Overdetermined systems

An overdetermined system of linear equations has more equations than unknowns. Such a system can either have only one solution or no solutions.

For example, the following system (3 equations and 1 unknown) has only one solution, that is $x = 2$:

$$\begin{aligned} 2x &= 4 \\ 3x &= 6 \\ 4x &= 8 \end{aligned}$$

However, the following system (3 equations and 1 unknown) has no solution:

$$\begin{aligned} 2x &= 4 \\ 3x &= 7 \\ 4x &= 9 \end{aligned}$$

When a system has no solution, we shall attempt to find the "best" approximate solution $\widehat{x}$. Such an approximate solution is called a least squares approximation.

Therefore the system

$$\begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix} [\, x \,] = \begin{pmatrix} b_1 \\ b_2 \\ b_3 \end{pmatrix}$$

has only one solution when $\begin{pmatrix} b_1 \\ b_2 \\ b_3 \end{pmatrix}$ is a scalar multiple of $\begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix}$, that is $\begin{pmatrix} b_1 \\ b_2 \\ b_3 \end{pmatrix}$ has to lie on the line spanned by $\begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix}$.

The following system (3 equations and 2 unknowns)

$$a_{11}x_1 + a_{12}x_2 = b_1 \tag{1}$$

$$a_{21}x_1 + a_{22}x_2 = b_2 \tag{2}$$

$$a_{31}x_1 + a_{32}x_2 = b_3 \tag{3}$$

can be written as

$$\begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \\ a_{31} & a_{32} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ b_3 \end{pmatrix}$$

or more concisely as

$$A\mathbf{x} = \mathbf{b}$$

Note that (1), (2) and (3) represent three straight lines. If these lines intersect each other at the same point, the system has one solution, otherwise it has no solutions in which case we have to find a least squares approximation $\widehat{\mathbf{x}}$ so that

$$||\mathbf{b} - A\widehat{\mathbf{x}}||$$

is as small as possible.

Least squares approximations

The system

$$\begin{pmatrix} 1 & 1 \\ 1 & 1 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix}$$

can also be written as

$$A\mathbf{x} = \mathbf{b},\ A = [\mathbf{a}_1, \mathbf{a}_2],\ \mathbf{a}_1 = \begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix},\ \mathbf{a}_2 = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix},\ \mathbf{b} = \begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix}$$

and has no solution, since $\mathbf{b}$ does not lie in the plane spanned by $\mathbf{a}_1$ and $\mathbf{a}_2$. The system can also be interpreted as three lines that do not intersect each other at the same point.

We therefore seek an approximate solution $\widehat{\mathbf{x}} = [\widehat{x}_1, \widehat{x}_2]^T$, so that

$$||\mathbf{b} - A\widehat{\mathbf{x}}||$$

is a minimum.

Consider the vector space V with the basis

$$\left\{ \mathbf{a}_1 = \begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix}; \quad \mathbf{a}_2 = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} \right\}$$

The vector $\mathbf{b} = [1, 2, 3]^T$ does not lie in V. We therefore want to find a vector $\widehat{\mathbf{b}}$ that lies in V and is as close as possible to $\mathbf{b}$. This implies that the norm of the difference between $\mathbf{b}$ and $\widehat{\mathbf{b}}$ has to be as small as possible.

Since $\widehat{\mathbf{b}}$ lies in V, $\widehat{\mathbf{b}}$ can be written as a linear combination of the basis vectors:

$$\widehat{\mathbf{b}} = \widehat{x}_1\mathbf{a}_1 + \widehat{x}_2\mathbf{a}_2$$

Let $\mathbf{e} = \mathbf{b} - \widehat{\mathbf{b}}$, that is

$$\mathbf{e} = \begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix} - \widehat{x}_1 \begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix} - \widehat{x}_2 \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$$

An alternative formulation is as follows:

$$\mathbf{e} = \mathbf{b} - A\widehat{\mathbf{x}}$$

with $\widehat{\mathbf{x}} = [\widehat{x}_1, \widehat{x}_2]^T$.

The vector $\widehat{\mathbf{x}}$ therefore has to be chosen in such a way that $\|\mathbf{e}\|$ is as small as possible. We can now follow one of two possible approaches:

— minimization by employing derivatives, or

— geometrical considerations and matrices.

Minimization by employing derivatives:

The square of the norm of $\mathbf{e}$ is given by

$$\|\mathbf{e}\|^2 = (1 - \widehat{x}_1 - \widehat{x}_2)^2 + (2 - \widehat{x}_1 - \widehat{x}_2)^2 + (3 - \widehat{x}_2)^2$$

We subsequently minimize $\|\mathbf{e}\|^2$ with respect to $\widehat{x}_1$ and $\widehat{x}_2$, that is

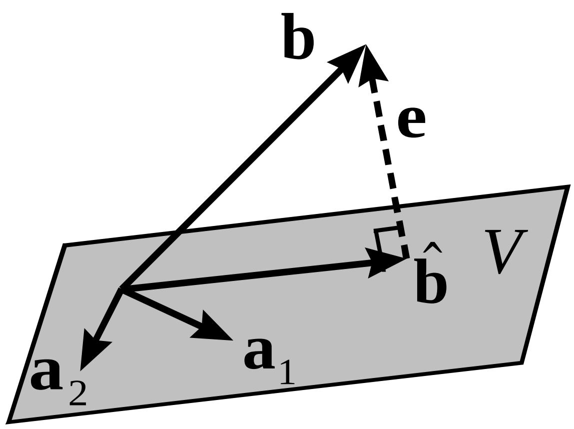
$$\frac{\partial \|\mathbf{e}\|^2}{\partial \widehat{x}_1} = 0 \quad \text{and} \quad \frac{\partial \|\mathbf{e}\|^2}{\partial \widehat{x}_2} = 0.$$

These two conditions lead to the following system of equations in $\widehat{x}_1$ and $\widehat{x}_2$,

$$\begin{array}{rcrcr} 4\widehat{x}_1 & + & 4\widehat{x}_2 & = & 6 \\ 4\widehat{x}_1 & + & 6\widehat{x}_2 & = & 12 \end{array}$$

and has the solution $[\widehat{x}_1, \widehat{x}_2]^T = [-1.5, 3.0]^T$.

Geometrical considerations and matrices:



For $\|\mathbf{e}\|$ to be as small as possible, $\mathbf{e}$ has to be orthogonal to each of the columns of A, therefore

$$A^T\mathbf{e} = \mathbf{0}$$

or

$$A^T(\mathbf{b} - A\widehat{\mathbf{x}}) = \mathbf{0}$$

Note that $\widehat{\mathbf{b}}$ is the projection of $\mathbf{b}$ onto V!

This leads to the well-known *normal equations*:

$$A^T A\widehat{\mathbf{x}} = A^T \mathbf{b}$$

For the above example we have that:

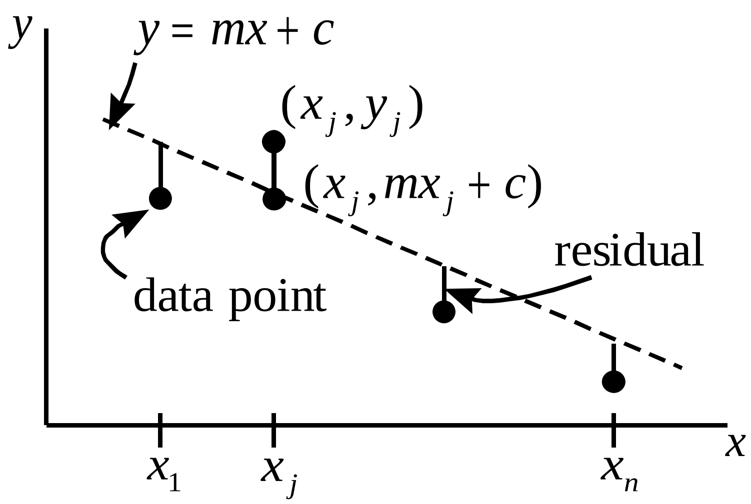
$$A = \begin{bmatrix} 1 & 1 \\ 1 & 1 \\ 0 & 1 \end{bmatrix}, \qquad A^T A = \begin{bmatrix} 2 & 2 \\ 2 & 3 \end{bmatrix} \qquad \text{and} \quad A^T \mathbf{b} = \begin{bmatrix} 3 \\ 6 \end{bmatrix}$$

Consequently $\widehat{\mathbf{x}} = [-1.5, 3.0]^T$.

The normal equations can be used to find least squares approximations for **any** overdetermined system $A\mathbf{x} = \mathbf{b}$, as long as the columns of A are linearly independent. We do not prove this theorem, but will subsequently utilize it to fit a curve through a set of points.

Application: Curve fitting

Suppose that we want to fit the best line $y = mx + c$ through a set of data points (x_1, y_1), (x_2, y_2),. . .,(x_n, y_n). One way to achieve this is to minimize the sum of the residuals below (using derivatives).



However, the problem can also be formulated as a system of linear equations:

$$\begin{aligned} mx_1 + c &= y_1 \\ mx_2 + c &= y_2 \\ \vdots &= \vdots \\ mx_n + c &= y_n \end{aligned}$$

This overdetermined system will only have a solution when all the data points lie on the same straight line. Since this is generally not the case, an approximate least squares solution has to be obtained. The system can also be expressed as a matrix equation:

$$\begin{pmatrix} x_1 & 1 \\ x_2 & 1 \\ \vdots & \vdots \\ x_n & 1 \end{pmatrix} \begin{pmatrix} m \\ c \end{pmatrix} = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix}, \quad \text{or} \quad X\mathbf{m} = \mathbf{y}$$

The least squares solution is therefore as follows:

$$\widehat{\mathbf{m}} = (X^T X)^{-1} X^T \mathbf{y}$$

<u>*Example 1:*</u> Find the equation $y = mx + c$ of the least squares line that fits best through the data points $(2, 1)$, $(5, 2)$, $(7, 3)$ and $(8, 3)$.

Solution:

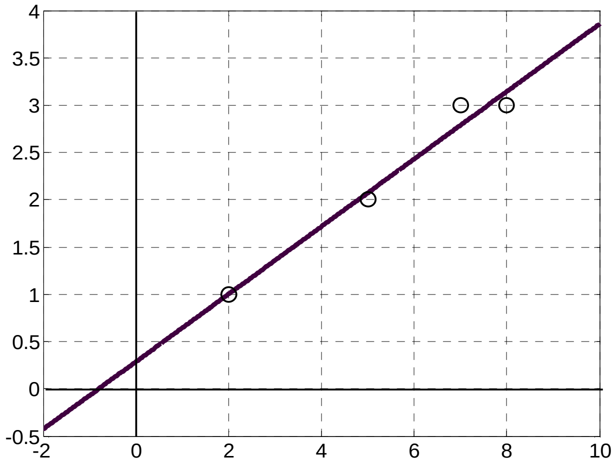
$$X = \begin{pmatrix} 2 & 1 \\ 5 & 1 \\ 7 & 1 \\ 8 & 1 \end{pmatrix}, \quad \mathbf{y} = \begin{pmatrix} 1 \\ 2 \\ 3 \\ 3 \end{pmatrix}$$

$$X^T X = \begin{pmatrix} 142 & 22 \\ 22 & 4 \end{pmatrix}$$

$$X^T \mathbf{y} = \begin{pmatrix} 57 \\ 9 \end{pmatrix}$$

$$\begin{pmatrix} \widehat{m} \\ \hat{c} \end{pmatrix} = \begin{pmatrix} 142 & 22 \\ 22 & 4 \end{pmatrix}^{-1} \begin{pmatrix} 57 \\ 9 \end{pmatrix} = \begin{pmatrix} 5/14 \\ 2/7 \end{pmatrix}$$

The line is therefore as follows: $y = \dfrac{5}{14}x + \dfrac{2}{7}$



Exercise: Show that the best parabola $y = ax^2 + bx + c$ through the data points $(-2, 0)$, $(0, -2)$, $(2, -1)$ and $(4, 2)$ is given by

$$y = \frac{5}{16}x^2 - \frac{11}{40}x - \frac{37}{20}$$