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Linear Least Squares

Presented at:

New Orleans Math & Science Conference July 24 & 25 2006

Generalizing the Method of Linear Least Squares

We wish to minimize the quantity,

$\sum_{i=1}^{n} (mx_i + b - y_i)^2 = SS$, where n equals the number of ordered pairs.

Expanding yields,

$$m^2\sum_{i=1}^{n} x^2{}_i + \sum_{i=1}^{n} b^2{}_i + \sum_{i=1}^{n} y_i^2 + 2mb\sum_{i=1}^{n} x_i - 2m\sum_{i=1}^{n} x_i y_i - 2b\sum_{i=1}^{n} y_i = SS$$

The above equation is of the form z = f(m,b). The function z is actually an elliptical paraboloid. Projecting the paraboloid onto the m-z plane for some fixed b value and similarly projecting the paraboloid onto the b-z plane for some fixed m value, yields the two parabolic equations respectively, (equivalently, assuming a plane parallel to the m-z plane through some specific b value interprets to projecting onto the m-z plane, and likewise for the b-z plane for some fixed m value).

1. $m^2\sum_{i=1}^{n} x_i^2 + m(2b\sum_{i=1}^{n} x_i - 2\sum_{i=1}^{n} x_i y_i)$ + other terms not in m = SS
2. $nb^2 + b(2m\sum_{i=1}^{n} x_i - 2\sum_{i=1}^{n} y_i)$ + other terms not in b = SS

The expression for the vertex of each parabola (-b/2a) respectively yields,

$$m_v = -(2b\sum_{i=1}^{n} x_i - 2\sum_{i=1}^{n} x_i y_i) / 2\sum_{i=1}^{n} x^2{}_i$$

$$b_v = -(2m\sum_{i=1}^{n} x_i - 2\sum_{i=1}^{n} y_i) / 2n,$$

The above are a set of linear equations with variables m and b. Eliminating the denominators and the factor of 2 yields,

A. $m_v \sum_{i=1}^{n} x^2{}_i = -b\sum_{i=1}^{n} x_i + \sum_{i=1}^{n} x_i y_i$

B. $b_v n = -m\sum_{i=1}^{n} x_i + \sum_{i=1}^{n} y_i$

Multiplying A by, n, and multiplying B by, - $\sum_{i=1}^{n} x_i$, and then adding the resulting two equations will solve for m. Multiplying A by $\sum_{i=1}^{n} x_i$, and multiplying B by - $\sum_{i=1}^{n} x^2{}_i$ and then adding the resulting equations will solve for b. The results are given below.

$$m = (n\sum_{i=1}^{n} x_i y_i - \sum_{i=1}^{n} x_i \sum_{i=1}^{n} y_i) / (n\sum_{i=1}^{n} x^2{}_i - (\sum_{i=1}^{n} x_i)^2$$

$$b = (\sum_{i=1}^{n} x^2{}_i \sum_{i=1}^{n} y_i - \sum_{i=1}^{n} x_i \sum_{i=1}^{n} x_i y_i) / (n\sum_{i=1}^{n} x^2{}_i - (\sum_{i=1}^{n} x_i)^2$$

Note: Using the partial derivatives, $\frac{\partial z}{\partial m}$ and $\frac{\partial z}{\partial b}$ applied to the previous set of parabolic equations, would immediately yield the set of linear equations A and B found above, which would lead to the solutions for m and b.

Let's check our previous result for the three points (0,1), (1,3), (2,2). Using the general equations for m and b we have,

m = 3

$$\sum_{i=1}^{n} x_i y_i = (0)(1) + (1)(3) + (2)(2) = 7$$

$$\sum_{i=1}^{n} x_i = 0 + 1 + 2 = 3$$

$$\sum_{i=1}^{n} y_i = 1 + 3 + 2 = 6$$

$$\sum_{i=1}^{n} x^2{}_i = 0^2 + 1^2 + 2^2 = 5$$

$$(\sum_{i=1}^{n} x_i)^2 = 3^2 = 9$$

Therefore m = [3(7) – (3)(6)] / [3(5) – 9] =1/2,
b = [(5)(6) –3(7)] / [(3)(5) – 9] = 3/2