Simple Linear Regression

Sometimes an experiment is set up where the experimenter has control over the values of one or more variables X and measures the resulting values of another variable Y, producing a field of observations.



The question then arises: What is the best line (or curve) to draw through this field of points?

Values of X are controlled by the experimenter, so the non-random variable x is called the **controlled** variable or the **independent** variable or the **regressor**.

Values of Y are random, but are influenced by the value of x. Thus Y is called the **dependent** variable or the **response** variable.

We want a "line of best fit" so that, given a value of x, we can predict the value of Y for that value of x.



The simple linear regression model is that the predicted value of y is

$$\hat{y} = \beta_0 + \beta_1 x$$

and that the **observed value** of Y is

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

where ε_i is the **error**.

It is assumed that the errors are normally distributed as $\varepsilon_i \sim N(0, \sigma^2)$, with a constant variance σ^2 . The point estimates of the errors ε_i are the **residuals** $e_i = y_i - \hat{y}_i$.

With the assumptions

1) $Y_i = \beta_0 + \beta_1 x_i + \varepsilon_i$ 2) $x = x_0 \implies Y \sim N(\beta_0 + \beta_1 x_0, \sigma^2) \implies (3) V[Y] \text{ is ind't of } x]$ in place, it then follows that $\hat{\beta}_0$ and $\hat{\beta}_1$ are unbiased estimators of the coefficients β_0 and β_1 .

$$\mathbf{E}\left[\hat{\beta}_{0} + \hat{\beta}_{1}x\right] = \beta_{0} + \beta_{1}x \qquad (\text{note lower case } x)$$

Methods for dealing with non-linear regression are available in the course text, but are beyond the scope of this course.

Examples illustrating violations of the assumptions in the simple linear regression model:



If the assumptions are true, then the probability distribution of Y | x is N($\beta_0 + \beta_1 x, \sigma^2$).



Example 12.01

Given that $Y_i = 10 - 0.5 x_i + \varepsilon_i$, where $\varepsilon_i \sim N(0, 2)$, find the probability that the observed value of y at x = 8 will exceed the observed value of y at x = 7.

$$Y_i \sim N(10 - 0.5 x_i, 2)$$

Let Y_7 = the observed value of y at x = 7and Y_8 = the observed value of y at x = 8, then $Y_7 \sim N(6.5, 2)$ and $Y_8 \sim N(6, 2)$

$$\Rightarrow \qquad Y_8 - Y_7 \sim N(6 - 6.5, 2 + 2)$$

$$\mu = -0.5 \qquad \sigma = \sqrt{4} = 2$$

$$P[Y_8 - Y_7 > 0] = P\left[Z > \frac{0 - (-0.5)}{2}\right] = 1 - \Phi(0.25) \approx .4013$$

Despite $\beta_1 < 0$, $P[Y_8 > Y_7] > 40\%$!

For any x_i in the range of the regression model, more than 95% of all Y_i will lie within 2σ (= 2 $\sqrt{2}$) either side of the regression line.



Derivation of the coefficients $\hat{\beta}_0$ and $\hat{\beta}_1$ of the regression line $y = \hat{\beta}_0 + \hat{\beta}_1 x$:

We need to minimize the errors.

Each error is estimated by the observed residual $e_i = y_i - \hat{y}_i$.

Minimize errors.

$$\sum |e_i|$$
 ? NO

Use the *SSE* (sum of squares due to errors)

$$S = \sum_{i=1}^{n} e_{i}^{2} = \sum_{i=1}^{n} (y_{i} - \hat{\beta}_{0} - \hat{\beta}_{1} x_{i})^{2} = f(\hat{\beta}_{o}, \hat{\beta}_{1})$$

Find $\hat{\beta}_0$ and $\hat{\beta}_1$ such that $\frac{\partial S}{\partial \hat{\beta}_0} = \frac{\partial S}{\partial \hat{\beta}_1} = 0$.

[Note:
$$\hat{\beta}_0, \hat{\beta}_1$$
 are variables, while x, y are constants.]

$$\frac{\partial S}{\partial \hat{\beta}_0} = 2 \sum_{i=1}^n \left(y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i \right) (0 - 1 - 0) = 0 \implies \hat{\beta}_0 \sum 1 + \hat{\beta}_1 \sum x = \sum y \qquad (1)$$

and

$$\frac{\partial S}{\partial \hat{\beta}_1} = 2\sum_{i=1}^n \left(y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i \right) \left(0 - 0 - x_i \right) = 0 \quad \Rightarrow \quad \hat{\beta}_0 \sum x + \hat{\beta}_1 \sum x^2 = \sum xy \quad (2)$$

or, equivalently,
$$\begin{bmatrix} n & \sum x \\ \sum x & \sum x^2 \end{bmatrix} \begin{bmatrix} \hat{\beta}_0 \\ \hat{\beta}_1 \end{bmatrix} = \begin{bmatrix} \sum y \\ \sum x y \end{bmatrix}$$
(3)

$$\Rightarrow \begin{bmatrix} \hat{\beta}_0 \\ \hat{\beta}_1 \end{bmatrix} = \begin{bmatrix} n & \sum x \\ \sum x & \sum x^2 \end{bmatrix}^{-1} \begin{bmatrix} \sum y \\ \sum xy \end{bmatrix} = \frac{1}{n S_{xx}} \begin{bmatrix} \sum x^2 & -\sum x \\ -\sum x & n \end{bmatrix} \begin{bmatrix} \sum y \\ \sum xy \end{bmatrix}$$
(4)



.

The solution to the linear system of two **normal equations** (1) and (2) is: from the lower row of matrix equation (4):

$$\hat{\beta}_{1} = \frac{S_{xy}}{S_{xx}}, \text{ (where } nS_{xy} = n\sum xy - \sum x\sum y$$
and
$$nS_{xx} = n\sum x^{2} - (\sum x)^{2} \text{)}$$
or, equivalently,
$$\hat{\beta}_{1} = \frac{\text{sample covariance of } (x, y)}{\text{sample variance of } x};$$
and, from equation (1):
$$\hat{\beta}_{0} = \frac{1}{n} \left(\sum y - \hat{\beta}_{1}\sum x\right).$$

A form that is less susceptible to round-off errors (but less convenient for manual computations) is

$$\hat{\beta}_1 = \frac{\sum_{i=1}^n (x_i - \overline{x})(y_i - \overline{y})}{\sum_{i=1}^n (x_i - \overline{x})^2} \text{ and } \hat{\beta}_0 = \overline{y} - \hat{\beta}_1 \overline{x}.$$

The regression line of Y on x is $y - \overline{y} = \hat{\beta}_1 (x - \overline{x})$.

Equation (1) guarantees that all simple linear regression lines pass through the centroid (\bar{x}, \bar{y}) of the data.

It turns out that the simple linear regression method remains valid even if the values of the regressor x are also random.

However, note that interchanging x with y, (so that Y is the regressor and X is the response), results in a *different* regression line (unless X and Y are perfectly correlated).

Example 12.02

(the same data set as Example 11.06: paired two sample t test)

Nine volunteers are tested before and after a training programme. Find the line of best fit for the posterior (after training) scores as a function of the prior (before training) scores.

Volunteer:	1	2	3	4	5	6	7	8	9
After training:	75	66	69	45	54	85	58	91	62
Before training:	72	65	64	39	51	85	52	92	58

Let Y = score after training and X = score before training.

In order to use the simple linear regression model, the assumptions

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

$$x = x_0 \implies Y \sim N(\beta_0 + \beta_1 x_0, \sigma^2)$$

must hold.

From a plot of the data

(in http://www.engr.mun.ca/~ggeorge/3423/demos/regress2.xls), and http://www.engr.mun.ca/~ggeorge/3423/demos/ex1202.mpj), one can see that the assumptions are reasonable.



i	\boldsymbol{x}_i	\boldsymbol{y}_i	x_i^2	$\boldsymbol{x}_i \boldsymbol{.} \boldsymbol{y}_i$	y_i^2
1	72	75	5184	5400	5625
2	65	66	4225	4290	4356
3	64	69	4096	4416	4761
4	39	45	1521	1755	2025
5	51	54	2601	2754	2916
6	85	85	7225	7225	7225
7	52	58	2704	3016	3364
8	92	91	8464	8372	8281
9	58	62	3364	3596	3844
Sum:	578	605	39384	40824	42397

 $nS_{xy} = n\sum xy - \sum x\sum y = 9 \times 40824 - 578 \times 605 = 17726$ [Note: $nS_{xy} = n(n-1) *$ sample covariance of (X, Y)] $nS_{xx} = n\sum x^2 - (\sum x)^2 = 9 \times 39384 - 578^2 = 20372$ [Note: $nS_{xx} = n(n-1) *$ sample variance of X] $\Rightarrow \hat{\beta}_1 = \frac{S_{xy}}{S_{xx}} = \frac{17726}{20372} = 0.870116$

and
$$\hat{\beta}_0 = \frac{1}{n} \left(\sum y - \hat{\beta}_1 \sum x \right) = \frac{1}{9} (605 - 0.807116 \times 578) = 11.34145$$

Each predicted value \hat{y}_i of Y is then estimated using $\hat{y}_i = \hat{\beta}_0 + \hat{\beta}_1 x_i \approx 11.34 + 0.87 x$ and the point estimates of the unknown errors ε_i are the observed residuals $e_i = y_i - \hat{y}_i$. [Use **un-rounded** values 11.34... and 0.87... to find residuals.]

A measure of the degree to which the regression line fails to explain the variation in Y is the sum of squares due to error,

SSE =
$$\sum_{i=1}^{n} e_i^2 = \sum_{i=1}^{n} (y_i - \hat{\beta}_0 - \hat{\beta}_1 x_i)^2$$

which is given in the adjoining table.

x_i	<i>Y</i> _i	\hat{y}_i	e_i	e_i^2
72	75	73.98979	1.0102	1.0205
65	66	67.89898	-1.8990	3.6061
64	69	67.02886	1.9711	3.8854
39	45	45.27597	-0.2760	0.0762
51	54	55.71736	-1.7174	2.9493
85	85	85.30130	-0.3013	0.0908
52	58	56.58747	1.4125	1.9952
92	91	91.39211	-0.3921	0.1537
58	62	61.80817	0.1918	0.0368
			SSE =	<u>13.8141</u>

An Alternative Formula for SSE:

$$\hat{\beta}_{0} = \bar{y} - \hat{\beta}_{1} \bar{x} \implies$$

$$SSE = \sum_{i=1}^{n} (y_{i} - (\bar{y} - \hat{\beta}_{1} \bar{x}) - \hat{\beta}_{1} x_{i})^{2} = \sum_{i=1}^{n} ((y_{i} - \bar{y}) - \hat{\beta}_{1} (x_{i} - \bar{x}))^{2}$$

$$= \sum_{i=1}^{n} (y_{i} - \bar{y})^{2} - 2\hat{\beta}_{1} \sum_{i=1}^{n} (x_{i} - \bar{x})(y_{i} - \bar{y}) + \hat{\beta}_{1}^{2} \sum_{i=1}^{n} (x_{i} - \bar{x})^{2}$$

$$= S_{yy} - 2\hat{\beta}_{1} S_{xy} + \hat{\beta}_{1}^{2} S_{xx}$$
But $\hat{\beta}_{1} = \frac{S_{xy}}{S_{xx}}$

$$\Rightarrow SSE = S_{yy} - \hat{\beta}_{1} S_{xy} \text{ or } SSE = \frac{S_{xx}S_{yy} - S_{xy}^{2}}{S_{xx}} \text{ or }$$

$$SSE = \frac{(nS_{xx})(nS_{yy}) - (nS_{xy})^{2}}{n \times (nS_{xx})}$$

In this example,

$$SSE = \frac{20372 \times 15548 - 17726^2}{9 \times 20372} = 13.814...$$

However, this formula is *very* sensitive to round-off errors: If all terms are rounded off prematurely to three significant figures, then

$$SSE = \frac{20400 \times 15500 - 17700^2}{9 \times 20400} = 15.85 \quad (2 \text{ d.p.})$$





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

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

The total variation in *Y* is the *SST* (sum of squares - total):

$$SST = \frac{n S_{yy}}{n} = \sum (y_i - \overline{y})^2 \quad \text{(which is } (n-1) \times \text{the sample variance of } y\text{)}.$$

In this example, SST = 15548 / 9 = 1727.555...

The total variation (*SST*) can be partitioned into the variation that can be explained by the regression line $(SSR = \sum (\hat{y}_i - \overline{y})^2)$ and the variation that remains unexplained by the regression line (*SSE*). SST = SSR + SSE

$$SST = SSR + SSE$$

$$\uparrow \qquad \uparrow$$

$$S_{yy} \qquad \hat{\beta}_{1} S_{xy}$$

The proportion of the variation in Y that is explained by the regression line is known as the **coefficient of determination**

$$r^2 = \frac{SSR}{SST} = 1 - \frac{SSE}{SST}$$

In this example, $r^2 = 1 - (13.81... / 1727.555...) = .992004...$

Therefore the regression model in this example explains 99.2% of the total variation in *y*. Note:

The coefficient of determination is just the square of the sample correlation coefficient r. Thus $r = \sqrt{r^2} \approx .996$. It is no surprise that the two sets of test scores in this example are very strongly correlated. Most of the points on the graph are very close to the regression line y = 0.87 x + 11.34. A point estimate of the unknown population variance σ^2 of the errors ε is the sample variance or **mean square error** $s^2 = MSE = SSE / (number of degrees of freedom).$

But the calculation of s^2 includes two parameters that are estimated from the data: $\hat{\beta}_0$ and $\hat{\beta}_1$. Therefore two degrees of freedom are lost and $MSE = \frac{SSE}{n-2}$. In this example, $MSE \approx 1.973$.

A concise method of displaying some of this information is the **ANOVA table** (used in Chapters 10 and 11 of Devore for analysis of variance). The f value in the top right corner of the table is the square of a t value that can be used in an **hypothesis test** on the value of the slope coefficient β_1 .

Sequence of manual calculations:

 $\{ n, \sum x, \sum y, \sum x^{2}, \sum xy, \sum y^{2} \} \rightarrow \{ n S_{xx}, n S_{xy}, n S_{yy} \} \rightarrow \{ \hat{\beta}_{1}, \hat{\beta}_{0}, SSR, SST \} \rightarrow \{ R^{2}, SSE \} \rightarrow \{ MSR, MSE \} \rightarrow f \rightarrow t$

Source	Degrees of Freedom	Sums of Squares	Mean Squares	f
Regression	1	<i>SSR</i> = 1713.741	MSR = SSR / 1 = 1713.741	= MSR/MSE = 868.4
Error	n-2 = 7	<i>SSE</i> = 13.81	MSE = SSE / (n-2) = 1.973	
Total	n-1 = 8	<i>SST</i> = 1727.555		

To test \mathcal{H}_{o} : $\beta_{1} = 0$ (no useful linear association) against \mathcal{H}_{a} : $\beta_{1} \neq 0$ (a useful linear association exists), we compare $|t| = \sqrt{f}$ to $t_{\alpha/2, (n-2)}$.

In this example, $|t| = \sqrt{868.4...} = 29.4... >> t_{.0005, 7}$ (the *p*-value is $< 10^{-7}$) so we reject \mathcal{H}_0 in favour of \mathcal{H}_a at any reasonable level of significance α .

The standard error s_b of $\hat{\beta}_1$ is $s / \sqrt{S_{xx}}$ so the *t* value is also equal to $\frac{\hat{\beta}_1 - 0}{\sqrt{\frac{n MSE}{n S_{xx}}}}$

Yet another alternative test of the significance of the linear association is an hypothesis test on the population correlation coefficient ρ , (\mathcal{H}_0 : $\rho = 0$ vs. \mathcal{H}_a : $\rho \neq 0$), using the test statistic $t = \frac{r\sqrt{n-2}}{\sqrt{1-r^2}}$, which is entirely equivalent to the other two *t* statistics above.

Example 12.03

(a) Find the line of best fit to the data

x	0	0	1	1	1	2	2	2	3	4
у	6.1	5.3	4.1	5.1	4.4	3.4	2.6	3.1	1.8	2.1

- (b) Estimate the value of y when x = 2.
- (c) Why can't the regression line be used to estimate y when x = 10?
- (d) Find the sample correlation coefficient.
- (e) Does a useful linear relationship between Y and x exist?
- (a) A plot of these data follows.



The Excel spreadsheet file for these data can be found at

"http://www.engr.mun.ca /~ggeorge/3423/demos /regress3.xls". The summary statistics are

$$\Sigma x = 16$$
 $\Sigma y = 38$ $n = 10$
 $\Sigma x^2 = 40$ $\Sigma xy = 45.6$ $\Sigma y^2 = 163.06$

From which

$$n S_{xy} = n \Sigma xy - \Sigma x \Sigma y = -152$$

 $n S_{xx} = n \Sigma x^{2} - (\Sigma x)^{2} = 144$ m

$$n S_{yy} = n \Sigma y^2 - (\Sigma y)^2 = 186.6$$



(b)
$$x=2 \Rightarrow y = 5.488... - 1.055... \times 2 = 3.38$$
 (2 d.p.)

(c)
$$x = 10 \Rightarrow y = 5.488... - 1.055... \times 10 = -5.07 < 0!$$
 (2 d.p.)

Problem: x = 10 is outside the sample range for x. \Rightarrow SLR model may be invalid. In one word: EXTRAPOLATION.

(d)
$$r = \frac{S_{xy}}{\sqrt{S_{xx}S_{yy}}} = \frac{-152}{\sqrt{144 \times 186.6}} = -.92727... \approx -.93$$

(e)
$$SSR = \frac{(n S_{xy})^2}{n (n S_{xx})} = \frac{(-152)^2}{10 \times 144} = 16.0\dot{4}$$

 $SST = S_{yy} = (186.6 / 10) = 18.66$

and SSE = SST - SSR = 18.66 - 16.04... = 2.615...

Source	d.f.	SS	MS	f
R	1	16.04444	16.04444	49.07
E	8	2.61555	0.3269	
Т	9	18.66000		

The ANOVA table is then:

from which $t = -\sqrt{f} \approx -7.005$ (3 d.p.) But $t_{.0005,8} = 5.041... |t| > t_{.0005,8}$

Therefore reject \mathcal{H}_{0} : $\beta_{1} = 0$ in favour of \mathcal{H}_{a} : $\beta_{1} \neq 0$ at any reasonable level of significance α . [*p*-value = .00011...]

OR $t = \frac{r\sqrt{n-2}}{\sqrt{1-r^2}} = \frac{-.92727...\times\sqrt{8}}{\sqrt{1-.85983...}} \approx -7.005$

 \Rightarrow reject $\mathcal{H}_{0}: \rho = 0$ in favour of $\mathcal{H}_{a}: \rho \neq 0$ (a significant linear association exists).

[Also, from the ANOVA table, $r^2 = \frac{SSR}{SST} = \frac{16.04...}{18.66} \approx .8598$

Therefore the regression line explains ~86% of the variation in y. $r = -\sqrt{r^2} = -.927$, as before.]

Confidence and Prediction Intervals

The simple linear regression model $Y_i = \beta_0 + \beta_1 x_i + \varepsilon_i$ leads to a line of best fit in the least squares sense, which provides an expected value of Y given a value for x :

$$\hat{y} = \hat{\beta}_0 + \hat{\beta}_1 x = E[Y | x] = \mu_{Y \bullet x}.$$

The uncertainty in this expected value has two components:

- the square of the standard error of the scatter of the observed points about the regression line (= σ^2 / n), and
- the uncertainty in the position of the regression line itself, which increases with the distance of the chosen x from the centroid of the data but decreases with increasing

spread of the full set of x values:
$$\sigma^2 \left(\frac{(x - \overline{x})^2}{S_{xx}} \right)$$

The unknown variance σ^2 of individual points about the true regression line is estimated by the mean square error $s^2 = MSE$. Thus a 100(1– α)% **confidence interval** for the expected value of Y at $x = x_0$ has endpoints at

$$(\hat{\beta}_0 + \hat{\beta}_1 x_o) \pm t_{\alpha/2,(n-2)} s \sqrt{\frac{1}{n} + \frac{(x_o - \overline{x})^2}{S_{xx}}}$$

The **prediction error** for a single point is the residual $E = Y - \hat{y}$, which can be treated as the difference of two independent random variables. The variance of the prediction error is then

$$\mathbf{V}[E] = \mathbf{V}[Y] + \mathbf{V}[\hat{y}] = \sigma^2 + \sigma^2 \left(\frac{1}{n} + \frac{n(x_\circ - \overline{x})^2}{n S_{xx}}\right)$$

Thus a $100(1-\alpha)$ % prediction interval for a single future observation of Y at $x = x_0$ has endpoints at

$$\left(\hat{\beta}_{0} + \hat{\beta}_{1} x_{o}\right) \pm t_{\alpha/2,(n-2)} s \sqrt{1 + \frac{1}{n} + \frac{(x_{o} - \overline{x})^{2}}{S_{xx}}}$$

The prediction interval is always wider than the confidence interval.

Example 12.03 (continued)

- (f) Find the 95% confidence interval for the expected value of Y at x = 2 and x = 5.
- (g) Find the 95% prediction interval for a future value of Y at x = 2 and at x = 5.
- (f) $\alpha = 5\% \implies \alpha/2 = .025$

Using the various values from parts (a) and (e):

n = 10 $t_{.025, 8} = 2.306...$ s = 0.57179... $\bar{x} = 1.6$

$$S_{xx} = 14.4$$
 $\hat{\beta}_0 = 5.4888...$ $\hat{\beta}_1 = -1.0555...$

$$\begin{aligned} x_{o} &= 2 \implies \text{the 95\% CI for } \mu_{Y|2} \text{ is} \\ \left(\hat{\beta}_{0} + \hat{\beta}_{1} x_{o}\right) &\pm t_{\alpha/2,(n-2)} s \sqrt{\frac{1}{n} + \frac{(x_{o} - \bar{x})^{2}}{S_{xx}}} = 3.3777... \pm 1.3185... \times \sqrt{0.1111...} \\ &= 3.3777... \pm 0.4395... \implies \underline{2.94} \le \mathrm{E}[Y|2] < 3.82 \text{ (to 3 s.f.)} \end{aligned}$$

$$\begin{aligned} x_o &= 5 \implies \text{the 95\% CI for } \mu_{Y|5} \text{ is} \\ \left(\hat{\beta}_0 + \hat{\beta}_1 x_o\right) &\pm t_{\alpha/2,(n-2)} s \sqrt{\frac{1}{n} + \frac{(x_o - \bar{x})^2}{S_{xx}}} = 0.2111... \pm 1.3185... \times \sqrt{0.902777...} \\ &= 0.2111... \pm 1.2528... \implies -1.04 \le \mathrm{E}[Y|5] \le 1.46 \text{ (to 3 s.f.)} \end{aligned}$$

(g) $x_0 = 2 \implies$ the 95% PI for Y is

$$\begin{pmatrix} \hat{\beta}_0 + \hat{\beta}_1 x_o \end{pmatrix} \pm t_{\alpha/2,(n-2)} s \sqrt{1 + \frac{1}{n} + \frac{(x_o - \overline{x})^2}{S_{xx}}} = 3.3777... \pm 1.3185... \times \sqrt{1.1111...} \\ = 3.3777... \pm 1.3898... \Rightarrow \underline{1.99 \le Y \le 4.77} \text{ (to 3 s.f.) at } x = 2 \\ x_o = 5 \Rightarrow \text{the 95\% PI for } Y \text{ is} \\ \begin{pmatrix} \hat{\beta}_0 + \hat{\beta}_1 x_o \end{pmatrix} \pm t_{\alpha/2,(n-2)} s \sqrt{1 + \frac{1}{n} + \frac{(x_o - \overline{x})^2}{S_{xx}}} = 0.2111... \pm 1.3185... \times \sqrt{1.902777...} \\ = 0.2111... \pm 1.8188... \Rightarrow \underline{-1.61 \le Y \le 2.03} \text{ (to 3 s.f.) at } x = 5$$

Note how the confidence and prediction intervals both become wider the further away from the centroid the value of x_0 is. The two intervals at x = 5 are wide enough to cross the *x*-axis, which is an illustration of the dangers of **extrapolation** beyond the range of *x* for which data exist.

Sketch of confidence and prediction intervals for Example 3 (f) and (g):

