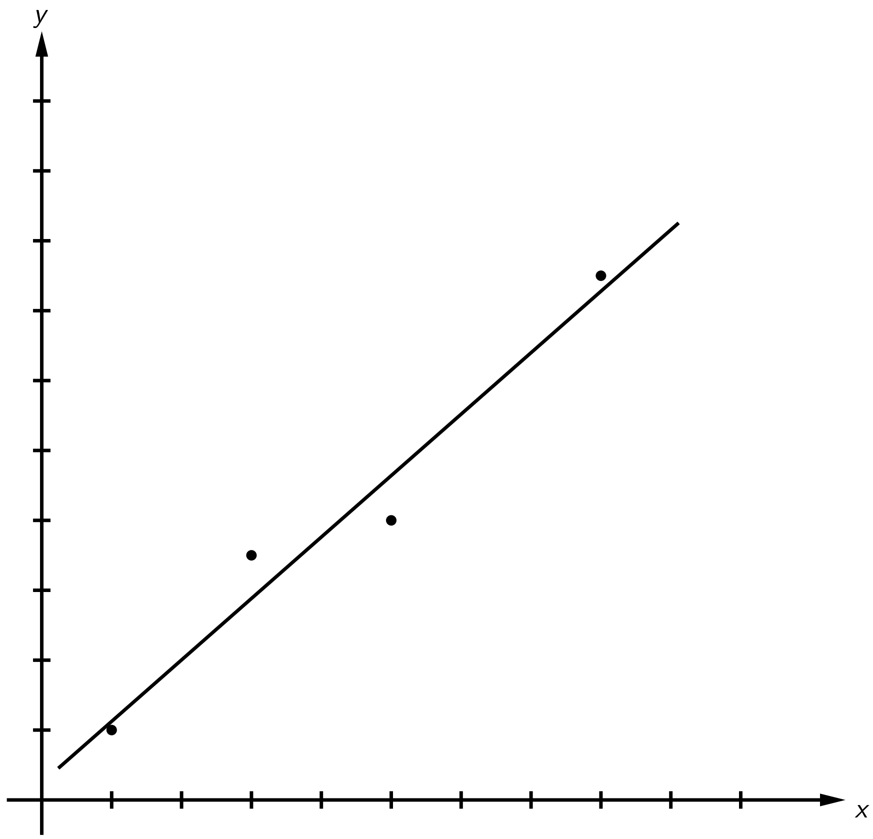
Problem

Experimental data is collected and the data is assumed to satisfy a linear relationship $y = ax + b$. Because of errors inherent in the measurements, the gathered data points do not all lie on a single line. For what values of a and b will the line best fit the data?

For example, here are data points $(1, 1)$, $(3, 3.5)$, $(5, 4)$ and $(8, 7.5)$ and a line that attempts to fit the data:



What is the equation $y = ax + b$ of the line of best fit?

Method of Least Squares

First recall sigma notation for abbreviating sums:

$$\sum_{i=1}^{n} x_i = x_1 + x_2 + \cdots + x_n$$

When the number of terms n is understood the range of the summation index i is often omitted, so we write $\sum x_i$ to mean $\sum_{i=1}^{n} x_i$.

Now suppose we have n data points (x_1, y_1), (x_2, y_2), $\ldots$, (x_n, y_n) through which we wish to fit a line $y = ax + b$. That is, we wish to find, if possible, a and b satisfying

$$\left.\begin{aligned} ax_1 + b &= y_1 \\ ax_2 + b &= y_2 \\ &\vdots \\ ax_n + b &= y_n \end{aligned}\right\} \tag{1}$$

This system is equivalent to

$$\begin{bmatrix} x_1 & 1 \\ x_2 & 1 \\ \vdots & \vdots \\ x_n & 1 \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix},$$

or more concisely $\mathbf{Au} = \mathbf{y}$ where

$$\mathbf{A} = \begin{bmatrix} x_1 & 1 \\ x_2 & 1 \\ \vdots & \vdots \\ x_n & 1 \end{bmatrix}, \quad \mathbf{u} = \begin{bmatrix} a \\ b \end{bmatrix}, \quad \mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}.$$

The system $\mathbf{Au} = \mathbf{y}$ has a solution if and only if $\mathbf{y}$ is in the subspace $\mathrm{col}(\mathbf{A})$, the column space of $\mathbf{A}$. This is the problem: if the data points contain errors, say as the result of taking measurements, it is unlikely that the data points all lie on a single line, and so $\mathbf{y}$ will likely not be in $\mathrm{col}(\mathbf{A})$: the system will be inconsistent. To get around this problem, we will instead solve the system

$$\mathbf{Au} = \mathbf{p}$$

where $\mathbf{p}$ is the vector in $\mathrm{col}(\mathbf{A})$ that is nearest $\mathbf{y}$. That is, $\mathbf{p}$ is the vector projection of $\mathbf{y}$ onto the column space of $\mathbf{A}$:

$$\mathbf{p} = \mathrm{proj}_{\mathrm{col}(\mathbf{A})}\mathbf{y}$$

We don't need to actually find $\mathbf{p}$, but we know it exists, and so $\mathbf{p} = \mathbf{Au}$ for some $\mathbf{u} = \begin{bmatrix} a \\ b \end{bmatrix}$.

Since $\mathbf{p} = \mathrm{proj}_{\mathrm{col}(\mathbf{A})}\mathbf{y}$ if follows that $\mathbf{y} - \mathbf{p}$ is orthogonal to $\mathrm{col}(\mathbf{A})$, and in particular

$$(\mathbf{y} - \mathbf{p}) \bullet \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = 0, \quad (\mathbf{y} - \mathbf{p}) \bullet \begin{bmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{bmatrix} = 0,$$

which is equivalent to

$$\mathbf{A}^T(\mathbf{y} - \mathbf{Au}) = \mathbf{0}\ ,$$

so

$$\mathbf{A}^T\mathbf{A}\mathbf{u} = \mathbf{A}^T\mathbf{y} \tag{2}$$

Equation (2) is called the **normal system** and the solution $\mathbf{u}$ is called the **least squares solution** to the original system (1).

Equation (2) has a unique solution $\mathbf{u}$ since the unique vector $\mathbf{p} = \text{proj}_{\text{col}(\mathbf{A})}\mathbf{y}$ exists, and so the square matrix $\mathbf{A}^T\mathbf{A}$ is invertible. The matrix $\mathbf{A}$ is $n \times 2$, so $\mathbf{A}^T$ is $n \times 2$ and $\mathbf{A}^T\mathbf{A}$ is 2×2, which has an easily computable inverse. Here are the details:

$$\mathbf{A}^T\mathbf{A}\mathbf{u} = \mathbf{A}^T\mathbf{y}$$

$$\begin{bmatrix} x_1 & x_2 & \cdots & x_n \\ 1 & 1 & \cdots & 1 \end{bmatrix} \begin{bmatrix} x_1 & 1 \\ x_2 & 1 \\ \vdots & \vdots \\ x_n & 1 \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} x_1 & x_2 & \cdots & x_n \\ 1 & 1 & \cdots & 1 \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$

$$\begin{bmatrix} \sum x_i^2 & \sum x_i \\ \sum x_i & n \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} \sum x_i y_i \\ \sum y_i \end{bmatrix}$$

$$\begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} \sum x_i^2 & \sum x_i \\ \sum x_i & n \end{bmatrix}^{-1} \begin{bmatrix} \sum x_i y_i \\ \sum y_i \end{bmatrix}$$

$$\begin{bmatrix} a \\ b \end{bmatrix} = \frac{1}{n(\sum x_i^2) - (\sum x_i)^2} \begin{bmatrix} n & -\sum x_i \\ -\sum x_i & \sum x_i^2 \end{bmatrix} \begin{bmatrix} \sum x_i y_i \\ \sum y_i \end{bmatrix}$$

$$\begin{bmatrix} a \\ b \end{bmatrix} = \frac{1}{n(\sum x_i^2) - (\sum x_i)^2} \begin{bmatrix} n(\sum x_i y_i) - (\sum x_i)(\sum y_i) \\ (\sum x_i^2)(\sum y_i) - (\sum x_i)(\sum x_i y_i) \end{bmatrix}$$

That is,

$$\boxed{a = \frac{n(\sum x_i y_i) - (\sum x_i)(\sum y_i)}{n(\sum x_i^2) - (\sum x_i)^2}, \qquad b = \frac{(\sum x_i^2)(\sum y_i) - (\sum x_i)(\sum x_i y_i)}{n(\sum x_i^2) - (\sum x_i)^2}}$$

Example:

(i) Find the least squares line through the points $(1, 1)$, $(3, 3.5)$, $(5, 4)$ and $(8, 7.5)$.

(ii) Find the the projection of $(1, 3.5, 4, 7.5)$ onto $\text{span}(\{(1, 3, 5, 8), (1, 1, 1, 1)\}$.

Solution:

(i) Here $n = 4$, and

$$\sum x_i = 1 + 3 + 5 + 8 = 17$$
$$\sum x_i^2 = 1^2 + 3^2 + 5^2 + 8^2 = 99$$
$$\sum y_i = 1 + 3.5 + 4 + 7.5 = 16$$
$$\sum x_i y_i = (1)(1) + (3)(3.5) + (5)(4) + (8)(7.5) = 91.5$$

so

$$a = \frac{(4)(91.5) - (17)(16)}{(4)(99) - (17)^2} = \frac{94}{107} \approx 0.88$$

and

$$b = \frac{(99)(16) - (17)(91.5)}{(4)(99) - (17)^2} = \frac{57}{214} \approx 0.27$$

So the least squares line is $y = \left(\frac{94}{107}\right)x + \left(\frac{57}{214}\right) \approx 0.88x + 0.27$.

This is the line shown on the graph on page 1.

(ii) Here $(1, 3.5, 4, 7.5) = (y_1, y_2, y_3, y_4)$ and $(1, 3, 5, 8) = (x_1, x_2, x_3, x_4)$. The projection of (y_1, y_2, y_3, y_4) onto span($\{(x_1, x_2, x_3, x_4), (1, 1, 1, 1)\}$ is $\mathbf{p} = \text{proj}_{\text{col}(\mathbf{A})}\mathbf{y}$, where

$$\mathbf{p} = \mathbf{Au} = \begin{bmatrix} x_1 & 1 \\ x_2 & 1 \\ x_3 & 1 \\ x_4 & 1 \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} .$$

So

$$\mathbf{p} = \begin{bmatrix} 1 & 1 \\ 3 & 1 \\ 5 & 1 \\ 8 & 1 \end{bmatrix} \begin{bmatrix} (94/107) \\ (57/214) \end{bmatrix} = \frac{1}{214} \begin{bmatrix} 245 \\ 621 \\ 997 \\ 1561 \end{bmatrix} \approx \begin{bmatrix} 1.14 \\ 2.90 \\ 4.66 \\ 7.29 \end{bmatrix}$$

Another Way to Think About Least Squares

From the derivation in the previous section it may not be clear why the technique is called the method of least squares. The derivation relies on the existence of a vector $\mathbf{p}$ in col($\mathbf{A}$) nearest to $\mathbf{y}$. That is, the vector for which $\|\mathbf{y} - \mathbf{p}\|$ is a minimum. $\|\mathbf{y} - \mathbf{p}\|$ is a minimum if and only if $\|\mathbf{y} - \mathbf{Au}\|^2$ is a minimum. But

$$\|\mathbf{y} - \mathbf{Au}\|^2 = \sum_{i=1}^{n} (y_i - ax_i - b)^2 . \tag{3}$$

So to solve the system $\mathbf{Au} = \mathbf{p}$ for $\mathbf{u}$ is to find the values of a and b which minimize the sum of squares (i.e. give the least squares) in equation (3).

Exercises

For each of the following sets of points:

(i) Find the least squares line through the points.

(ii) Find $\mathbf{p} = \text{proj}_{\text{col}(\mathbf{A})}\mathbf{y}$, where $\mathbf{A}$ and $\mathbf{y}$ correspond to the matrices in equation (2).

1. $(2, -1)$, $(3, 0)$, $(5, 1)$. (ans: $y = 0.64x - 2.14$)
2. $(1, 7)$, $(2, 5)$, $(4, 3)$, $(7, -2)$. (ans: $y = -1.45x + 8.33$)
3. $(-2, 0)$, $(2, 3)$, $(6, 6)$; notice these points lie on a single line. (ans: $y = 0.75x + 1.5$)