735	-6.221	.000	-134.399	-68.152

a. Dependent Variable: Total dissolved solids conc

The unstandardized coefficients are the coefficients of the estimated regression model. Thus the expected *TDS* value is given by:

$$TDS = 1103.967 - 101.275\ln(Discharge).$$

Thus we can see that for each one unit increase in ln(*Discharge*), the *TDS* value is expected to decrease by 101.275 units. The intercept for this example could be interpreted as the *TDS* value (1103.967) when the ln(*Discharge*) flow is zero (i.e. Discharge = 1 m^3/s.

The standardized coefficients are appropriate in multiple regression when we have explanatory variables that are measured on different units. These coefficients are obtained from regression after the explanatory variables are all standardized. The idea is that the coefficients of explanatory variables can be more easily compared with each other as they are then on the same scale. In simple linear regression they are of little concern.

The standard errors give us estimates of the variability of the (unstandardised) coefficients and are used for significance tests for the coefficients and for the displayed 95% confidence intervals. The *t* values and corresponding significance vales are tests assessing the worth of the (unstandardised) coefficients. It is usually of importance to be assessing the worth of our predictor variable and hence evaluating the significance of the coefficient β_1 in our model formulation. That is we are assessing for evidence of a significant non-zero slope. If the coefficient is not significantly different to zero then this implies the predictor variable does not influence our response variable.

Here we have both test are highly significant ($p<0.001$), indicating that we have very strong evidence of need both the coefficients in our model. The resulting confidence intervals expand our understanding of the problem. For example, with 95% confidence we believe that the interval between -134.399 and -68.152 covers the true unknown *TDS* value change per ln(*Discharge*) unit.

The remaining output is concerned with checking the model assumptions of normality, linearity, homoscedasticity and independence of the residuals. Residuals are the differences between the observed and predicted responses. The residual scatterplots allow you to check:

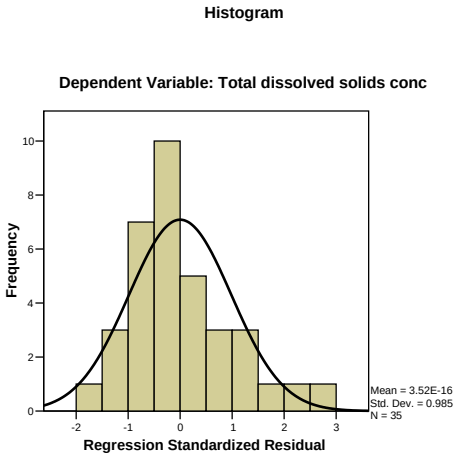
- *Normality*: the residuals should be normally distributed about the predicted responses;
- *Linearity*: the residuals should have a straight line relationship with the predicted responses;
- *Homoscedasticity*: the variance of the residuals about predicted responses should be the same for all predicted responses.

Residuals Statistics[a]

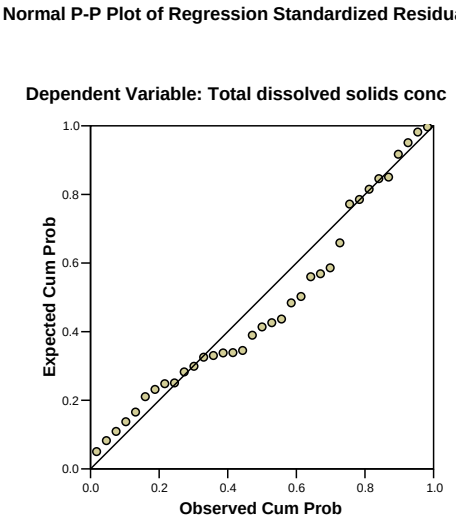
	Minimum	Maximum	Mean	Std. Deviation	N
Predicted Value	198.53	558.19	454.00	83.491	35
Residual	-128.404	214.702	.000	77.101	35
Std. Predicted Value	-3.060	1.248	.000	1.000	35
Std. Residual	-1.641	2.743	.000	.985	35

a. Dependent Variable: Total dissolved solids conc

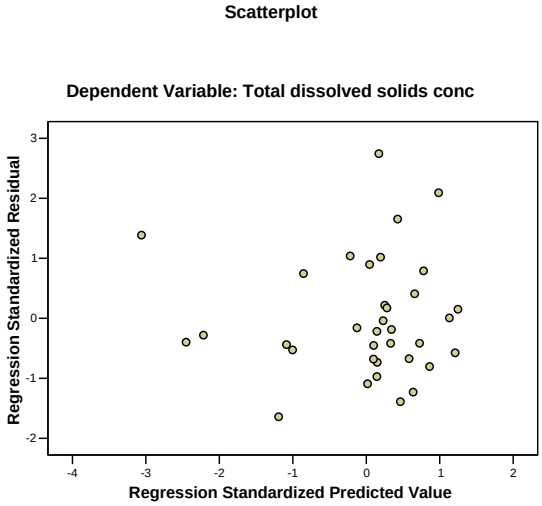
The above table summarises the predicted values and residuals in unstandarised and standardised forms. It is usual practice to consider standardised residuals due to their ease of interpretation. For instance outliers (observations that do not appear to fit the model that well) can be identified as those observations with standardised residual values above 3.3 (or less than -3.3). From the above we can see that we do not appear to have any outliers.



The above plot is a check on normality; the histogram should appear normal; a fitted normal distribution aids us in our consideration. Serious departures would suggest that normality assumption is not met. Here we have a slight suggestion of positive skewness but considering we have only 35 data points we have no real cause for concern.



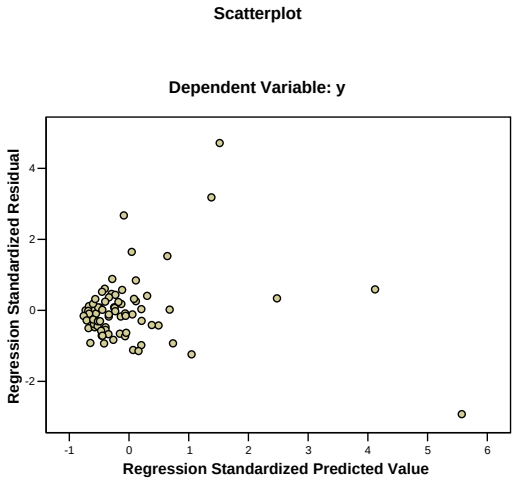
The above plot is a check on normality; the plotted points should follow the straight line. Serious departures would suggest that normality assumption is not met. Here we have no major cause for concern.



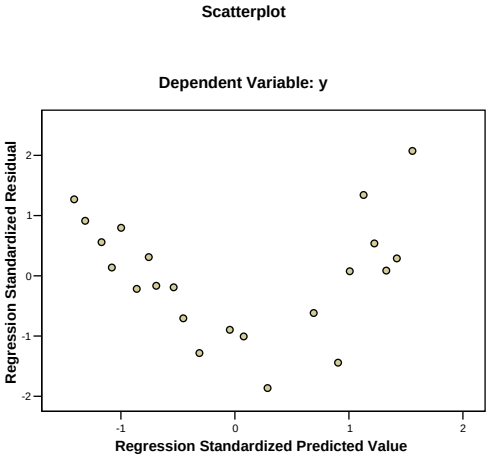
The above scatterplot of standardised residuals against predicted values should be a random pattern centred around the line of zero standard residual value. The points should have the same dispersion about this line over the predicted value range. From the above we can see no clear relationship between the residuals and the predicted values which is consistent with the assumption of linearity. The dispersion of residuals over the predicted value range between -1 and 1 looks constant, for predicted values below -1 there is too few points to provide evidence against a change in variability.

Model violations

So what do residual scatterplots of models that violate the model look like? Here are two common examples together with suggested remedies for the next regression to try.



In the plot above there is clear evidence of heteroscedasticty; change of variance with predicted value. Try log natural or square root transformation of *y* to stabilise variance.



In the plot above there is a clear curved pattern in the residuals. Try transforming *x* to obtain a linear relationship between it and the response variable.

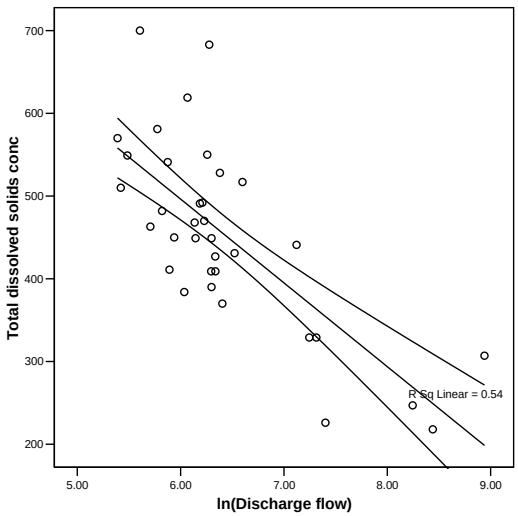
Example (revisited)

In order to get *TDS* predictions for particular *Discharge* values we can use the fitted line, say for a Discharge of 2000 m^3/s:

$$\begin{aligned} TDS &= 1103.967 - 101.275\ln(2000) \\ &= 334.186 \end{aligned}$$

Alternatively, we could let a statistics like SPSS to do the work and calculate confidence or prediction intervals at the same time. We shall now consider some of the other output that SPSS gives us.

The following gives the fitted line together with 95% confidence interval for the expected *TDS* response.



When requesting a predicted value we can also obtain the following:

- the predicted values for the various Discharges together with the associated standard errors of the predictions;
- 95% CI for the expected response;
- 95% CI for individual predicted responses;

For example for a *Discharge* of 2000 m^3/s:

- the expected TDS is 334.18 mg/L (s.e. = 23.366);
- we are 95% certain that interval from 286.64 to 381.72 mg/L covers the unknown expected TDS value;
- we are 95% certain that interval from 168.01 to 500.35 mg/L covers the range of predicted individual TDS observations.

Caution: beware of extrapolation! It would be unwise to predict the TDS for a Discharge value of 12,000 m^3/s as this is far beyond the observed data range.