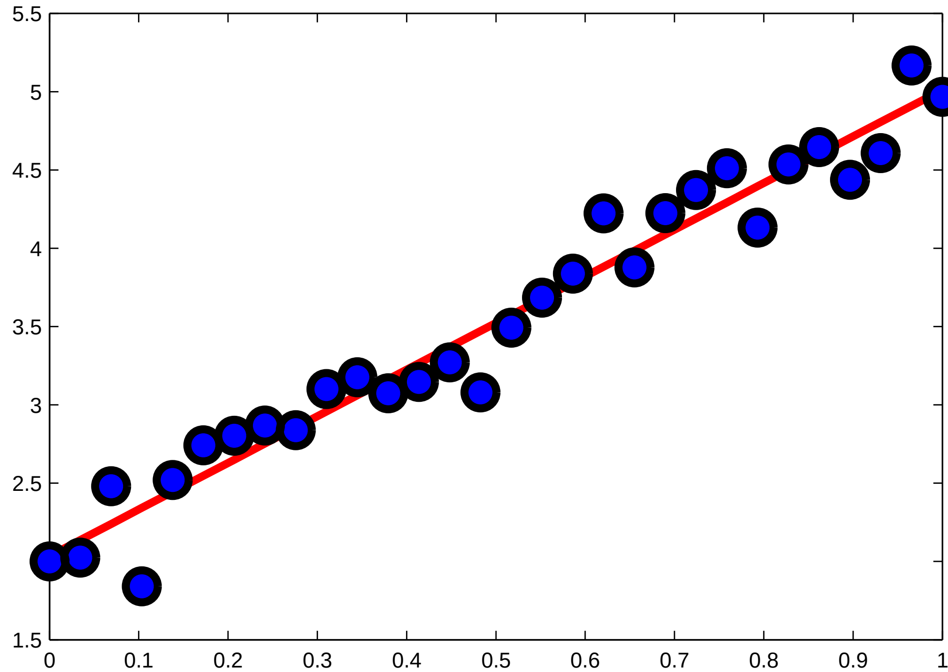
2 Least squares



The outcomes of many physical experiments are modeled by linear relations of the form:

$$y = m\,x + b. \tag{12}$$

There are two primary reasons for that. Firstly, many physical laws are linear in nature[1]. For instance, Equation (12) could be an expression of Hooke's Law, or Ohm's Law; these, as you know, describe a vast number of mechanical and electrical phenomena. Secondly, even if the relation between x and y is nonlinear to begin with, it can often be transformed into a linear one by a suitable choice of coordinates. For instance $y = y_0\,e^{-k\,x}$ is, clearly, a nonlinear relation between x and y. However, the relationship between x and $z = \ln(y)$ is linear:

$$z = \ln(y_0) - k\,x.$$

[1]Why do you think that is?

A human eye is incapable of distinguishing a plot of a decaying exponential from, say, a similarly shaped hyperbola—to us all such plots look the same. Yet, we can easily determine through visual examination whether a plot is a straight line or not. The best way to confirm exponential relation is to plot the data in semi-logarithmic coordinates. This explains the popularity of logarithmic plots in subjects like Physical Chemistry where decaying exponentials are extremely common.

The figure at the start of this section shows the best linear fit (red line) for a set of thirty noisy observations (blue circles). The coefficients of the linear relation were computed by solving the linear system:

$$\begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_{30} \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_{30} \end{bmatrix} \tag{13}$$

The system (13) is an immediate consequence of the assumed linear relation (12). If there were no noise in the data, we could solve the equations through simple elimination of variables. However, as is evident from the figure, the data is noisy and the system (13) is clearly inconsistent. Formally, there is no solution because the data points are not perfectly aligned. And yet, the points are "close" to being on the same line. Therefore we would like to be able to solve the system and find the line that provides the "best" linear fit.

There are, actually, many possibilities for the best linear fit depending on what one means by "best". The most common approach, based on the use of the inner (dot) product, is known as the *least squares fit* and will now be described.

Quite generally, suppose we have discrete data (x_1, y_1), (x_2, y_2), $\ldots$, (x_N, y_N) modeled by the linear relation (12) and we wish to estimate the parameters m and b. Let us introduce the following vectors in $\mathbb{R}^N$:

$$\mathbf{1} = \begin{bmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{bmatrix}, \quad \mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_N \end{bmatrix}, \quad \mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{bmatrix}.$$

The assumption that Equation (12) holds for each data point (x_k, y_k) can be expressed by a single vector relation:

$$\mathbf{y} = m\,\mathbf{x} + b\,\mathbf{1}. \tag{14}$$

Let us rewrite Equation (14) as a matrix-vector product. To this end we introduce the N-by-2 matrix

$$A = \begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_N \end{bmatrix} = [\mathbf{1} \mid \mathbf{x}]$$

and aggregate the unknowns into a single vector:

$$\mathbf{u} = \begin{bmatrix} b \\ m \end{bmatrix}.$$

Then Equation (14) can now be recast as:

$$A\,\mathbf{u} = \mathbf{y}.$$

If $N = 2$ the matrix A is square and we could, in principle, write $\mathbf{u} = A^{-1}\,\mathbf{y}$: this would give us the familiar equations for the intercept and the slope of a line passing through two given points. However, for $N > 2$ the matrix A is rectangular and therefore non-invertible. Even if $N = 2$ the inverse A^{-1} may be impossible to compute. For instance, the following matrix

$$A = \begin{bmatrix} 1 & 0 \\ 1 & 10^{-16} \end{bmatrix}$$

is nonsingular, yet its numerical inversion is extremely unstable [2]. This brings us to the main question of this section:

> How do we solve $A\,\mathbf{u} = \mathbf{y}$ when A^{-1} is badly scaled or does not exist?

Normal equations

Let us consider the general two-by-two linear system

$$\begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \end{bmatrix} \tag{15}$$

and search for a solving strategy not involving the possibly nonexistent A^{-1}. When looking for new ways of solving a problem, it is often helpful to examine the following question:

[2] Such matrices are called ill-conditioned

Given a possible solution, how can we validate it?

Let us pretend that we have found $\mathbf{u}$. To check whether it solves Equation (15) we can compute the residual vector

$$\mathbf{r} = A\,\mathbf{u} - \mathbf{y},$$

and see if it is zero: clearly, if $\mathbf{r} = \mathbf{0}$ then $\mathbf{u}$ is a solution of Equation (15).

Now, how do we check if a vector is zero? The question is not as silly as it sounds, especially, if we are doing this on a computer. We could iterate over the components of the vector and check if any of them are *nonzero* for then the whole vector is nonzero. However, running a long `for...do` loop may be slow. A faster approach, at least in `Matlab`, is to compute the square[3] of the length $\|\mathbf{r}\|^2 = \mathbf{r}^T\,\mathbf{r}$ and see if it is zero: surely, if $\|\mathbf{r}\|^2 = 0$ then $\mathbf{u}$ is a solution of Equation (15).

Next, let us think of the likely case where $\|\mathbf{r}\|^2$ is not zero but is instead "small"? Strictly speaking, $\mathbf{u}$ is not a solution, however, intuitively, we would expect it to be close to one. And if we could somehow diminish $\|\mathbf{r}\|^2$ we would get closer still. This suggests the following method for solving Equation (15) *and any other linear system*:

Minimize $\|\mathbf{r}\|^2 = \|A\,\mathbf{u} - \mathbf{y}\|^2$ with respect to $\mathbf{u}$.

To simplify notation, let us denote $f(\mathbf{u}) = \|A\,\mathbf{u} - \mathbf{y}\|^2$. Using Equation (15) we can compute f explicitly as:

$$f(u_1, u_2) = (a_{11}\,u_1 + a_{12}\,u_2 - y_1)^2 + (a_{21}\,u_1 + a_{22}\,u_2 - y_2)^2. \tag{16}$$

To find the minimum of (16), set the gradient to zero. This leads to the following system of linear equations:

$$\begin{aligned} 2\,(a_{11}\,u_1 + a_{12}\,u_2 - y_1)\,a_{11} + 2\,(a_{21}\,u_1 + a_{22}\,u_2 - y_2)\,a_{21} &= 0 \\ 2\,(a_{11}\,u_1 + a_{12}\,u_2 - y_1)\,a_{12} + 2\,(a_{21}\,u_1 + a_{22}\,u_2 - y_2)\,a_{22} &= 0 \end{aligned}$$

Let us rewrite this system in matrix-vector form. First, cancel the twos, take the y-terms to the right-hand side and collect the like terms on the left:

$$\begin{aligned} (a_{11}^2 + a_{21}^2)\,u_1 + (a_{11}\,a_{12} + a_{21}\,a_{22})\,u_2 &= a_{11}\,y_1 + a_{21}\,y_2 \\ (a_{11}\,a_{12} + a_{21}\,a_{22})\,u_1 + (a_{12}^2 + a_{22}^2)\,u_2 &= a_{12}\,y_1 + a_{22}\,y_2 \end{aligned}$$

[3]Computing the square of the length rather than the length itself allows us to avoid the square root.

It is clear that the right hand side is the matrix-vector product:

$$\begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix}^T \begin{bmatrix} y_1 \\ y_2 \end{bmatrix} = A^T \mathbf{y}.$$

Quick experimentation shows that the left-hand side is the product:

$$\begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix}^T \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \end{bmatrix} = A^T A \, \mathbf{u}.$$

We conclude that, in order to minimize f and thus solve $A\,\mathbf{u} = \mathbf{y}$, we need to solve the *normal equations*:

$$A^T A \, \mathbf{u} = A^T \mathbf{y}. \tag{17}$$

It is clear that Equation (17) is equivalent to the original system $A\,\mathbf{u} = \mathbf{y}$. However, it is also clear that normal equations are nicer to work with. Unlike A, the matrix $A^T A$ is guaranteed to be square. Better still, $A^T A$ is symmetric and therefore has orthonormal eigenvectors and real eigenvalues. And that is not all! The eigenvalues of $A^T A$ are all nonnegative (Exercise).

Let us return to the original problem of finding the best linear fit for a set of N discrete data points. In statistical analysis this is part of *linear regression*.

Normal equations for linear regression

To find the normal equations, multiply both sides of $[\mathbf{1} \mid \mathbf{x}]\,\mathbf{u} = \mathbf{y}$ by the transpose $[\mathbf{1} \mid \mathbf{x}]^T$. On the left-hand side, we get

$$\begin{bmatrix} \mathbf{1}^T \\ \hline \mathbf{x}^T \end{bmatrix} [\mathbf{1} \mid \mathbf{x}] \begin{bmatrix} b \\ m \end{bmatrix} = \begin{bmatrix} \mathbf{1}^T \mathbf{1} & \mathbf{1}^T \mathbf{x} \\ \mathbf{x}^T \mathbf{1} & \mathbf{x}^T \mathbf{x} \end{bmatrix} \begin{bmatrix} b \\ m \end{bmatrix},$$

while the right-hand side becomes:

$$\begin{bmatrix} \mathbf{1}^T \\ \hline \mathbf{x}^T \end{bmatrix} \mathbf{y} = \begin{bmatrix} \mathbf{1}^T \mathbf{y} \\ \mathbf{x}^T \mathbf{y} \end{bmatrix}.$$

The normal equations are therefore:

$$\begin{bmatrix} \mathbf{1}^T \mathbf{1} & \mathbf{1}^T \mathbf{x} \\ \mathbf{x}^T \mathbf{1} & \mathbf{x}^T \mathbf{x} \end{bmatrix} \begin{bmatrix} b \\ m \end{bmatrix} = \begin{bmatrix} \mathbf{1}^T \mathbf{y} \\ \mathbf{x}^T \mathbf{y} \end{bmatrix}. \tag{18}$$

As long as

$$\det \begin{bmatrix} \mathbf{1}^T \mathbf{1} & \mathbf{1}^T \mathbf{x} \\ \mathbf{x}^T \mathbf{1} & \mathbf{x}^T \mathbf{x} \end{bmatrix} \neq 0,$$

the solution of Equation (18) can be written in the form:

$$\begin{bmatrix} b \\ m \end{bmatrix} = \begin{bmatrix} \mathbf{1}^T\mathbf{1} & \mathbf{1}^T\mathbf{x} \\ \mathbf{x}^T\mathbf{1} & \mathbf{x}^T\mathbf{x} \end{bmatrix}^{-1} \begin{bmatrix} \mathbf{1}^T\mathbf{y} \\ \mathbf{x}^T\mathbf{y} \end{bmatrix}. \qquad (19)$$

However, since we are not making any assumptions about the data, we need to investigate the case when the determinant of the normal system is zero.

Exceptional case

Denote

$$F(N) = \det \begin{bmatrix} \mathbf{1}^T\mathbf{1} & \mathbf{1}^T\mathbf{x} \\ \mathbf{x}^T\mathbf{1} & \mathbf{x}^T\mathbf{x} \end{bmatrix} = N\sum_{n=1}^{N} x_n^2 - \left(\sum_{n=1}^{N} x_n\right)^2.$$

It is easy to check that

$$\begin{aligned} F(2) &= 2\,(x_1^2+x_2^2) - (x_1+x_2)^2 = (x_1-x_2)^2 \\ F(3) &= 3\,(x_1^2+x_2^2+x_3^2) - (x_1+x_2+x_3)^2 = (x_1-x_2)^2+(x_1-x_3)^2+(x_2-x_3)^2 \\ F(4) &= 4\,(x_1^2+x_2^2+x_3^2+x_4^2) - (x_1+x_2+x_3+x_4)^2 \\ &= (x_1-x_2)^2+(x_1-x_3)^2+(x_1-x_4)^2+(x_2-x_3)^2+(x_2-x_4)^2+(x_3-x_4)^2 \end{aligned}$$

The pattern is, clearly,

$$F(N) = \frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N}(x_i-x_j)^2,$$

which tells us that

$$\det \begin{bmatrix} \mathbf{1}^T\mathbf{1} & \mathbf{1}^T\mathbf{x} \\ \mathbf{x}^T\mathbf{1} & \mathbf{x}^T\mathbf{x} \end{bmatrix} = \frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N}(x_i-x_j)^2 = 0$$

if and only if $x_i = x_j$ for every pair of indices i and j. In words: the x-coordinates of all data points must be the same. This, of course, is highly unlikely. Nevertheless, let us suppose that $x_n = x_1$ for all n. Then the normal equations (18) are easily seen to be:

$$\begin{bmatrix} N & N\,x_1 \\ N\,x_1 & N\,x_1^2 \end{bmatrix} \begin{bmatrix} b \\ m \end{bmatrix} = \begin{bmatrix} \sum_{n=1}^{N} y_n \\ x_1\,\sum_{n=1}^{N} y_n \end{bmatrix}.$$

This is a consistent system of two linearly dependent equations. As such, it has infinitely many solutions satisfying:

$$N\,b + N\,x_1\,m = \sum_{n=1}^{N} y_n.$$

As one solution, we could return the horizontal line:

$$b = \frac{1}{N}\sum_{n=1}^{N} y_n, \quad m = 0.$$

However, it might make more sense to return an error message.

The limiting case

Suppose that the data is generated by sampling a continuous function $y = f(x)$ on the interval $\alpha \le x \le \beta$. That is, $\mathbf{y} = f(\mathbf{x})$. Is stands to reason that in the limit, as $N \to \infty$, the best linear fit will yield the straight line closest to the graph of $y = f(x)$ on the interval $[\alpha, \beta]$. This suggests that there should be a continuous analogue of Equations (18) and (19).

Let $\Delta x = \frac{\beta-\alpha}{N}$ be the horizontal distance between the points in the sample. Multiplying both sides of Equation (18) by Δx, we get

$$\begin{bmatrix} \mathbf{1}^T \mathbf{1}\,\Delta x & \mathbf{1}^T \mathbf{x}\,\Delta x \\ \mathbf{x}^T \mathbf{1}\,\Delta x & \mathbf{x}^T \mathbf{x}\,\Delta x \end{bmatrix} \begin{bmatrix} b \\ m \end{bmatrix} = \begin{bmatrix} \mathbf{1}^T \mathbf{y}\,\Delta x \\ \mathbf{x}^T \mathbf{y}\,\Delta x \end{bmatrix}.$$

Now

$$\lim_{N\to\infty} \mathbf{1}^T \mathbf{1}\,\Delta x = \lim_{N\to\infty} N\,\Delta x = \beta - \alpha = \int_\alpha^\beta 1\,dx.$$

In the same manner, other dot products after being scaled by Δx can be recognized as Riemann sums tending to definite integrals:

$$\begin{aligned}
\lim_{N\to\infty} \mathbf{1}^T \mathbf{x}\,\Delta x &= \lim_{N\to\infty} \mathbf{x}^T \mathbf{1}\,\Delta x = \lim_{N\to\infty} \sum_{n=1}^{N} x_n\,\Delta x = \int_\alpha^\beta x\,dx = \frac{\beta^2-\alpha^2}{2} \\
\lim_{N\to\infty} \mathbf{x}^T \mathbf{x}\,\Delta x &= \lim_{N\to\infty} \sum_{n=1}^{N} x_n^2\,\Delta x = \int_\alpha^\beta x^2\,dx = \frac{\beta^3-\alpha^3}{3} \\
\lim_{N\to\infty} \mathbf{1}^T \mathbf{y}\,\Delta x &= \lim_{N\to\infty} \sum_{n=1}^{N} f(x_n)\,\Delta x = \int_\alpha^\beta f(x)\,dx \\
\lim_{N\to\infty} \mathbf{x}^T \mathbf{y}\,\Delta x &= \lim_{N\to\infty} \sum_{n=1}^{N} x_n\,f(x_n)\,\Delta x = \int_\alpha^\beta x\,f(x)\,dx
\end{aligned}$$

We conclude that in the continuous case the normal equations become:

$$\begin{bmatrix} \int_\alpha^\beta 1\,dx & \int_\alpha^\beta x\,dx \\ \int_\alpha^\beta x\,dx & \int_\alpha^\beta x^2\,dx \end{bmatrix} \begin{bmatrix} b \\ m \end{bmatrix} = \begin{bmatrix} \int_\alpha^\beta f(x)\,dx \\ \int_\alpha^\beta x\,f(x)\,dx \end{bmatrix}. \tag{20}$$

As an illustration, let $\alpha = 0$, $\beta = \frac{\pi}{2}$ and $f = \sin(x)$. Equation (20) becomes:

$$\begin{bmatrix} \frac{\pi}{2} & \frac{\pi^2}{8} \\ \frac{\pi^2}{8} & \frac{\pi^3}{24} \end{bmatrix} \begin{bmatrix} b \\ m \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

From which the best linear fit for the sine function on the interval $[0, \frac{\pi}{2}]$ is found to be:

$$y = \frac{8}{\pi} - \frac{24}{\pi^2} + \left(\frac{96}{\pi^3} - \frac{24}{\pi^2}\right) x.$$

Figure below 5 shows that the linear fit is reasonably good.

Polynomial regression

Suppose we would like to model the data with a quadratic relation:

$$y = a + b\,x + c\,x^2.$$

Finding the vector of coefficients

$$\mathbf{u} = \begin{bmatrix} a \\ b \\ c \end{bmatrix}$$

requires that we solve the following 3-by-N system:

$$\left[\mathbf{1} \mid \mathbf{x} \mid \mathbf{x}^2\right] \mathbf{u} = \mathbf{y}.$$

Here by $\mathbf{x}^2$ we denote the vector of squares:

$$\mathbf{x}^2 = \begin{bmatrix} x_1^2 \\ x_2^2 \\ \vdots \\ x_N^2 \end{bmatrix}$$

This time solving the normal equations leads to:

$$\begin{bmatrix} a \\ b \\ c \end{bmatrix} = \begin{bmatrix} \mathbf{1}^T\mathbf{1} & \mathbf{1}^T\mathbf{x} & \mathbf{1}^T\mathbf{x}^2 \\ \mathbf{x}^T\mathbf{1} & \mathbf{x}^T\mathbf{x} & \mathbf{x}^T\mathbf{x}^2 \\ \mathbf{x}^{2,T}\mathbf{1} & \mathbf{x}^{2,T}\mathbf{x} & \mathbf{x}^{2,T}\mathbf{x}^2 \end{bmatrix}^{-1} \begin{bmatrix} \mathbf{1}^T\mathbf{y} \\ \mathbf{x}^T\mathbf{y} \\ \mathbf{x}^{2,T}\mathbf{y} \end{bmatrix}.$$

Fitting higher order polynomials is completely analogous.

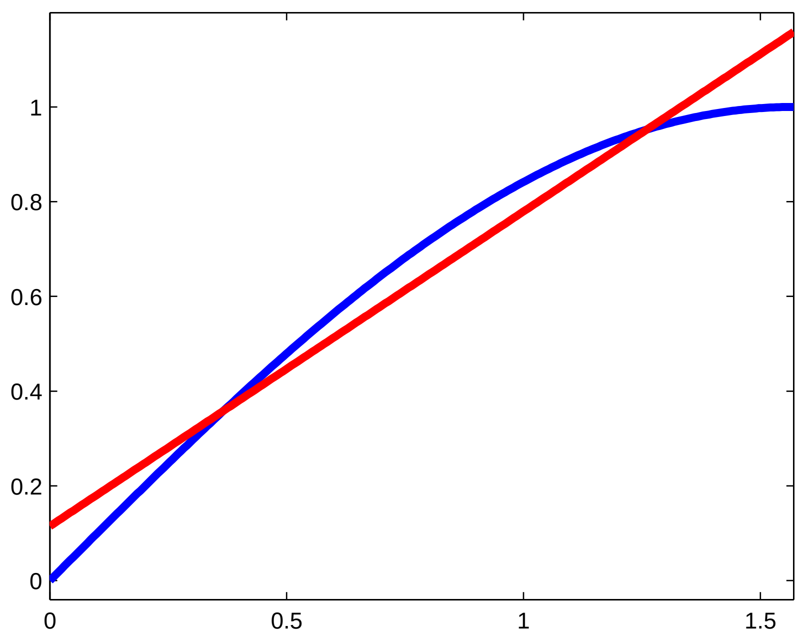


Figure 5: Continuous linear regression

Exercises

1. Use the following code to generate (noisy) data `x` and `y`:

```
x = linspace(0,2*pi)';
a = 2; b = -1;
y = a*cos(x) + b*sin(x) + .1*randn(size(x));
```

   Then use least squares to estimate `a` and `b`. Present a plot showing the best fit accompanied with the code that implements least squares fitting.

2. The following data is modeled by the exponential relation: $y = a\, e^{k\, x}$; the first

column are the values of x while the second column is the corresponding values of y:

0	1.3938
0.2000	1.1084
0.4000	0.8505
0.6000	0.9341
0.8000	0.5149
1.0000	0.5802

Use least squares to estimate k and a.

3. Find the best cubic fit $y = a_0 + a_1\,x + a_2\,x^2 + a_3\,x^3$ for the data in the previous problem. Present a plot accompanied with code.

Extra Credit: Find the *continuous* quadratic approximation for the sine function on $[0, \frac{\pi}{2}]$ and illustrate it with a plot similar to Figure 5.