Curve fitting: least squares methods

Curve fitting is a problem that arises very frequently in science and engineering.
Suppose that from some experiment n observations, i.e. values of a dependent variable y measured at specified values of an independent variable x, have been collected. In other words, we have a set of n data points

$$(x_1, y_1),\ (x_2, y_2),\ (x_3, y_3),\ \ldots, (x_n, y_n)$$

The first step in constructing a mathematical model of the underlying physical process is to plot these data points and postulate a function form $f(x)$ to describe the general trend in the data.
Some simple functions commonly used to fit data are:

- straight line: $f(x) = ax + b$
- parabola: $f(x) = ax^2 + bx + c$
- polynomial: $f(x) = a_m x^m + a_{m-1}x^{m-1} + \cdots + a_2 x^2 + a_1 x + a_0$ (includes the previous two cases)
- exponential: $f(x) = c\exp(ax)$
- Gaussian, e.g. $f(x) = c\exp(-bx^2)$
- sine or cosine, e.g. $f(x) = a\cos(bx) + c$

The coefficients a, b, c etc. in the formula of $f(x)$ are *parameters* that we can adjust.

Of course, since there are inevitable measurement errors in the data, in general we would not expect $f(x)$ to fit the data perfectly. The best we can do is try to choose the parameters of the function so as to *minimize* the fitting *error*—the distance between the data values y_i and the y-values $f(x_i)$ on the fitted curve. The *residuals* are defined to be the differences between the observed y-values and those given by the fitted curve at the x-values where the data was originally collected:

$$r_i = y_i - f(x_i) \quad \text{for } i = 1, 2, \ldots n.$$

The length-n array of r_i values is called the residual vector $\mathbf{r}$, and we aim to minimize the *norm* of this vector. Recall from last lecture the three vector norms that are most widely used in applications; they give rise to the following three standard error measures:

- Average error: $E_1(f) = \dfrac{1}{n}\|\mathbf{r}\|_1 = \dfrac{1}{n}\sum_{i=1}^{n}|r_i| = \sum_{i=1}^{n}|y_i - f(x_i)|$
- Root-mean-square error: $E_2(f) = \dfrac{1}{\sqrt{n}}\|\mathbf{r}\|_2 = \left(\dfrac{1}{n}\sum_{i=1}^{n}|r_i|^2\right)^{1/2} = \sqrt{\dfrac{1}{n}\sum_{i=1}^{n}\big(y_i - f(x_i)\big)^2}$
- Maximum error: $E_\infty(F) = \|\mathbf{r}\|_\infty = \max\limits_{i=1,2,\ldots,n}|r_i| = \max\limits_{i=1,2,\ldots,n}|y_i - f(x_i)|$

Suppose that the formula of f contains the parameters $\alpha_1, \alpha_2, \ldots, \alpha_K$. Then the error quantity $E(f)$ that we wish to minimize will depend on these parameters, so we write it as $E(\alpha_1, \alpha_2, \ldots, \alpha_K)$. From multivariable calculus we know that to minimize $E(\alpha_1, \alpha_2, \ldots, \alpha_K)$, we should solve the K equations

$$\left.\begin{aligned} \frac{\partial E}{\partial \alpha_1} &= 0 \\ \frac{\partial E}{\partial \alpha_2} &= 0 \\ &\vdots \\ \frac{\partial E}{\partial \alpha_K} &= 0 \end{aligned}\right\} \quad \text{for } \alpha_1, \alpha_2, \ldots, \alpha_K$$

If we choose the parameters of f in order to minimize the root-mean-square error, then the process is called "least squares fitting".

Minimizing the root-mean-square error $E_2(f) = \sqrt{\frac{1}{n}\sum_{i=1}^{n}\big(y_i - f(x_i)\big)^2}$ is equivalent to minimizing

$$\|\mathbf{r}\|_2^2 = \sum_{i=1}^{n}\big(y_i - f(x_i)\big)^2$$

Write

$$E(\alpha_1, \alpha_2, \ldots, \alpha_K) = \sum_{i=1}^{n}\big(y_i - f(x_i)\big)^2$$

Then

$$\frac{\partial E}{\partial \alpha_k} = \sum_{i=1}^{n} 2\,\big(y_i - f(x_i)\big)\cdot\left(-\frac{\partial f(x_i)}{\partial \alpha_k}\right),$$

so we need to solve the equations

$$(\star) \qquad \sum_{i=1}^{n}\big(f(x_i) - y_i\big)\,\frac{\partial f(x_i)}{\partial \alpha_k} = 0, \qquad k = 1, 2, \ldots, K$$

When $f(x)$ is a polynomial of degree m (with $m+1$ coefficients), $(\star)$ can be written as a *linear* system $M\boldsymbol{\alpha} = \boldsymbol{\beta}$ where

$$M = \begin{pmatrix} \sum_{i=1}^{n} x_i^{2m} & \sum_{i=1}^{n} x_i^{2m-1} & \cdots & \sum_{i=1}^{n} x_i^{m} \\ \sum_{i=1}^{n} x_i^{2m-1} & \sum_{i=1}^{n} x_i^{2m-2} & \cdots & \sum_{i=1}^{n} x_i^{m-1} \\ \vdots & \vdots & \ddots & \vdots \\ \sum_{i=1}^{n} x_i^{m} & \sum_{i=1}^{n} x_i^{m-1} & \cdots & n \end{pmatrix}, \qquad \boldsymbol{\beta} = \begin{pmatrix} \sum_{i=1}^{n} x_i^{m} y_i \\ \sum_{i=1}^{n} x_i^{m-1} y_i \\ \vdots \\ \sum_{i=1}^{n} y_i \end{pmatrix}$$

and $\boldsymbol{\alpha}$ is the array of parameters (i.e. coefficients of the polynomial) that we solve for.