QUESTION:
Do the values of the constants of the model correspond to a minimum? Is the least squares regression straight line unique?

ANSWER:
Given n data pairs, $(x_1, y_1), \ldots, (x_n, y_n)$, the best fit for the straight line regression model

$$y = a_0 + a_1 x, \qquad (1)$$

is found by method of least squares.
Starting with the sum of the square of the residuals, S_r we get

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

and using

$$\frac{\partial S_r}{\partial a_0} = 0 \qquad (3)$$

$$\frac{\partial S_r}{\partial a_1} = 0 \qquad (4)$$

gives two simultaneous linear equations whose solution is

$$a_1 = \frac{n\sum_{i=1}^{n} x_i y_i - \sum_{i=1}^{n} x_i \sum_{i=1}^{n} y_i}{n\sum_{i=1}^{n} x_i^2 - \left(\sum_{i=1}^{n} x_i\right)^2} \qquad (5a)$$

$$a_0 = \frac{\sum_{i=1}^{n} x_i^2 \sum_{i=1}^{n} y_i - \sum_{i=1}^{n} x_i \sum_{i=1}^{n} x_i y_i}{n\sum_{i=1}^{n} x_i^2 - \left(\sum_{i=1}^{n} x_i\right)^2} \qquad (5b)$$

But does this give the minimum of value of S_r? The first derivative only tells us about a local extreme, not whether it is a minimum or a maximum.

We need to conduct a second derivative test to find out whether the point (a_0, a_1) from Equation (5) gives the minimum or maximum of S_r.

What is the second derivative test for a minimum if we have a function of two variables?

If you have a function $f(x, y)$ and we found a critical point (a, b) from the first derivative test, then (a, b) is a minimum point if

$$\frac{\partial^2 f}{\partial x^2}\frac{\partial^2 f}{\partial y^2} - \left(\frac{\partial^2 f}{\partial x \partial y}\right)^2 > 0\text{, and} \qquad (6)$$

$$\frac{\partial^2 f}{\partial x^2} > 0 \text{ OR } \frac{\partial^2 f}{\partial y^2} > 0 \qquad (7)$$

From Equation (2)

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

$$= -2\sum_{i=1}^{n}(y_i - a_0 - a_1 x_i) \qquad (8)$$

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

$$= -2\sum_{i=1}^{n}(x_i y_i - a_0 x_i - a_1 x_i^2) \qquad (9)$$

then

$$\frac{\partial^2 S_r}{\partial a_0^2} = -2\sum_{i=1}^{n} -1$$

$$= 2n \qquad (10)$$

$$\frac{\partial^2 S_r}{\partial a_1^2} = 2\sum_{i=1}^{n} x_i^2 \qquad (11)$$

$$\frac{\partial^2 S_r}{\partial a_o \partial a_1} = 2\sum_{i=1}^{n} x_i \qquad (12)$$

So we satisfy condition (7) as from Equation (10),

2n is a positive number and

from equation (11)

$2\sum_{i=1}^{n} x_1^2$ is a positive number as assuming that all data points are NOT zero is reasonable.

Is the other condition for being a minimum as given by Equation (6) met? Yes, we can show (*but the proof is not given*)

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

$$= 4\left[n\sum_{i=1}^{n} x_i^2 - \left(\sum_{i=1}^{n} x_i\right)^2\right] > 0$$

(13)

So the values of a_0 and a_1 that we have in Equations (5a) and (5b), are in fact a minimum. Also, this minimum is an absolute minimum because the first derivative is zero for only one point as given by Equations (5a) and (5b). Hence, this also makes the straight-line regression model unique.