

Linear Regression

Chemical Engineering Majors

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Transforming Numerical Methods Education for STEM
Undergraduates

Linear Regression

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What is Regression?

What is regression? Given n data points $(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)$ best fit $y = f(x)$ to the data. The best fit is generally based on minimizing the sum of the square of the residuals, S_r .

Residual at a point is

$$\varepsilon_i = y_i - f(x_i)$$

Sum of the square of the residuals

$$S_r = \sum_{i=1}^n (y_i - f(x_i))^2$$

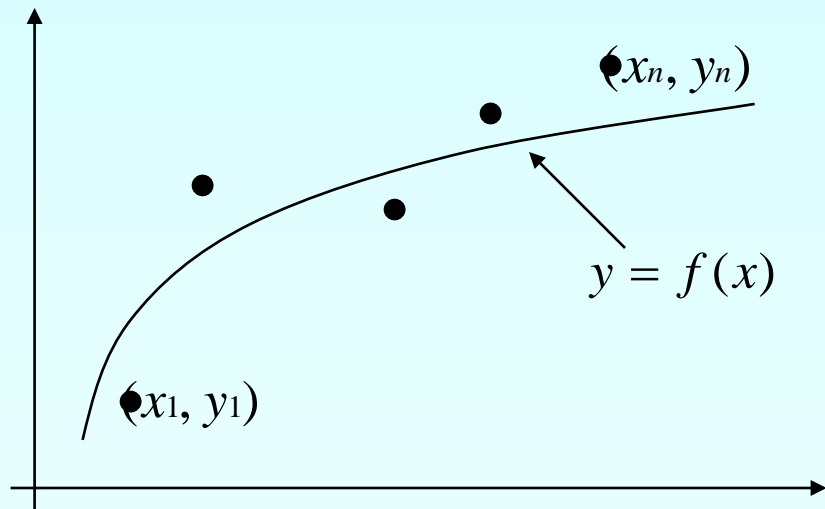


Figure. Basic model for regression

Linear Regression-Criterion#1

Given n data points $(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)$ best fit $y = a_0 + a_1x$ to the data.

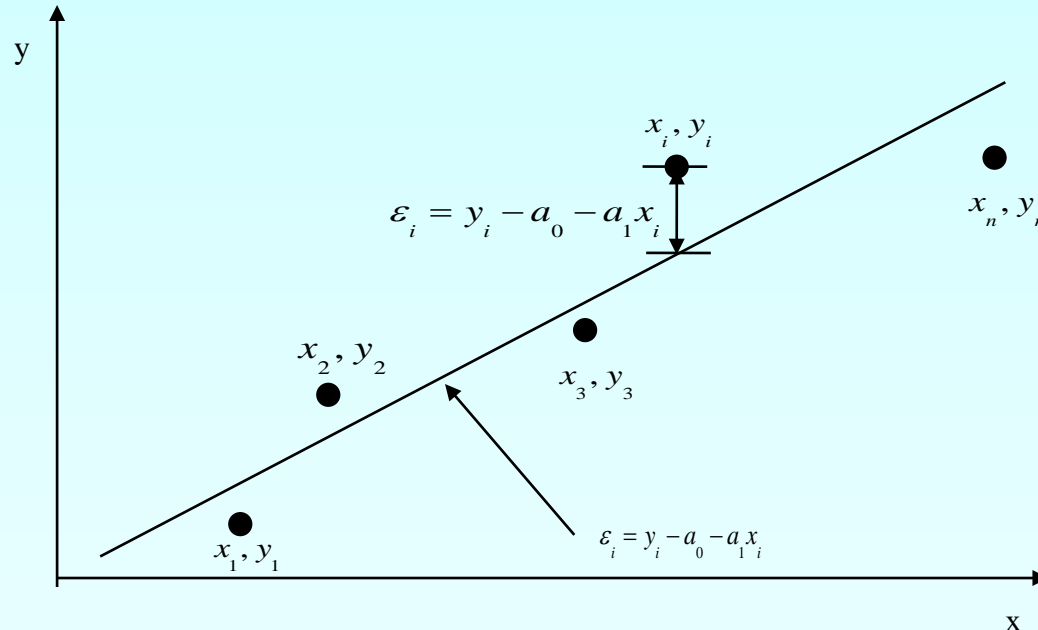


Figure. Linear regression of y vs. x data showing residuals at a typical point, x_i .

Does minimizing $\sum_{i=1}^n \varepsilon_i$ work as a criterion, where $\varepsilon_i = y_i - (a_0 + a_1x_i)$

Example for Criterion#1

Example: Given the data points $(2,4)$, $(3,6)$, $(2,6)$ and $(3,8)$, best fit the data to a straight line using Criterion#1

Table. Data Points

x	y
2.0	4.0
3.0	6.0
2.0	6.0
3.0	8.0

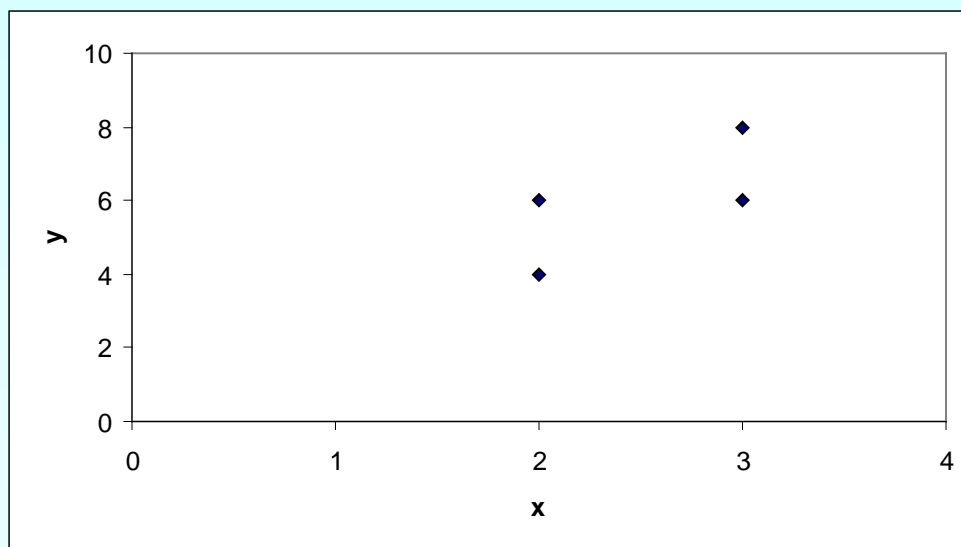


Figure. Data points for y vs. x data.

Linear Regression-Criteria#1

Using $y=4x-4$ as the regression curve

Table. Residuals at each point for regression model $y = 4x - 4$.

x	y	$y_{\text{predicted}}$	$\varepsilon = y - y_{\text{predicted}}$
2.0	4.0	4.0	0.0
3.0	6.0	8.0	-2.0
2.0	6.0	4.0	2.0
3.0	8.0	8.0	0.0
			$\sum_{i=1}^4 \varepsilon_i = 0$

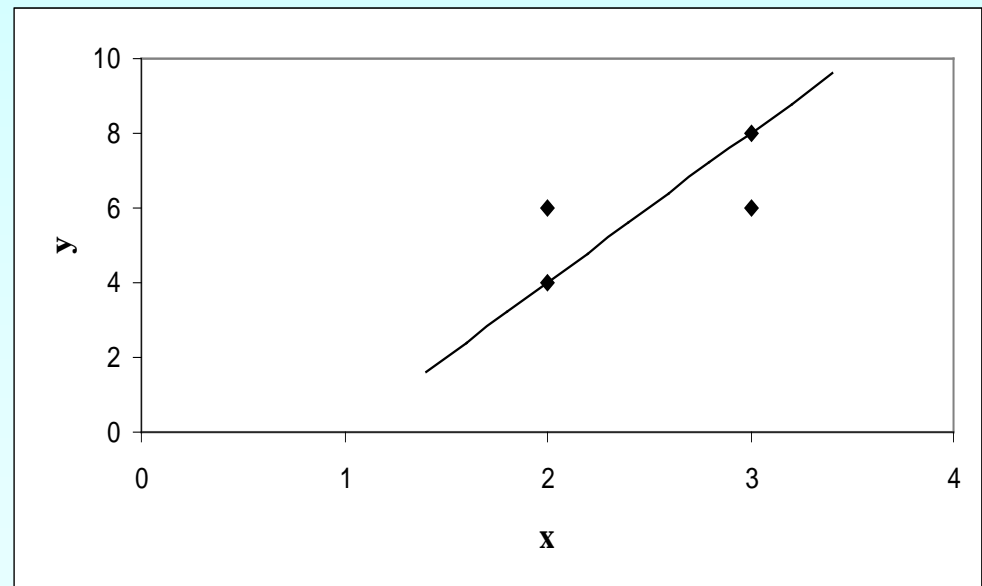


Figure. Regression curve for $y=4x-4$, y vs. x data

Linear Regression-Criteria#1

Using $y=6$ as a regression curve

Table. Residuals at each point for $y=6$

x	y	$y_{\text{predicted}}$	$\varepsilon = y - y_{\text{predicted}}$
2.0	4.0	6.0	-2.0
3.0	6.0	6.0	0.0
2.0	6.0	6.0	0.0
3.0	8.0	6.0	2.0
			$\sum_{i=1}^4 \varepsilon_i = 0$

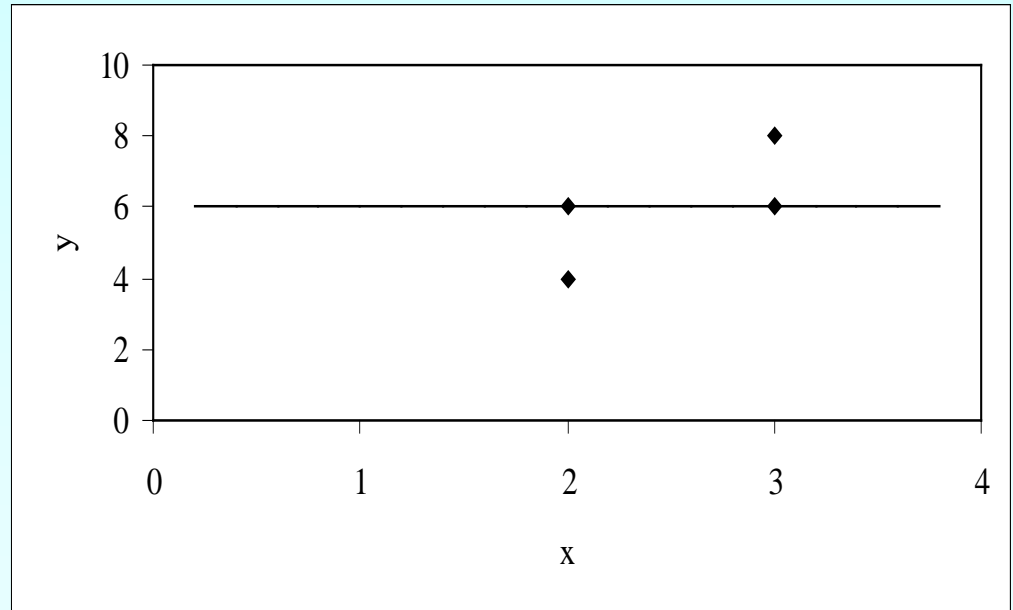


Figure. Regression curve for $y=6$, y vs. x data

Linear Regression – Criterion #1

$$\sum_{i=1}^4 \varepsilon_i = 0 \quad \text{for both regression models of } y=4x-4 \text{ and } y=6.$$

The sum of the residuals is as small as possible, that is zero, but the regression model is not unique.

Hence the above criterion of minimizing the sum of the residuals is a bad criterion.

Linear Regression-Criterion#2

Will minimizing $\sum_{i=1}^n |\epsilon_i|$ work any better?

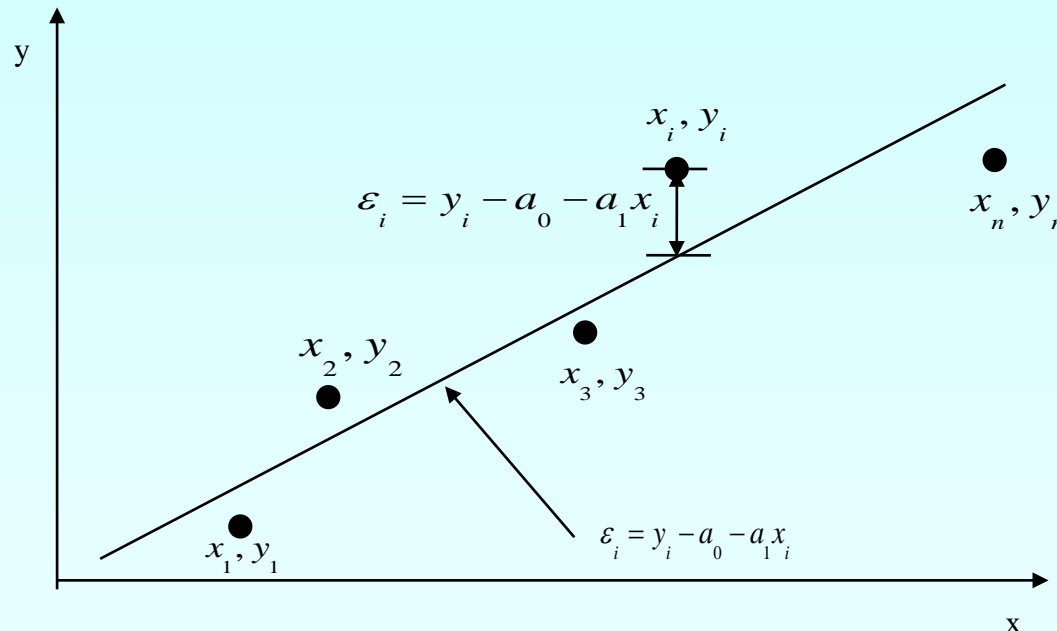


Figure. Linear regression of y vs. x data showing residuals at a typical point, x_i .

Linear Regression-Criteria 2

Using $y=4x-4$ as the regression curve

Table. The absolute residuals employing the $y=4x-4$ regression model

x	y	$y_{\text{predicted}}$	$ \epsilon = y - y_{\text{predicted}} $
2.0	4.0	4.0	0.0
3.0	6.0	8.0	2.0
2.0	6.0	4.0	2.0
3.0	8.0	8.0	0.0
			$\sum_{i=1}^4 \epsilon_i = 4$

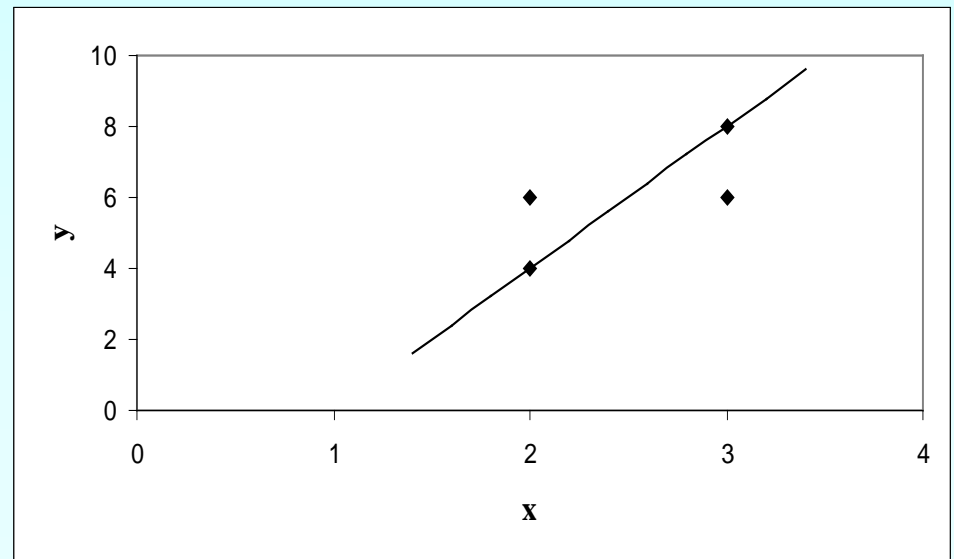


Figure. Regression curve for $y=4x-4$, y vs. x data

Linear Regression-Criteria#2

Using $y=6$ as a regression curve

Table. Absolute residuals employing the $y=6$ model

x	y	$y_{\text{predicted}}$	$ \varepsilon = y - y_{\text{predicted}} $
2.0	4.0	6.0	2.0
3.0	6.0	6.0	0.0
2.0	6.0	6.0	0.0
3.0	8.0	6.0	2.0
			$\sum_{i=1}^4 \varepsilon_i = 4$

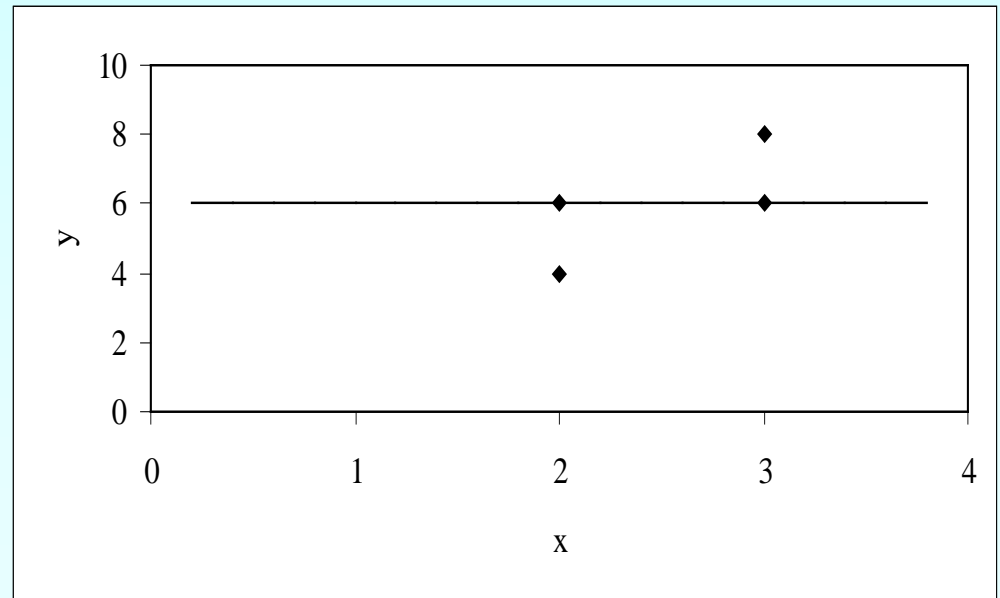


Figure. Regression curve for $y=6$, y vs. x data

Linear Regression-Criterion#2

$$\sum_{i=1}^4 |\varepsilon_i| = 4 \text{ for both regression models of } y=4x-4 \text{ and } y=6.$$

The sum of the errors has been made as small as possible, that is 4, but the regression model is not unique.

Hence the above criterion of minimizing the sum of the absolute value of the residuals is also a bad criterion.

Can you find a regression line for which $\sum_{i=1}^4 |\varepsilon_i| < 4$ and has unique regression coefficients?

Least Squares Criterion

The least squares criterion minimizes the sum of the square of the residuals in the model, and also produces a unique line.

$$S_r = \sum_{i=1}^n \varepsilon_i^2 = \sum_{i=1}^n (y_i - a_0 - a_1 x_i)^2$$

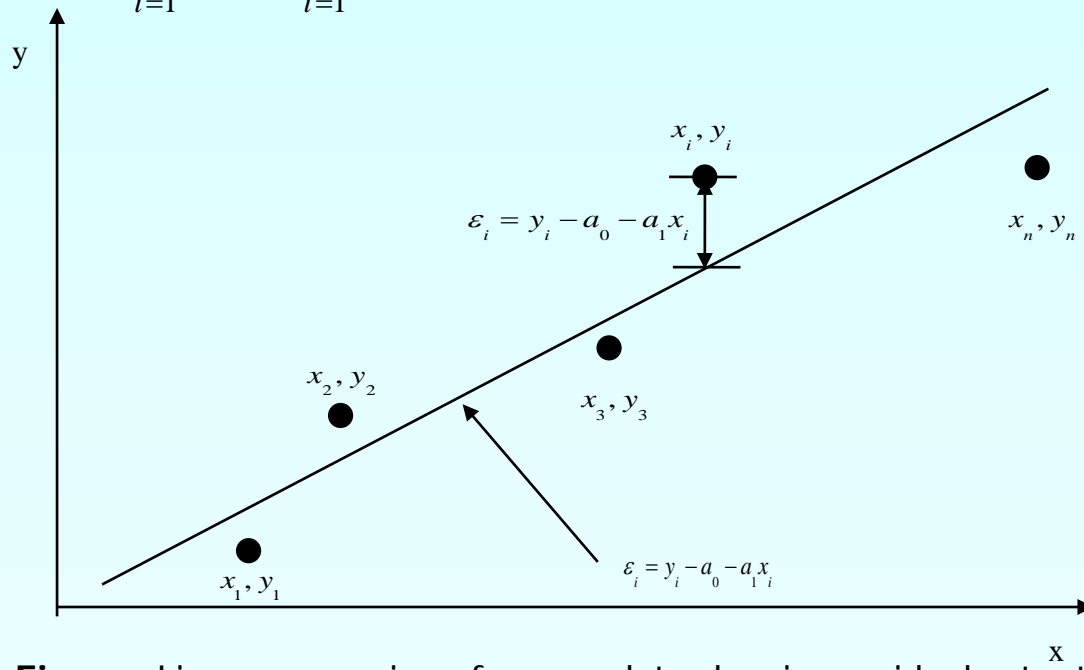


Figure. Linear regression of y vs. x data showing residuals at a typical point, x_i .

Finding Constants of Linear Model

Minimize the sum of the square of the residuals: $S_r = \sum_{i=1}^n \varepsilon_i^2 = \sum_{i=1}^n (y_i - a_0 - a_1 x_i)^2$

To find a_0 and a_1 we minimize S_r with respect to a_1 and a_0 .

$$\frac{\partial S_r}{\partial a_0} = -2 \sum_{i=1}^n (y_i - a_0 - a_1 x_i)(-1) = 0$$

$$\frac{\partial S_r}{\partial a_1} = -2 \sum_{i=1}^n (y_i - a_0 - a_1 x_i)(-x_i) = 0$$

giving

$$\sum_{i=1}^n a_0 + \sum_{i=1}^n a_1 x_i = \sum_{i=1}^n y_i$$

$$(a_0 = \bar{y} - a_1 \bar{x})$$

$$\sum_{i=1}^n a_0 x_i + \sum_{i=1}^n a_1 x_i^2 = \sum_{i=1}^n y_i x_i$$

Finding Constants of Linear Model

Solving for a_0 and a_1 directly yields,

$$a_1 = \frac{n \sum_{i=1}^n x_i y_i - \sum_{i=1}^n x_i \sum_{i=1}^n y_i}{n \sum_{i=1}^n x_i^2 - \left(\sum_{i=1}^n x_i \right)^2}$$

and

$$a_0 = \frac{\sum_{i=1}^n x_i^2 \sum_{i=1}^n y_i - \sum_{i=1}^n x_i \sum_{i=1}^n x_i y_i}{n \sum_{i=1}^n x_i^2 - \left(\sum_{i=1}^n x_i \right)^2} \quad (a_0 = \bar{y} - a_1 \bar{x})$$

Example 1

The torque, T needed to turn the torsion spring of a mousetrap through an angle, is given below. Find the constants for the model given by

$$T = k_1 + k_2\theta$$

Table: Torque vs Angle for a torsional spring

Angle, θ	Torque, T
<i>Radians</i>	<i>N-m</i>
0.698132	0.188224
0.959931	0.209138
1.134464	0.230052
1.570796	0.250965
1.919862	0.313707

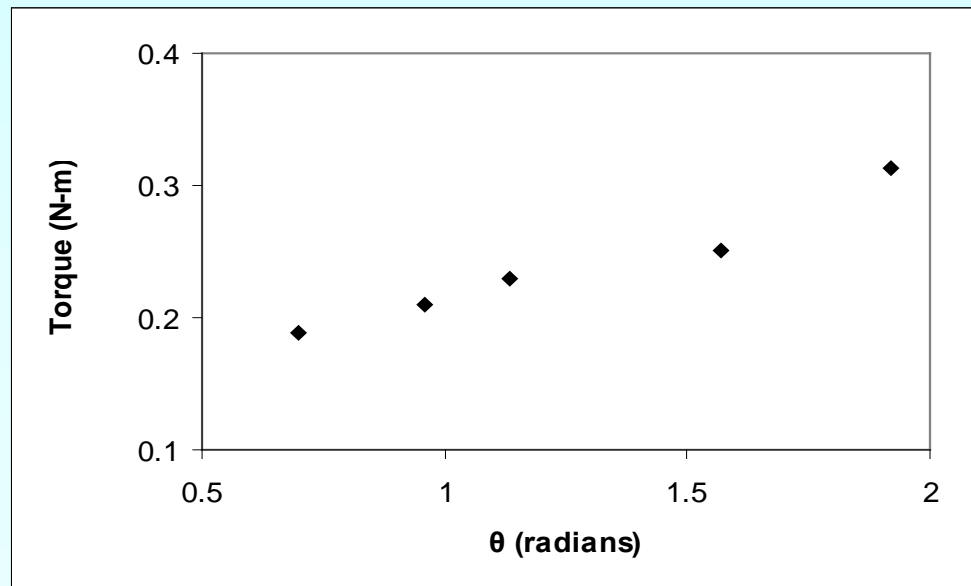


Figure. Data points for Angle vs. Torque data

Example 1 cont.

The following table shows the summations needed for the calculations of the constants in the regression model.

Table. Tabulation of data for calculation of important summations

θ	T	θ^2	$T\theta$
<i>Radians</i>	<i>N-m</i>	<i>Radians²</i>	<i>N-m-Radians</i>
0.698132	0.188224	0.487388	0.131405
0.959931	0.209138	0.921468	0.200758
1.134464	0.230052	1.2870	0.260986
1.570796	0.250965	2.4674	0.394215
1.919862	0.313707	3.6859	0.602274
$\sum_{i=1}^5 = 6.2831$	1.1921	8.8491	1.5896

Using equations described for a_0 and a_1 with $n = 5$

$$\begin{aligned}
 k_2 &= \frac{n \sum_{i=1}^5 \theta_i T_i - \sum_{i=1}^5 \theta_i \sum_{i=1}^5 T_i}{n \sum_{i=1}^5 \theta_i^2 - \left(\sum_{i=1}^5 \theta_i \right)^2} \\
 &= \frac{5(1.5896) - (6.2831)(1.1921)}{5(8.8491) - (6.2831)^2} \\
 &= 9.6091 \times 10^{-2} \text{ N-m/rad}
 \end{aligned}$$

Example 1 cont.

Use the average torque and average angle to calculate k_1

$$\begin{aligned}\bar{T} &= \frac{\sum_{i=1}^5 T_i}{n} \\ &= \frac{1.1921}{5}\end{aligned}$$

$$= 2.3842 \times 10^{-1}$$

$$\begin{aligned}\bar{\theta} &= \frac{\sum_{i=1}^5 \theta_i}{n} \\ &= \frac{6.2831}{5}\end{aligned}$$

$$= 1.2566$$

Using,

$$\begin{aligned}k_1 &= \bar{T} - k_2 \bar{\theta} \\ &= 2.3842 \times 10^{-1} - (9.6091 \times 10^{-2})(1.2566) \\ &= 1.1767 \times 10^{-1} \text{ N-m}\end{aligned}$$

Example 1 Results

Using linear regression, a trend line is found from the data

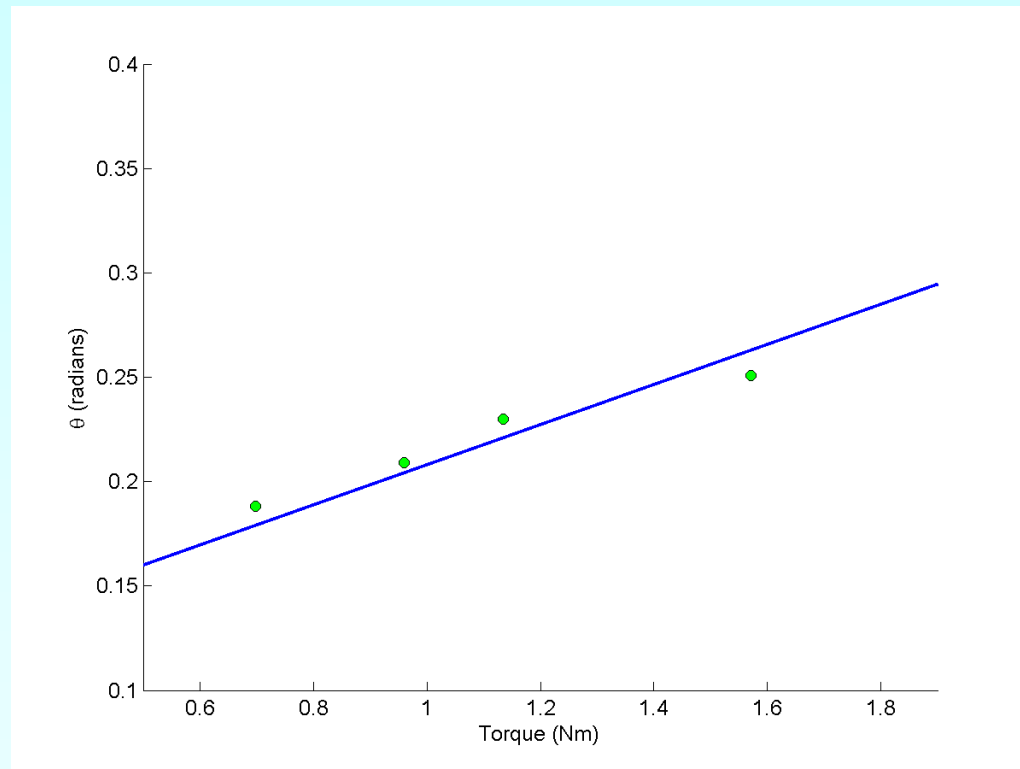


Figure. Linear regression of Torque versus Angle data

Can you find the energy in the spring if it is twisted from 0 to 180 degrees?

Example 2

To find the longitudinal modulus of composite, the following data is collected. Find the longitudinal modulus, E using the regression model

Table. Stress vs. Strain data

Strain (%)	Stress (MPa)
0	0
0.183	306
0.36	612
0.5324	917
0.702	1223
0.867	1529
1.0244	1835
1.1774	2140
1.329	2446
1.479	2752
1.5	2767
1.56	2896

$\sigma = E\varepsilon$ and the sum of the square of the residuals.

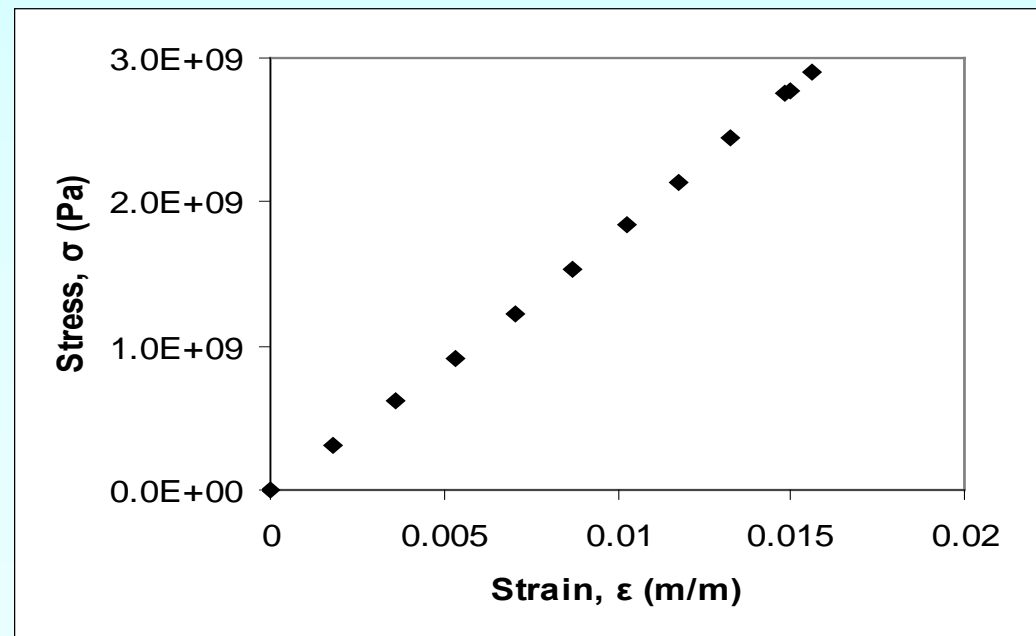


Figure. Data points for Stress vs. Strain data

Example 2 cont.

Residual at each point is given by

$$\gamma_i = \sigma_i - E\varepsilon_i$$

The sum of the square of the residuals then is

$$\begin{aligned} S_r &= \sum_{i=1}^n \gamma_i^2 \\ &= \sum_{i=1}^n (\sigma_i - E\varepsilon_i)^2 \end{aligned}$$

Differentiate with respect to E

$$\frac{\partial S_r}{\partial E} = \sum_{i=1}^n 2(\sigma_i - E\varepsilon_i)(-\varepsilon_i) = 0$$

Therefore

$$E = \frac{\sum_{i=1}^n \sigma_i \varepsilon_i}{\sum_{i=1}^n \varepsilon_i^2}$$

Example 2 cont.

Table. Summation data for regression model

i	ϵ	σ	ϵ^2	$\epsilon\sigma$
1	0.0000	0.0000	0.0000	0.0000
2	1.8300 10^{-3}	3.0600 10^8	3.3489 10^{-6}	5.5998 10^5
3	3.6000 10^{-3}	6.1200 10^8	1.2960 10^{-5}	2.2032 10^6
4	5.3240 10^{-3}	9.1700 10^8	2.8345 10^{-5}	4.8821 10^6
5	7.0200 10^{-3}	1.2230 10^9	4.9280 10^{-5}	8.5855 10^6
6	8.6700 10^{-3}	1.5290 10^9	7.5169 10^{-5}	1.3256 10^7
7	1.0244 10^{-2}	1.8350 10^9	1.0494 10^{-4}	1.8798 10^7
8	1.1774 10^{-2}	2.1400 10^9	1.3863 10^{-4}	2.5196 10^7
9	1.3290 10^{-2}	2.4460 10^9	1.7662 10^{-4}	3.2507 10^7
10	1.4790 10^{-2}	2.7520 10^9	2.1874 10^{-4}	4.0702 10^7
11	1.5000 10^{-2}	2.7670 10^9	2.2500 10^{-4}	4.1505 10^7
12	1.5600 10^{-2}	2.8960 10^9	2.4336 10^{-4}	4.5178 10^7
$\sum_{i=1}^{12}$			1.2764 10^{-3}	2.3337 10^8

With

$$\sum_{i=1}^{12} \epsilon_i^2 = 1.2764 \times 10^{-3}$$

and

$$\sum_{i=1}^{12} \sigma_i \epsilon_i = 2.3337 \times 10^8$$

Using

$$\begin{aligned}
 E &= \frac{\sum_{i=1}^{12} \sigma_i \epsilon_i}{\sum_{i=1}^{12} \epsilon_i^2} \\
 &= \frac{2.3337 \times 10^8}{1.2764 \times 10^{-3}} \\
 &= 182.84 \text{ GPa}
 \end{aligned}$$

Example 2 Results

The equation $\sigma = 182.84\varepsilon$ describes the data.

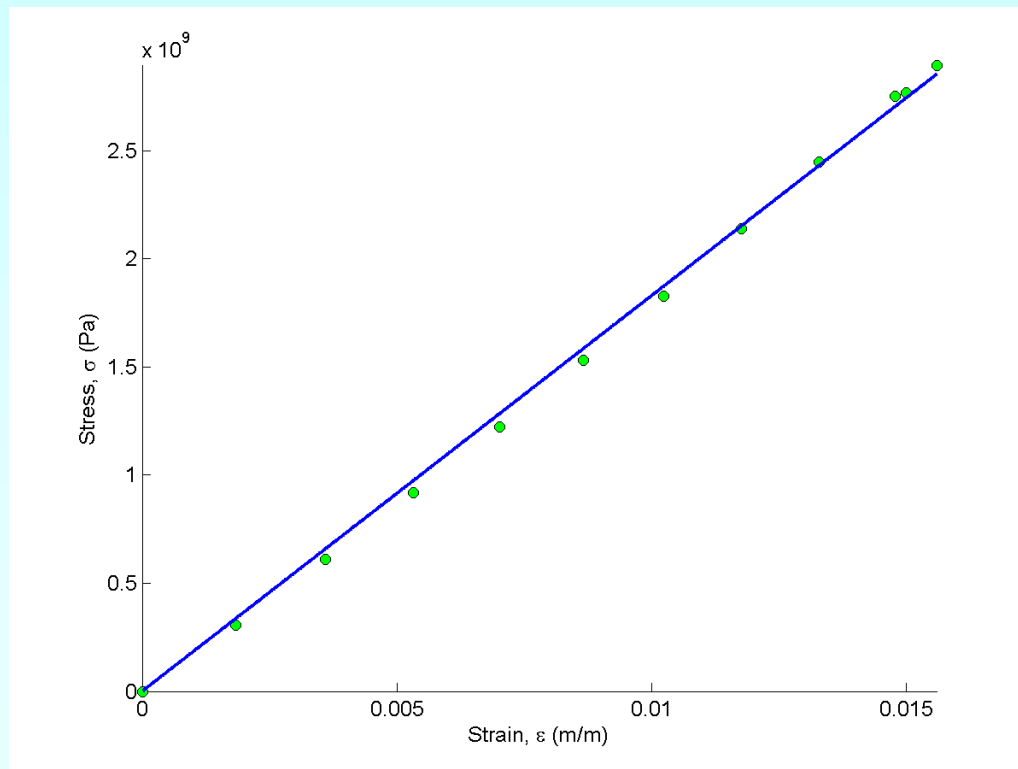


Figure. Linear regression for Stress vs. Strain data

Additional Resources

For all resources on this topic such as digital audiovisual lectures, primers, textbook chapters, multiple-choice tests, worksheets in MATLAB, MATHEMATICA, MathCad and MAPLE, blogs, related physical problems, please visit

http://numericalmethods.eng.usf.edu/topics/linear_regression.html

THE END

<http://numericalmethods.eng.usf.edu>