Nonlinear Regression for Dependent Variables

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Nonlinear regression methods can be used to fit functions for two related variables where both variables are subject to error. A computer program for nonlinear estimation described previously has been modified to fit such functions for a given set of data. A numerical example is provided for a second-degree equation in x and y. A closer fit to an observed set of data is possible if the error structure for the variables is specified. KEY WORDS: curve fitting, regression analysis.

INTRODUCTION

Curve fitting by nonlinear regression has become a familiar tool in quantitative geology. Given observations on two related variables x and y, it is possible to fit such data to nearly any specified function. As in linear regression, however, it may happen that both x and y are subject to error. The classical least-squares approach assumes the error to be associated with either x or y. Moreover, the error in both x and y may differ from one observation to the next. Clearly, in these instances, a different form of curve fitting is demanded.

The problem of least-squares curve fitting of a function to a set of data \( (x_i, y_i), 1 \leq i \leq n, \) when \( x_i \) and \( y_i \) are both subject to error specified by weights \( \omega(x_i) \) and \( \omega(y_i) \), in fact, was described and reviewed some years ago by Deming (1943). Deming defined the best-fitting curve as that given by minimizing the sum in the equation:

\[
S = \sum_i \left[ \omega(x_i)(x_i - x_i^*)^2 + \omega(y_i)(y_i - y_i^*)^2 \right] \quad (1)
\]

where \( x_i, y_i \) are the observations, \( x_i^*, y_i^* \) are calculated values which lie on the best-fitting curve, and \( \omega(x_i), \omega(y_i) \) are the weights for \( x_i, y_i \) specified for the different observations. This work was reviewed by York (1966, 1967, 1968) who has developed subsequently a method for the situation where the function to be fitted is a straight line. Similar approaches to fitting a straight line have been described by McIntyre and others (1966), Williamson (1968), and

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A statistical treatment of linear regression when both variables are subject to error can be found in Kendall and Stuart (1961, Chap. 29). More recently, statistical articles by Richardson and Wu (1970) and Halperin and Gurian (1971) have appeared. A method for minimizing (1) to any given accuracy for a polynomial of specified degree has been described by O'Neill, Sinclair, and Smith (1969) and since has been improved upon by Grossman (1971). Thus, the problem has not been ignored. It is, however, a problem which is not readily handled by those engaged in analyzing data.

The purpose of this paper is to show how a computer program for nonlinear regression presently available to geologists (McCammon, 1969) can be modified to fit any function by least squares when both x and y are subject to error. In this paper, only the modifications necessary in the program are presented, and therefore the reader should refer to the original program for the details of operation. Also, the reader is referred to Draper and Smith (1967, Chap. 10) for a general discussion of the methods used in nonlinear estimation.

NONLINEAR FUNCTION EVALUATION

Suppose we have a function

\[ y = f(x; \theta) \]  

(2)

in which the unknown parameter vector \( \theta \) is nonlinear with respect to \( x \) and \( y \), and suppose we wish to estimate \( \theta \) for a given set of observations in \( x \) and \( y \) where both \( x \) and \( y \) are subject to error. We assume that the data do not fit the function exactly and we proceed by estimating \( \theta \) by least-squares methods. If the error is assumed to be in \( x \) alone, the usual method would involve expanding (2) in a Taylor series out to the first-order terms which represent the partial derivatives of \( y \) with respect to each \( \theta_i \), solving the resulting system of linear equations for the corrections to the parameters and, finally, applying the corrections in a manner which would reduce the total error sum of squares. It is an iterative process which would converge in most situations to the estimates of the parameters which would yield the minimum error sum of squares. When the error is assumed in both \( x \) and \( y \), we can proceed in a similar manner the difference being that the corrections to the parameters involve \( x \) and \( y \) jointly. For example, consider the situation illustrated in Figure 1a for the situation where the error in \( x \) and \( y \) is assumed to be equal. Referring to (1), this implies \( \omega(x_i) = \omega(y_j) \), and without loss of generality we assume \( \omega(x_i) = \omega(y_j) = 1 \) and therefore the function to be minimized is the squared perpendicular distance from the observation point to the point which lies along the function to be fitted. To evaluate (1) for a given estimate \( \theta^* \), we