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1993 Meas. Sci. Technol. 4 635

(http://iopscience.iop.org/0957-0233/4/5/016)

Meas. Sci. Technol. 4 (1993) 635–636. Printed in the UK

RAPID COMMUNICATION

Parameters' variances of a least-squares determined straight line with errors in both coordinates

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Received 23 December 1992, accepted for publication 15 February 1993

Abstract. A year ago, a paper dealing with parameters' errors of a least-squares determined curve was published by Cecchi. Very recently, Kalantar correctly pointed out that the results quoted by Cecchi for the variance estimates of a straight-line fit do not agree with those previously reported by other authors. Nevertheless, for straight-line fits the formalism discussed by Cecchi is essentially correct. In the present communication, complete agreement between results is achieved after some detailed calculations.

To facilitate the discussion, the formalism followed by Cecchi [1] will be briefly outlined. To obtain the parameters' variances, Cecchi starts from the least-squares canonical equations and from the standard error propagation law. The least-squares canonical equations ([1] equation (5)) are

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

where S is the weighted sum of squared residuals and a_j are the m parameters to be determined. For the special case of a straight line fitting ($y = a + bx$), S reduces to

$$S = \sum_{i=1}^{n} \frac{(y_i - a - bx_i)^2}{(s_{y_i})^2 + (bs_{x_i})^2} \tag{2}$$

where n is the number of measured pairs (x_i, y_i), each one having uncertainties denoted by (s_{x_i}, s_{y_i}) respectively. The standard error propagation law, applied under common assumptions (small, independent and random errors), leads to the following expression for the variance of a

$$s_a^2 = \sum_{i=1}^{n} \left[\left(\frac{\partial a}{\partial x_i} s_{x_i} \right)^2 + \left(\frac{\partial a}{\partial y_i} s_{y_i} \right)^2 \right] \tag{3}$$

and a similar expression holds for s_b^2.

The next step for evaluating s_a is to obtain the partial derivatives appearing in (3). Following Cecchi, differentiating equation (1) with respect to x at each (x_i, y_i), the system of equations quoted below is obtained for the special case we are interested in

$$\frac{\partial^2 S}{\partial a^2} \frac{\partial a}{\partial x_i} + \frac{\partial^2 S}{\partial b \partial a} \frac{\partial b}{\partial x_i} = -\frac{\partial^2 S}{\partial x_i \partial a} \qquad i = 1, \ldots, n \tag{4a}$$

$$\frac{\partial^2 S}{\partial a \partial b} \frac{\partial a}{\partial x_i} + \frac{\partial^2 S}{\partial b^2} \frac{\partial b}{\partial x_i} = -\frac{\partial^2 S}{\partial x_i \partial b} \qquad i = 1, \ldots, n. \tag{4b}$$

The unknowns $\partial a/\partial x_i$ and $\partial b/\partial x_i$ can be easily obtained by solving the system of equations (4). These are an n set of a 2×2 inhomogeneous linear system, whose coefficients are the second derivatives of S, which can be evaluated from (2). By differentiating equation (1), now with respect to y, a system completely analogous to (4) is obtained. This allows the calculation of $\partial a/\partial y_i$ and $\partial b/\partial y_i$.

The second derivatives appearing in the two systems are

$$\frac{\partial^2 S}{\partial a^2} = \sum_{i=1}^{n} w_i = -A \tag{5a}$$

$$\frac{\partial^2 S}{\partial a \partial b} = \frac{\partial^2 S}{\partial b \partial a} = \sum_{i=1}^{n} w_i F_i' = -B \tag{5b}$$

$$\frac{\partial^2 S}{\partial b^2} = \sum_{i=1}^{n} [w_i F_i'^2 - d_i^2 w_i^2 s_{x_i}^2] = -C \tag{5c}$$

$$\frac{\partial^2 S}{\partial x_i \partial a} = bw_i \tag{5d}$$

$$\frac{\partial^2 S}{\partial x_i \partial b} = -w_i(d_i - bF_i') \tag{5e}$$

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$$\frac{\partial^2 S}{\partial y_i \partial a} = -w_i \tag{5f}$$

$$\frac{\partial^2 S}{\partial y_i \partial b} = -w_i F_i' \tag{5g}$$

where an overall factor 2 was cancelled throughout because it does not affect either the solution of system (4) or that of its analogy for the y variables, and $d_i = y_i - a - bx_i$, $w_i = 1/(s_{y_i}^2 + (bs_{x_i})^2)$, $F_i' = x_i + 2bd_i w_i s_{x_i}^2$. Using expressions (5) the following results are obtained

$$\frac{\partial a}{\partial x_i} = w_i[bC + B(d_i - bF_i')]/\Delta \tag{6a}$$

$$\frac{\partial a}{\partial y_i} = w_i[BF_i' - C]/\Delta \tag{6b}$$

$$\frac{\partial b}{\partial x_i} = -w_i[bB + A(d_i - bF_i']/\Delta \tag{6c}$$

$$\frac{\partial b}{\partial y_i} = w_i[B - AF_i']/\Delta \tag{6d}$$

where $\Delta = AC - B^2$.

For comparison purposes, the same notation used by Cecchi was kept, with the exception of F_i', which differs from Cecchi's F_i by a factor of 2 in the second term. Note, however, that our set of equations (6) present other differences from the equivalent set (equations (11)) given by Cecchi.

Applying expressions (6) to Pearson data with York weights [2] (taking $a = 5.47991$ and $b = -0.48053$ from [1] or [3], for instance) one can easily find $s_a = 0.291934$ and $s_b = 0.057617$. These results are in complete agreement with those reported in the literature [3–5].

It is worthwhile mentioning that formulae (5) (or, equivalently, results (6)) lead to the so-called recurrence y/x when x is (or is considered to be) error free, as one would expect. This feature is not fulfilled by the results quoted in reference [1]. It also must be mentioned that the agreement found between the results obtained following the former distinct analytical approaches (those of [3, 4], the Monte Carlo method mentioned by Kalantar, and that used by Cecchi) is highly satisfying. However we want to stress the fact that the method of Cecchi discussed is more direct.

In conclusion, the method discussed by Cecchi leads to well known results for s_a and s_b, provided formulae (6) are used in expression (3) and its analogy for s_b.

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