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Linear least-squares fits with errors in both coordinates. II: Comments on parameter variances

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Corrected expressions for parameter variances in linear (straight-line) least-squares fits given in an earlier paper [B. C. Reed, Am. J. Phys. **57**, 642–646 (1989)] are presented and discussed. In addition, some simplifications to the solution given in that paper are presented, and some comments made as to the role of weighting.

I. INTRODUCTION

In the July 1989 edition of this Journal, this author published a paper concerning linear least-squares fits (that is, straight-line fits) in cases where there are errors in both coordinates[1] (hereafter Paper I). This paper drew attention to various numerical problems that can arise on attempting to implement the iterative solution to this problem originally put forth by York,[2] showed how one can circumvent these problems in practice, and made available a simple program for doing the computations on a PC. In addition, it was shown that York's solution is exact, and immune from problems encountered in attempts to modify conventional least-squares algorithms.[3–6] Since publication of this paper, many interested parties have written to the author with detailed accounts of their experiences with a variety of algorithms claiming to address this problem. These experiences are clearly converging on two conclusions: (i) the various algorithms *agree* as to the correct values of the slope m and intercept c, and (ii) there is considerable *disagreement* as to the *variances* σ_m and σ_c of the slope and intercept that various methods report. Unfortunately, the expressions quoted for σ_m and σ_c in Paper I have proven to be erroneous.

Given that users who have developed programs based on Paper I may not be aware of this shortcoming, a discussion giving a corrected treatment is needed. This is the main purpose of the present paper. However, this paper is also much more than an erratum, for a number of sundry issues are also addressed. Specifically, a simplification of the "least-squares cubic" is discussed, attention is drawn to some relevant references the author was not aware of at the time of writing Paper I, results for a commonly used example are discussed in detail, and some remarks on the role of weighting are made. Since the literature on this problem goes back over a century, the present paper will surely not be the last word on it; the purpose here is therefore not so much to introduce new results as to clarify old ones and to provide detailed examples against which others can check their own algorithms.

The outline of this paper is as follows. In Sec. II York's solution to the best-fit line is summarized and simplified. In Sec. III the difficulty with York's expression for σ_m is examined, and a corrected expression offered. Detailed results for a well-known example ("Pearson's data with York's weights") are presented, along with revised results for examples I and II in Paper I. Section IV discusses some sundry points. Explicit expressions for σ_m and σ_c appear in the Appendix.

II. YORK'S SOLUTION

Assume that one has a set of N data-point pairs (x_i, y_i); each point has its own weighting factors in x and y, designated as $W(x_i)$ and $W(y_i)$, which are conventionally assigned as the inverses of the squares of the measurement uncertainties (see Sec. IV). The problem is to find the values of the parameters m and c that yield the "best-fit" of the model equation

$$Y = mX + c \tag{1}$$

to the data, where X and Y are the *predicted* or *calculated* values of the data points, that is, their values after adjustment to the best-fit line. "Best-fit" is defined as minimizing the sum of the weighted squared residuals, commonly designated as **S**:

$$\mathbf{S} = \sum_{i=1}^{N} [W(x_i)(x_i - X_i)^2 + W(y_i)(y_i - Y_i)^2]. \tag{2}$$

[Note: In most textbook treatments, (X,Y) designates an observed point, and (x,y) the predicted. We reverse this notation to remain consistent with Paper I]. York[2] showed that the best-fit slope is given by solving the equation

$$f(m) = m^3 - 3\alpha m^2 + 3\beta m - \gamma = 0, \tag{3}$$

where

$$\alpha = \left(2\sum \frac{W_i^2 U_i V_i}{W(x_i)}\right)(3\delta)^{-1}, \tag{4}$$

$$\beta = \left(\sum \frac{W_i^2 V_i^2}{W(x_i)} - \sum W_i U_i^2\right)(3\delta)^{-1}, \tag{5}$$

$$\gamma = \left(-\sum W_i U_i V_i\right)\delta^{-1}, \tag{6}$$

with

$$\delta = \sum \frac{W_i^2 U_i^2}{W(x_i)}, \tag{7}$$

and where the "overall" or "effective" weight W_i for a given point is given by

$$W_i = \frac{W(x_i)W(y_i)}{m^2 W(y_i) + W(x_i)}. \tag{8}$$

In Eqs. (4)–(7), U_i and V_i are defined by

$$U_i = x_i - \langle x \rangle, \tag{9}$$

$$V_i = y_i - \langle y \rangle, \tag{10}$$

where $\langle x \rangle$ and $\langle y \rangle$ are given by

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$$\langle x\rangle = \sum W_i x_i \left(\sum W_i\right)^{-1} \tag{11}$$

and

$$\langle y\rangle = \sum W_i y_i \left(\sum W_i\right)^{-1}, \tag{12}$$

with all sums in Eqs. (4)–(12) running from 1 to N.

The central problem in finding the best-fit slope is then to find that root of Eq. (3) that minimizes **S**. York derived Eq. (3) by applying the method of undetermined multipliers to Eq. (1) and demanding that **S** be minimized; he termed Eq. (3) the "least-squares cubic" because it *appears* to have the form of a cubic equation in m. However, this is illusory as the "coefficients" α, β, and γ, are in fact all functions of m through the U_i, V_i, W_i, and δ. As discussed in Paper I, the simplest approach is to plot $f(m)$ vs m and examine the zeros.

Once m is known, the intercept c is given by

$$c = \langle y\rangle - m\langle x\rangle, \tag{13}$$

and the value of **S** can be expressed as

$$\mathbf{S} = \sum W_i (y_i - c - mx_i)^2 = \sum W_i (V_i - mU_i)^2. \tag{14}$$

York gives (erroneously) the variances in the slope and intercept as

$$\sigma_m^2 = \frac{\mathbf{S}}{N-2}\left(\sum W_i U_i^2\right)^{-1} \tag{15}$$

and

$$\sigma_c^2 = \left[\sum W_i x_i^2 \left(\sum W_i\right)^{-1}\right]\sigma_m^2. \tag{16}$$

Before examining the difficulties with these last two equations, we give a simpler formulation[7] of Eq. (3). Cancelling factors of 3 and clearing the factor of δ in the denominator of Eq. (3) yields, after some slight rearrangement

$$m^3\left(\sum \frac{W_i^2 U_i^2}{W(x_i)}\right) - 2m^2\left(\sum \frac{W_i^2 U_i V_i}{W(x_i)}\right) + m\left(\sum \frac{W_i^2 V_i^2}{W(x_i)}\right) = m\left(\sum W_i U_i^2\right) - \left(\sum W_i U_i V_i\right). \tag{17}$$

Now, Eq. (8) can be expressed as

$$\left(\frac{m^2}{W(x_i)} + \frac{1}{W(y_i)}\right) W_i = 1. \tag{18}$$

If Eq. (18) is inserted *within the sums* of the two terms on the right side of Eq. (17) (equivalent to multiplying through by 1), one finds after a little algebra that the "least-squares cubic" can be expressed, with no loss of generality, as a "least-squares quadratic":

$$m^2\left(\sum \frac{W_i^2 U_i V_i}{W(x_i)}\right) + m\sum W_i^2\left(\frac{U_i^2}{W(y_i)} - \frac{V_i^2}{W(x_i)}\right) - \left(\sum \frac{W_i^2 U_i V_i}{W(y_i)}\right) = 0, \tag{19}$$

which we write for convenience as

$$g(m) = Am^2 + Bm - C = 0. \tag{20}$$

Do not confuse the coefficient C defined in Eqs. (19) and (20) with the best-fit intercept c. Williamson,[8] who also investigated (and corrected) problems with York's parameter-variance expressions, has shown that the equation for the best-fit slope can actually be cast into a pseudo-*linear* form. In the present paper, however, I will stick to the form of Eq. (20) to effect a completely independent analysis from that of Williamson.

III. PARAMETER VARIANCES

A proper treatment of error propagation[9,10] shows that the variance in the slope of the best-fit line should be computed via

$$\sigma_m^2 = \frac{\mathbf{S}}{N-2}\sum_j \left[\frac{1}{W(y_j)}\left(\frac{\partial m}{\partial y_j}\right)^2 + \frac{1}{W(x_j)}\left(\frac{\partial m}{\partial x_j}\right)^2\right], \tag{21}$$

with a similar expression holding for σ_c^2 but with derivatives of c instead of m. In writing Eq. (21), we have assumed that weights are assigned in the usual inverse-square fashion: $W(x_i) = 1/\sigma^2(x_i)$ and $W(y_i) = 1/\sigma^2(y_i)$.

The factor of $S/(N-2)$ (the "external standard deviation") appearing in Eq. (21) deserves some comment. Some authors (Williamson) do not include this factor, although the majority of statistical authorities do so. An intuitive justification for its inclusion can be given as follows. Suppose that one optimistically assigns each of the $W(x_i)$ and $W(y_i)$ to be ten times greater than their true values. The derived slope, intercept, residuals, and values of $(\partial m/\partial x_j)$ and $(\partial m/\partial y_j)$ will all be unchanged, but the sum over j in Eq. (21) would come out ten times too small. On the intuitive belief that σ_m should remain invariant under such a scaling (after all, the *relative* weights of each point are unchanged), it becomes necessary to multiply by a factor (such as **S**) directly proportional to the weights. A further aspect of Eq. (21) is that inasmuch as it incorporates only the lowest-order terms in a Taylor-series expansion, it cannot be said to yield "exact" values of the parameter variances, contrary to what Williamson claims in his paper. [The values of m and c derived from Eqs. (3) or (20) are, however, exact in that no approximations have been made in their derivations].

The derivatives appearing in Eq. (21) are straightforward if tedious to compute. One proceeds by differentiating Eq. (20) with respect to x_j:

$$(2mA + B)\left(\frac{\partial m}{\partial x_j}\right) + m^2\left(\frac{\partial A}{\partial x_j}\right) + m\left(\frac{\partial B}{\partial x_j}\right) - \left(\frac{\partial C}{\partial x_j}\right) = 0, \tag{22}$$

and solving for $(\partial m/\partial x_j)$. Since A, B, and C are also all functions of m the result is a tedious calculation involving extensive application of the chain rule. The results are given explicitly in Appendix A, where it can be seen that they are considerably more complex than York's approximate expression, Eq. (15).

York appears to have derived Eq. (15) from Deming's treatment of this problem.[9] While it is difficult to say precisely from where York's expression derives, an informed speculation can be made from the form of his result. Comparing Eqs. (15) and (21) indicates that York has taken

$$\sum_j \left[\frac{1}{W(y_j)}\left(\frac{\partial m}{\partial y_j}\right)^2 + \frac{1}{W(x_j)}\left(\frac{\partial m}{\partial x_j}\right)^2\right] \approx \left(\sum_j W_j U_j^2\right)^{-1}. \tag{23}$$

The sum on the right side of this result turn up in York's work in the case where the x_i are *not* subject to error. In this case $W_i = W(y_i)$ [Eq. (8) with $W(x_i) \to \infty$; the

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$(\partial m/\partial x_j)$ term in Eq. (21) vanishes], and his least-squares cubic reduces to

$$m\left(\sum W(y_i)U_i^2\right)-\left(\sum W(y_i)U_iV_i\right)=0.$$

York's expression for σ_m^2 then follows if one adopts the approximation $W(y_i)/\Sigma W(y_i)\approx 0$. Whatever the detail of its derivation, York's result appears to involve some inappropriate approximations, and discontinuance of its use in favor in Eq. (21) is urged forthwith.

A. Observed versus calculated points

Another aspect to this problem not often discussed is that some statistical authorities prefer to evaluate the derivatives in Eq. (21) at the *calculated* (as opposed to observed) values of the data points.[11] This is because the Taylor-series used to calculate σ_m is actually expanded about the calculated points; see, in particular, Sec. 53 of Deming.[9] In practical circumstances this difference is a small one for well-correlated data, as the examples below indicate. In terms of the observed points (x_i,y_i) the calculated points (X_i,Y_i) were shown by York to be given by

$$X_i = x_i - \lambda_i m/W(x_i) \tag{24}$$

and

$$Y_i = y_i + \lambda_i/W(y_i), \tag{25}$$

where the Lagrangian multipliers λ_i are given by

$$\lambda_i = W_i(c + mx_i - y_i). \tag{26}$$

It is worthwhile to point out that if one takes this approach, then all of A, B, C, U_i, V_i, etc., *must be reevaluated at the calculated points after the best-fit slope has been determined*, before proceeding with the computation of σ_m and σ_c.

B. Examples

As a guide for readers debugging their own programs, I give here some examples. The first is a case commonly seen in the literature[5,12,13]—"Pearson's data with York's weights." The original data traces back to a paper by Karl Pearson in 1901;[14] the weights are from York's 1966 paper. The data are given in Table I. The best-fit slope and intercept are found to be $(m,c) = (-0.4805, 5.4799)$; the sum of weighted squared residuals is $\mathbf{S} = 11.866$. These figures are in agreement with those quoted in Refs. 5, 12, and 13. Equation (21), and its counterpart for σ_c with derivatives evaluated at the *observed* points,[15] gives $(\sigma_m,\sigma_c) = (0.0702,0.3555)$. Evaluating at the *calculated* points gives only very slightly different results: $(\sigma_m,\sigma_c) = (0.0706,0.3592)$.

Table I. Pearson's data with York's weights.

i	x_i	y_i	$W(x_i)$	$W(y_i)$
1	0.0	5.9	1000	1
2	0.9	5.4	1000	1.8
3	1.8	4.4	500	4
4	2.6	4.6	800	8
5	3.3	3.5	200	20
6	4.4	3.7	80	20
7	5.2	2.8	60	70
8	6.1	2.8	20	70
9	6.5	2.4	1.8	100
10	7.4	1.5	1	500

For the data of example I in Paper I, $(m,c) = (1.1668, -0.3652)$, $\mathbf{S} = 578.05$, $(\sigma_m,\sigma_c)_{\text{obs}} = (0.1704,0.1561)$, and $(\sigma_m,\sigma_c)_{\text{calc}} = (0.1470,0.1348)$. For the data example II in Paper I $(m,c) = (4.5437, -17.484)$, $(\sigma_m,\sigma_c)_{\text{obs}} = (14.476, 72.898)$, $(\sigma_m,\sigma_c)_{\text{calc}} = (7.0432,35.551)$, and $\mathbf{S} = 13.956$. In this latter case a significant difference appears between the parameter variances computed using the observed versus calculated points; this is because the data were produced by a random number generator and are poorly correlated. The author's experience is that σ_{calc} is generally less than σ_{obs}.

For all three of these examples, Chong[16] has verified independently that these results (with derivatives evaluated at the observed points) are in exact agreement with those predicted by Williamson's expressions, and Jefferys[17] has confirmed that the results obtained for example I are in agreement with his own software, which utilizes the calculated values of the data points.

IV. SUNDRY REMARKS

The most important lesson from these results is that when one quotes parameter variances for a least-squares fit, *define exactly how the variances were obtained.*

A revised FORTRAN program to find the best-fit m via the roots of the "least-squares quadratic," and generate corresponding estimates for σ_m and σ_c based on Eq. (21) using both observed and calculated coordinates is available from the author. Including extensive comments, the program runs to about 315 lines. A challenging project for anyone with a lot of patience or a good symbolic manipulator would be to compute the second-order contributions to σ_m and σ_c.

To close, it seems worthwhile to make a few remarks on the role of weighting. Standard practice is to assign weights as the inverse squares of the measurement uncertainties; this is based fundamentally on the assumption of normally distributed measurement errors;[9,10] in fact, Deming defines weights in this way in his Sec. 11. A more intuitively appealing argument for this approach can be given as follows. Imagine a situation where the data are such that $0\leqslant x\leqslant 1$, $0\leqslant y\leqslant 10$, $\sigma(x_i)\approx 0.1$, and $\sigma(y_i)\approx 1$. In both dimensions the (uncertainty/data) ratio is typically 0.1, but if weights are assigned in the usual way, then we would have $W(x_i)\approx 100$ vs $W(y_i)\approx 1$, which appears to "unfairly" favor the x direction. To preserve the sense that x and y should contribute equally to the solution, one might be tempted to divide all of the y_i and $\sigma(y_i)$ by 10 to produce equal weights in each dimension. But if one changes the weights, will not the best-fit slope change? The answer to this can be obtained by working through the effect of such a scaling in the least-squares quadratic: *only when weights are assigned as inverse-squares of the errors will the scaled best-fit slope come out to be exactly one-tenth of the unscaled slope.* Thus if weights are assigned as the inverse squares of the errors, one need never invoke any scaling; x and y will contribute to the solution "as they should."

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examine this problem further. In particular, Dr. Delano Chong, Dr. Bill Jefferys, and Dr. Matthew Lybanon shared a number of results and valuable comments. This work was supported by Natural Sciences and Engineering Research Council of Canada operating Grant A8580.

APPENDIX: EXPRESSIONS FOR PARAMETER DERIVATIVES

Here, we give explicit expressions for the derivatives appearing in Eq. (21) and its counterpart for σ_c^2. After many hours of algebra, one finds

$$\frac{\partial m}{\partial x_j} = -\frac{(m^2 DD_j + mEE_j - FF_j)}{(2mA + B - AAm^2 + BBm - CC)}, \quad \text{(A1)}$$

$$\frac{\partial m}{\partial y_j} = -\frac{(m^2 GG_j - 2mDD_j - EE_j/2)}{(2mA + B - AAm^2 + BBm - CC)}. \quad \text{(A2)}$$

A and B are defined in Eqs. (19) and (20). The other factors are defined by

$$AA = 4m \sum \frac{W_i^3 U_i V_i}{W^2(x_i)} - \frac{W(HH)(JJ)}{m}, \quad \text{(A3)}$$

$$BB = -\sum W_i^2 \left[4m \frac{W_i}{W(x_i)} \left(\frac{U_i^2}{W(y_i)} - \frac{V_i^2}{W(x_i)} \right) - \frac{2V_i(HH)}{W(x_i)} + \frac{2U_i(JJ)}{W(y_i)} \right], \quad \text{(A4)}$$

$$CC = -\sum \frac{W_i^2}{W(y_i)} \left[4m \frac{W_i U_i V_i}{W(x_i)} + V_i(JJ) + U_i(HH) \right], \quad \text{(A5)}$$

$$DD_j = \sum \frac{W_i^2 V_i}{W(x_i)} \left(\delta_{ij} - \frac{W_j}{W} \right), \quad \text{(A6)}$$

$$EE_j = 2 \sum \frac{W_i^2 U_i}{W(y_i)} \left(\delta_{ij} - \frac{W_j}{W} \right), \quad \text{(A7)}$$

$$FF_j = \sum \frac{W_i^2 V_i}{W(y_i)} \left(\delta_{ij} - \frac{W_j}{W} \right), \quad \text{(A8)}$$

and

$$GG_j = \sum \frac{W_i^2 U_i}{W(x_i)} \left(\delta_{ij} - \frac{W_j}{W} \right), \quad \text{(A9)}$$

where

$$W = \sum W_i, \quad \text{(A10)}$$

$$HH = -\frac{2m}{W} \sum \frac{W_i^2 V_i}{W(x_i)}, \quad \text{(A11)}$$

$$JJ = -\frac{2m}{W} \sum \frac{W_i^2 U_i}{W(x_i)}, \quad \text{(A12)}$$

and where δ_{ij} is the usual Kronecker delta. All sums are over $i = 1$ to N. Expressions for the derivatives of the intercept c with respect to x_j and y_j follow from the above and Eqs. (11)–(13):

$$\frac{\partial c}{\partial x_j} = [(HH) - m(JJ) - \langle x \rangle] \left(\frac{\partial m}{\partial x_j} \right) - \frac{mW_j}{W}, \quad \text{(A13)}$$

$$\frac{\partial c}{\partial y_j} = [(HH) - m(JJ) - \langle x \rangle] \left(\frac{\partial m}{\partial y_j} \right) + \frac{W_j}{W}. \quad \text{(A14)}$$

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