Chapter XXIII
The Method of Least Squares

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ABSTRACT

The method of least squares is a geometric principle of curve fitting. The unknown parameters of a function are calculated in such a way that the sum of squared differences between function values and measurements gets minimal. Examples are given for a linear and a nonlinear curve fitting problem. Consequences of model linearizations are explained.

INTRODUCTION

Model fit is a general task in data mining. It is a basic component of general problems like optimization, statistical data evaluation, data imaging, and so forth. The method of least squares (MLS) is a widely used principle of geometric character to fit a model to given data. The method goes back to the work of C. F. Gauss and A. M. Legendre.

Suppositions concern merely the model to be adapted: The data must be numbers. Many data-related optimization criteria are extensions of the classic least squares method. Statistical parameter estimation and the method of least squares are closely connected in linear statistical models (e.g., the Gauss-Markov theorem in mathematical statistics).

The method of least squares is explained at its simplest examples in the following paragraphs. In addition, difficulties occurring in the model linearization are demonstrated.

The so-called method of least squares is a universal method for the calculation of the parameters $\alpha_1, \ldots, \alpha_k$ of a model function $y = f_{\alpha_1,\ldots,\alpha_1}(x)$, which in the best possible way goes through a given set of points (x_i, y_i), i = 1, ..., n. The basic idea is to minimize the sum of the squared distances between the function $f_{\alpha_1,\ldots,\alpha_k}(x_i)$ and the measurement y_i:

$$g(\alpha_1,\ldots,\alpha_k) = \sum_{i=1}^{n} \left(f_{\alpha_1,\ldots,\alpha_k}(x_i) - y_i \right)^2 .$$

For that, the equations

$$\frac{\partial g(\alpha_1,...,\alpha_k)}{\partial \alpha_j} = 0\,,\ \text{j = 1, ..., k}$$

formulate the necessary conditions. These k equations are the system for the determination of the unknown parameters α_1, ..., α_k. The solutions must still be examined to determine whether they satisfy the sufficient conditions for a minimum.

EXAMPLE 1

A linear function $y = f(x) = ax + b$ shall be fitted to the set of points. The function:

$$g(a,b) = \sum_{i=1}^{n} \left((ax_i + b) - y_i\right)^2$$

depends on the unknown a and b and shall be minimized.

The necessary conditions for the existence of a minimum are:

$$\frac{\partial g(a,b)}{\partial a} = \sum_{i=1}^{n} 2\left((ax_i + b) - y_i\right)x_i = 0 \quad \text{and}$$

$$\frac{\partial g(a,b)}{\partial b} = \sum_{i=1}^{n} 2\left((ax_i + b) - y_i\right) = 0\,.$$

The conditions lead to a linear system of equations:

$$(I)\quad \left(\sum_{i=1}^{n} x_i^{\,2}\right)a + \left(\sum_{i=1}^{n} x_i\right)b = \left(\sum_{i=1}^{n} x_i y_i\right)$$

$$(II)\quad \left(\sum_{i=1}^{n} x_i\right)a + nb = \left(\sum_{i=1}^{n} y_i\right)\,.$$

The solution (a_0, b_0) of this system of equations is uniquely determined in case the determinant of the coefficients of the linear system is different from zero.

Unfortunately, there are only a few model functions that lead to such an easily solvable system of equations. Nonlinear systems of equations result mostly. In these cases, one must be content with iterative approximate solutions.

EXAMPLE 2

The model function $y = f(x) = c \cdot \exp(dx)$ leads to nonlinear equations for the determination of the parameters c and d. It is calculated from:

$$g_1(c,d) = \sum_{i=1}^{n} \left((c \cdot \exp(dx_i)) - y_i\right)^2 \qquad (*),$$

$$\frac{\partial g_1(c,d)}{\partial c} = \sum_{i=1}^{n} 2\left((c \cdot \exp(dx_i)) - y_i\right)\exp(dx_i) = 0\,, \text{ and}$$

$$\frac{\partial g_1(c,d)}{\partial d} = \sum_{i=1}^{n} 2\left((c \cdot \exp(dx_i)) - y_i\right)\left(c \cdot \exp(dx_i)\right)x_i = 0\,.$$

The resulting system of nonlinear equations follows:

$$(I)\quad \left(\sum_{i=1}^{n} \left(\exp(dx_i)\right)^2\right)c - \sum_{i=1}^{n} y_i \exp(dx_i) = 0$$

$$(II)\quad \left(\sum_{i=1}^{n} \left(\exp(dx_i)\right)^2\right)c^2 - \left(\sum_{i=1}^{n} x_i y_i \exp(dx_i)\right)c = 0$$

One can get the solution using a numeric approximation method, for example, the Gauss-Newton method. Most iterative procedures need a start value (c_s, d_s). This start value shall be contained in a close neighbourhood of the solution. However, this is not a sufficient condition for the convergence of the algorithm toward the desired solution.