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 \( y = f_{\alpha_1, \ldots, \alpha_k}(x) \), which in the best possible way goes through a given set of points \((x_i, y_i)\), \(i = 1, \ldots, n\). 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
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