
FROM PRIMER FOR LINEAR ALGEBRA
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3.2. The Least Squares Solution of Overdetermined Linear Systems

Systems having more equations than unknowns often arise in data fitting problems. In the simplest case a researcher might assume that the output, y , of an experiment is a linear function of the input, x . In other words,

$$y = ax + b$$

is assumed where the parameters a and b are to be found to fit the observed experimental data. Typically, the experiment is performed many times. This generates data $(x_1, y_1), (x_2, y_2), \dots, (x_N, y_N)$ which are supposed to satisfy

$$y_i = ax_i + b, \quad i = 1, 2, 3, \dots, N, \quad (1)$$

for some numbers a and b . This can be viewed as a system of linear equations for a and b :

$$\begin{bmatrix} x_1 & 1 \\ x_2 & 1 \\ \vdots & \vdots \\ x_N & 1 \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} y_1 \\ \vdots \\ y_N \end{bmatrix} \quad (2)$$

If $N \geq 3$, then (2) will in general have no solution. For example, in the $N \geq 3$ case the column space of the matrix is either a line or a plane and the chance that the vector of outputs $\begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix}$ is in the column space is small. In higher dimensions it doesn't get better. Nevertheless, there is the need to make some good sense out of (2).

One standard way of treating systems like (2) is to replace the right hand side by a vector in the column space of the coefficient matrix. The best vector to choose would be the member of the column space closest to the right hand side. We formulate this as a general principle.

Least Squares Principle. If the system $Ax = b$ has no solution, then replace b by the member of the

column space closest to \mathbf{b} , say \mathbf{b}^* , and then solve $A\mathbf{x} = \mathbf{b}^*$. If $A\mathbf{x} = \mathbf{b}^*$ has a unique solution, it is called the *least squares solution* of $A\mathbf{x} = \mathbf{b}$.

There are still problems to be overcome. First, how do we find \mathbf{b}^* ? Next, what should we do if $A\mathbf{x} = \mathbf{b}^*$ does not have a unique solution?

Our present treatment avoids the first problem and ignores the second. However, in some simple cases, like system (2), one can readily check if $A\mathbf{x} = \mathbf{b}^*$ has a unique solution.

Theorem 1. If A is an $N \times 2$ matrix and neither column is a multiple of the other, then the system $A\mathbf{x} = \mathbf{b}$ has either no solutions or exactly one solution.

The following result is more general but the hypotheses are not easy to check.

Theorem 2. If A is an $n \times k$ matrix and if no column is a linear combination of the others, then the system $A\mathbf{x} = \mathbf{b}$ has either no solutions or exactly one solution.

Remark. The condition on the columns in Theorem 2 is called *linear independence*. □

Under the conditions of Theorem 1 or Theorem 2, there will be a unique solution to $A\mathbf{x} = \mathbf{b}^*$.

Now, consider the case of a 3×2 matrix whose column space is a plane. From basic facts about projections onto planes, we have

Fact. \mathbf{b}^* is the point in the column space of A closest to \mathbf{b} if and only if $\mathbf{b} - \mathbf{b}^*$ is perpendicular to every vector in the column space of A . That is, for every \mathbf{z} in \mathbf{R}^2 , $A\mathbf{z}$ is perpendicular to $\mathbf{b} - \mathbf{b}^*$:

$$(A\mathbf{z})^t(\mathbf{b} - \mathbf{b}^*) = 0. \quad (3)$$

Since we know \mathbf{b}^* is in the column space of A , we can write $A\mathbf{x}^* = \mathbf{b}^*$. Also, we have

$$(A\mathbf{z})^t = \mathbf{z}^t A^t$$

so (3) becomes

so
$$A^t A = \begin{bmatrix} 2 & 3 \\ 3 & 6 \end{bmatrix} \quad \text{and} \quad A^t \mathbf{b} = \begin{bmatrix} 13 \\ 20 \end{bmatrix}.$$

The solution of

$$\begin{aligned} 2x + 3y &= 13 \\ 3x + 6y &= 20 \end{aligned}$$

is $x = 6$, $y = \frac{1}{3}$. □

Example 2. The data in the table below appear to lie near a straight line $y = mx + b$. Find the values of m and b that give the least squares fit to the data.

x_i	0.78	0.80	0.82	0.84	0.86	0.88
y_i	0.70	0.72	0.73	0.74	0.76	0.77

Solution. The linear system for m and b is given by the equations

$$mx_i + b = y_i \quad i = 1, 2, \dots, 6.$$

$$\begin{bmatrix} 0.78 & 1 \\ 0.80 & 1 \\ 0.82 & 1 \\ 0.84 & 1 \\ 0.86 & 1 \\ 0.88 & 1 \end{bmatrix} \begin{bmatrix} m \\ b \end{bmatrix} = \begin{bmatrix} 0.70 \\ 0.72 \\ 0.73 \\ 0.74 \\ 0.76 \\ 0.77 \end{bmatrix}.$$

Now,

$$A^t = \begin{bmatrix} 0.78 & 0.80 & 0.82 & 0.84 & 0.86 & 0.88 \\ 1 & 1 & 1 & 1 & 1 & 1 \end{bmatrix}$$

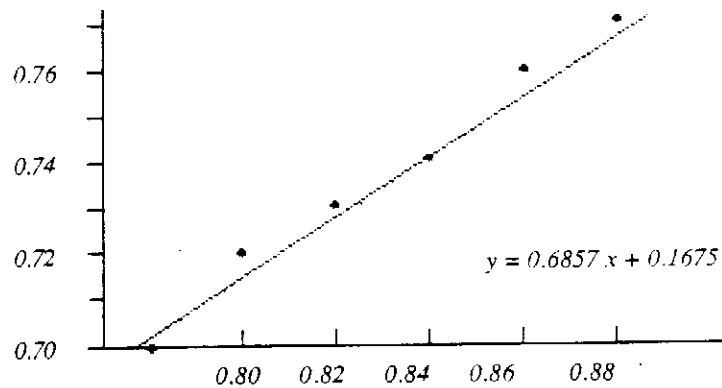
$$A^t \mathbf{y} = \begin{bmatrix} 3.6734 \\ 4.4200 \end{bmatrix} \quad \text{and} \quad A^t A = \begin{bmatrix} 4.1404 & 4.9800 \\ 4.9800 & 6 \end{bmatrix}.$$

So, we must solve

$$4.1404m^* + 4.98b^* = 3.6734$$

$$4.98m^* + 6b^* = 4.42.$$

With a hand calculator we obtain $m^* = 0.6857$ and $b^* = 0.1675$. Here is a sketch of the straight line together with the data points.



Example 3. A researcher obtained the data in the table below and suspects that the data points all lie on or near a quadratic so it is reasonable to set up the system

$$y_i = ax_i^2 + bx_i + c, \quad i = 1, 2, \dots, 6$$

and find the least squares solution a^*, b^*, c^* .

i	x_i	y_i
1	0	5
2	2	11
3	4	32
4	6	73
5	8	122
6	10	200

Solution. We have a 6×3 system, $Ax = y$, where the entries of y can be read directly from the table, the last column of A contains all 1's, the middle column contains the x_i 's and the first column contains

the squares of the x_i 's.

$$\begin{bmatrix} 0 & 0 & 1 \\ 4 & 2 & 1 \\ 16 & 4 & 1 \\ 36 & 6 & 1 \\ 64 & 8 & 1 \\ 100 & 10 & 1 \end{bmatrix} \begin{bmatrix} a \\ b \\ c \end{bmatrix} = \begin{bmatrix} 5 \\ 11 \\ 32 \\ 73 \\ 122 \\ 200 \end{bmatrix}.$$

We compute

$$A^t A = \begin{bmatrix} 15,664 & 1,800 & 220 \\ 1,800 & 220 & 30 \\ 220 & 30 & 6 \end{bmatrix} \quad \text{and} \quad A^t y = \begin{bmatrix} 30,992 \\ 3,564 \\ 443 \end{bmatrix}$$

and solve

$$15,664a^* + 1800b^* + 220c^* = 30,992$$

$$1,800a^* + 220b^* + 30c^* = 3,564$$

$$220a^* + 30b^* + 6c^* = 443.$$

From a programmable hand calculator we get $a^* = 2.11$, $b^* = -1.80$, $c^* = 5.57$.

3.2. EXERCISES

1. Find the least squares solution of $Ax = b$ if

$$(a) \quad A = \begin{bmatrix} 2 & 1 \\ 4 & 2 \\ 1 & 1 \end{bmatrix}, \quad b = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}, \quad b = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}$$

$$(b) \quad A = \begin{bmatrix} 1 & 3 \\ -1 & 1 \\ 2 & 1 \end{bmatrix}, \quad b = \begin{bmatrix} 0 \\ 1 \\ 1 \end{bmatrix}, \quad b = \begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix}$$

2. For each system in Exercise 1, verify that $b - Ax^*$ is perpendicular to the columns of A .

