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Error analysis of the parameters of a least-squares determined curve when both variables have uncertainties

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Abstract. By means of the least-squares canonical equations and the error propagation law only, the uncertainties in the parameters of the functional expression used to fit a set of experimental points, with both coordinates subject to error, are analytically determined.

1. Introduction

Recently [1, 2] Neri *et al*, using a procedure based only on the least-squares principle and on the error propagation formula, determined the parameters of a fitting curve with both observables having uncertainties. The number of 'exact' figures of the parameters is limited exclusively by the computer precision. However, not all the calculated digits are significant, because the errors affecting the experimental points obviously propagate to the parameters of the model.

The error analysis of the parameters determined in least-squares fits has been discussed recently by Burrell [3], who also used a new procedure to calculate the errors themselves when the regression curve is non-linear and error-affected in only one coordinate. In this paper, this calculation method has been extended to the general case of curves involving errors in both variables. The obtained expressions have been written in detail for the linear regression, and they have been applied to a practical example.

2. Determination of the parameters

The calculation starts from the results obtained by Neri *et al* [1, 2] which, for convenience, are recalled in the following. Let the observations consist of n pairs (x_i, y_i) and let s_{x_i} be the error in x_i and s_{y_i} the error in y_i. They are to be fitted to the model

$$y=f(x;\, a_1, \ldots, a_j, \ldots, a_m) \tag{1}$$

where the a_j quantities are the parameters to be determined.

The vertical distance between the ith point and the curve (1) at the abscissa x_i is

$$d_i=y_i-f(x_i;\, a_1, \ldots, a_j \ldots, a_m) \tag{2}$$

and

$$s_i^2=s_{y_i}^2+\left(\frac{\partial f}{\partial x_i}\, s_{x_i}\right)^2 \tag{3}$$

is the variance of d_i. The function to be minimized is

$$S(a_1, \ldots, a_j, \ldots, a_m)=\sum_{i=1}^{n} w_i d_i^2 \tag{4}$$

where $w_i=(1/s_i^2)$ is the weight of the ith observation. The least-squares canonical equations are

$$\frac{\partial S}{\partial a_j}=0 \qquad j=1, \ldots, m. \tag{5}$$

The above system of m equations can be solved with standard numeric methods implemented easily into a computer program. The parameters a_j are obtained with an accuracy limited only by the computer precision.

3. Evaluation of the uncertainties in the parameters

3.1. General case

If s_{x_i} and s_{y_i} with $i=1, \ldots, n$ are small, completely independent and random, the variances of the a_j quantities are calculated with the classical error propagation law:

$$s_{a_j}^2=\sum_{i=1}^{n}\left[\left(\frac{\partial a_j}{\partial x_i}\, s_{x_i}\right)^2+\left(\frac{\partial a_j}{\partial y_i}\, s_{y_i}\right)^2\right] \qquad j=1, \ldots, m. \tag{6}$$

In order to obtain the $2mn$ derivatives $\partial a_j/\partial x_i$ and $\partial a_j/\partial y_i$, equations (5) are differentiated with respect to x and y at each of the experimental points, i.e. at (x_i, y_i)

the following equations are obtained

$$\sum_{k=1}^{m}\left[\left(\frac{\partial^2 S}{\partial a_j \partial a_k}\right)\frac{\partial a_k}{\partial x_i}\right]+\frac{\partial^2 S}{\partial a_j \partial x_i}=0 \qquad j=1,\ldots,m \quad (7a)$$

$$\sum_{k=1}^{m}\left[\left(\frac{\partial^2 S}{\partial a_j \partial a_k}\right)\frac{\partial a_k}{\partial y_i}\right]+\frac{\partial^2 S}{\partial a_j \partial y_i}=0 \qquad j=1,\ldots,m. \quad (7b)$$

This is a linear system in the $2m$ unknown derivatives $\partial a_k/\partial x_i$ and $\partial a_k/\partial y_i$, with $k=1,\ldots,m$. The constants

$$\frac{\partial^2 S}{\partial a_j \partial a_k}, \qquad \frac{\partial^2 S}{\partial a_j \partial x_i}, \qquad \frac{\partial^2 S}{\partial a_j \partial y_i}$$

with $j, k=1,\ldots,m$ and $i=1,\ldots,n$, are the second derivatives of the expression (4) at the point (x_i, y_i).

From a general point of view, this reasoning cannot be developed any more because, to calculate these derivatives, the fitting curve (1) must be known explicitly. To show the method in detail, the important case of linear regression is now worked out.

3.2. The linear regression

Equations (1), (2) and (3) become

$$y=a+bx \qquad (8)$$

$$d_i=y_i-a-bx_i \qquad (9)$$

$$s_i^2=(s_{y_i})^2+(bs_{x_i})^2. \qquad (10)$$

Let

$$x_i+bd_iw_is_{x_i}^2=F_i$$

$$-\sum_{i=1}^{n} w_i=A$$

$$-\sum_{i=1}^{n} w_iF_i=B$$

$$\sum_{i=1}^{n}\left[(s_{x_i}d_iw_i)^2-w_iF_i^2\right]=C.$$

Carrying out some simple mathematical calculations we obtain the solution of the system (7) for the ith experimental point:

$$\frac{\partial a}{\partial x_i}=\frac{d_i}{AC-B^2}\left[bC+B(d_i-bF_i)\right] \qquad (11a)$$

$$\frac{\partial a}{\partial y_i}=\frac{d_i}{AC-B^2}(BF_i-C) \qquad (11b)$$

$$\frac{\partial b}{\partial x_i}=\frac{-d_i}{AC-B^2}\left[bB+A(d_i-bF_i)\right] \qquad (11c)$$

$$\frac{\partial b}{\partial y_i}=\frac{d_i}{AC-B^2}(B-AF_i). \qquad (11d)$$

Substituting these results in the sums (6), the analytical expressions of the uncertainties s_a and s_b are obtained.

3.3. Numerical example

Neri *et al* [1, 2], as a practical example, used Pearson's data [4] with York's [5] weights w_{x_i} and w_{y_i} to calculate the parameters a and b of the linear fit (8). They found $a=5.479\,910\,219\,48$ and $b=-0.480\,553\,402\,6$. In order to calculate the uncertainties in a and b with the formulae given by equation (6), Pearson's data [4], with the errors calculated from York's weights [5] (as indicated in table 1) are used. A double precision calculation has been performed on an IBM PC, using a BASIC program; in a few seconds the values of the parameter uncertainties are obtained: $s_a=0.10$ and $s_b=0.024$.

Table 1. Pearson's data [4] and errors calculated with York's weights [5].

x_i	$s_{x_i}=w_{x_i}^{-1/2}$	y_i	$s_{y_i}=w_{y_i}^{-1/2}$
0.0	$1000^{-1/2}$	5.9	1.0
0.9	$1000^{-1/2}$	5.4	$1.8^{-1/2}$
1.8	$500^{-1/2}$	4.4	$4^{-1/2}$
2.6	$800^{-1/2}$	4.6	$8^{-1/2}$
3.3	$200^{-1/2}$	3.5	$20^{-1/2}$
4.4	$80^{-1/2}$	3.7	$20^{-1/2}$
5.2	$60^{-1/2}$	2.8	$70^{-1/2}$
6.1	$20^{-1/2}$	2.8	$70^{-1/2}$
6.5	$1.8^{-1/2}$	2.4	$100^{-1/2}$
7.4	1.0	1.5	$500^{-1/2}$

This result shows that the number of significant digits of a and b values is small. However, the importance of calculating the parameters with the maximum possible number of 'exact' figures is evident: it, in fact, directly influences the calculations of the parameter errors, as shown by the formulae deduced above.

4. Conclusions

This paper describes a method for estimating the uncertainties of the parameters of a theoretical model, taking into consideration the errors affecting both coordinates of the experimental points. It has the following features:

(i) it requires only the least-squares formula and the error propagation law to be used;

(ii) the errors can be analytically expressed, for many kinds of fitting curve: the mathematical concepts involved are common, but the calculations that must be carried out may be laborious;

(iii) the whole mathematical procedure is easily translated into a program that could be run on a common personal computer.

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