Experimental data and theoretical curves: Consider a scientific experiment when collected data relate two variables, say x and y. Assume that a theoretical dependence is known but experimental data are not exactly on the theoretical curve due to measurement errors. The problem is to estimate parameters of the theoretical curve from the set of experimental data points.

Example: Consider a spring suspended from a ceiling. Let x be a spring deformation and Y be a spring force. The theory (Hooke's law) predicts a straight line:

$$y = ax + b,$$

where (a, b) are parameters. There experimental measurements gave three points $(9, 33)$; $(12, 43)$; and $(19, 61)$. The problem is to estimate parameters (a, b) from the three points.

Least squares approximations

Consider a total square error in the measurement of y for a fixed value of x:

$$E = (y_1 - ax_1 - b)^2 + ... + (y_n - ax_n - b)^2$$

and find the values of (a, b) such that the values of E are minimal.

Let us introduce vectors and matrices

$$\mathbf{y} = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix}, \qquad \mathbf{z} = \begin{bmatrix} a \\ b \end{bmatrix}, \qquad M = \begin{bmatrix} x_1 & 1 \\ \vdots & \vdots \\ x_n & 1 \end{bmatrix}$$

Then,

$$E = \|\mathbf{y} - M\mathbf{z}\|^2$$

Geometric interpretation for $n = 3$

Let $\mathbf{v} = M\mathbf{z}$ be a three-dimensional vector in a space. It is clear that

$$\mathbf{v} = a \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} + b \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} = a\mathbf{x} + b\mathbf{1},$$

which defines a plane that contains two vectors $\mathbf{x}$ and $\mathbf{1}$. The equation for the plane $\mathbf{v} = M\mathbf{z}$ is

$$(x_2 - x_3)v_1 + (x_3 - x_1)v_2 + (x_1 - x_2)v_3 = 0.$$

Example:

$$\mathbf{x} = \begin{bmatrix} 9 \\ 12 \\ 19 \end{bmatrix}, \qquad \mathbf{y} = \begin{bmatrix} 33 \\ 43 \\ 61 \end{bmatrix}$$

Solution in the case $n = 3$:

Find the vector $\mathbf{v}_0$ in the plane $\mathbf{v} = M\mathbf{z}$, such that $\|\mathbf{y} - \mathbf{v}_0\|$ is a minimal distance from $\mathbf{y}$ to the point $\mathbf{v}_0$ in the plane. Then, $M\mathbf{z}_0 = \mathbf{v}_0$ gives the parameters (a, b) in the vector $\mathbf{z}_0$.

Then,

$$(M\mathbf{z}) \cdot (\mathbf{y} - M\mathbf{z}_0) = 0,$$

such that

$$\mathbf{z} \cdot \left(M^T\mathbf{y} - M^T M\mathbf{z}_0\right) = 0,$$

such that

$$M^T M\mathbf{z}_0 = M^T\mathbf{y}$$

Since $M^T M$ is a 2×2 matrix and $M^T\mathbf{y}$ is a 2×1 matrix, the linear system above is square. This system, called the normal equation for least square approximation, has a unique solution if at least two values from (x_1, x_2, x_3) are distinct.

Example:

$$M = \begin{bmatrix} 9 & 1 \\ 12 & 1 \\ 19 & 1 \end{bmatrix}, \qquad \mathbf{y} = \begin{bmatrix} 33 \\ 43 \\ 61 \end{bmatrix}$$

Extensions:

- The same normal equation is valid for any $n \geq 3$ (see calculus)
- A closed form expression can be obtained for parameters a and b of the linear function $y = ax + b$ (see statistics)
- A similar problem and the normal equation can be obtained for polynomial least squares approximation, when $y = c_0 + c_1 + ... + c_m x^m$ and $m < n$ (see numerical methods)
- The problem of polynomial least squares approximation becomes the problem of polynomial interpolation, when $m = n$ (see Section 3.4 of the main text).