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A least-squares-based method for determining the ratio between two measured quantities

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Abstract. A numerical procedure to find the ratio between two measured quantities is discussed in the framework of the least-squares method with errors in both coordinates. Constant, as well as variable, amounts of statistical uncertainties are considered for each variable along their measured range. Analytical solutions for particular cases are given. The variance of the ratio is given as a closed analytical expression valid for the general case. Limiting cases of the presented results are compared with those obtained using classical least-squares expressions. A comparison with the weighted average method is also discussed.

1. Introduction

The ratio between two measured quantities is often needed in laboratories. As examples, the experimental determination of the following proportionality factors can be cited: calibration constant of Rogowski coils; attenuation factor of voltage dividers; relative calibration between similar sensors; determination of sensibility constants of linear transducers, etc. The quotient between two quantities (output to input, or output to output) must be obtained in all these cases and, frequently, both measured quantities have similar amounts of experimental uncertainties.

The problem of finding the ratio between two quantities x and y from which the data set (x_i, y_i) $1 \leq i \leq N$ has been measured, can be faced by finding the factor k that relates x and y in the form $y = kx$. When $N > 1$, the problem of finding k is clearly overdetermined. Among the standard numerical procedures to find k in these cases, the least-squares method is the most common. It is so widespread that it is included in many spreadsheets. Moreover, it has an analytical solution when measurement errors in only one coordinate are taken into account (Bevington 1969). Nevertheless, the problem loses its simplicity when one has to consider statistical uncertainties in both x_i and y_i measurements: α_i and β_i respectively. These uncertainties not only determine the variance of k, but they also affect the estimation of k.

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Among the least-squares-based procedures to fit experimental data when none of the coordinates are error free, the model $y = mx + b$ was extensively treated in the literature (see, for instance, the precursor articles of York (1966) and Williamson (1968); the more recent works of Reed (1992) and Press and Teukolsky (1992); and the review by Macdonald and Thompson (1992) with 35 references therein). In spite of the work already undertaken, this model still attracts attention, mainly in the parameters' variance evaluation (Cecchi 1991, 1993, Kalantar 1992, Moreno and Bruzzone 1993).

The least-squares fitting to the model $y = kx$ has almost the same subtle points as $y = mx + b$, but it has not been discussed in the literature with the same detail. Moreover, the results already known for $y = mx + b$ cannot be used in a straightforward manner to evaluate either k or its variance, because the fitted slope depends on whether an intercept b is included in the model or not.

In the current work we develop the model $y = kx$ in a self-contained form, based on the generalized least-squares method proposed by Deming (1943); the standard error propagation formula will then be used to obtain the variance of k. A particular case covering three situations of experimental interest for which an analytical solution exists will be treated in detail. Limiting cases will be analysed when possible, and a comparison with the weighted average method will be discussed. Finally, the conclusions of the work will be drawn.

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2. Method

When dealing with errors in both coordinates, the Deming criterion states that the expression

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

must be minimized to obtain the fitting points (X_i, Y_i), which, in turn, satisfies a relation like $f(X, Y, \underline{p}) = 0$, $\underline{p}$ being the set of $m < N$ parameters to be determined, and f is the so called model to fit the data. The coefficients ω_{x_i} and ω_{y_i} are weighting factors, usually to be the reciprocal of the variance of the observations α_i^{-2} and β_i^{-2} respectively, when Gaussian error theory is applicable. When this is not the case, other weighting procedures, and even expressions for S other than that proposed by Deming, must be used. For example, in the case of Poisson statistics (closely related to counting processes), weights are usually assigned as the reciprocal of the measured values, and expression (1) is kept as a simplifying approximation (Bevington 1969). Combinations of weighting schemes can be considered in the framework of the maximum likelihood theory. In this work we will consider only the Gaussian case for the sake of brevity. Nevertheless, when the Poisson distribution can be approximated by a Gaussian curve (number of counts greater than 50, say) both the formalism we are going to discuss and the results we will obtain can be extended to Poisson statistics by redefining the weighting factors as stated above.

2.1. Relation between Deming criterion and the effective variance method

For the case we are interested in, there is an explicit relationship $Y = f(X)$ between the fitting points. Therefore, expression (1) may be rewritten as

$$S = \sum_{i=1}^{N} \{\omega_{x_i}(x_i - X_i)^2 + \omega_{y_i}[y_i - f(X_i)]^2\} \tag{2}$$

where $f(X_i) = kX_i$ is the proposed model to fit the data.

Following Orear's derivation (1982), the minimization of equation (2) for a well behaved function f, can be approximately done by minimizing

$$S = \sum_{i=1}^{N} \frac{[y_i - f(x_i)]^2}{\beta_i^2 + \left(\frac{\mathrm{d}f}{\mathrm{d}x}|_{x_i}\right)^2 \alpha_i^2} \tag{3}$$

with respect to f which, in turn, can be a member of some parametrized family.

Formula (3) is the so-called effective variance method (Barker and Diana 1974) which, as Orear has shown, is equivalent to the Deming criterion equation(2) when f is a linear function.

Applying expression (3) to the model $f(x) = kx$, we have

$$S = \sum_{i=1}^{N} \frac{(y_i - kx_i)^2}{\beta_i^2 + k^2\alpha_i^2} \tag{4}$$

which must be minimized by varying k. This condition means

$$\frac{\partial S}{\partial k} = 0 \tag{5}$$

which leads to

$$-2\sum_{i=1}^{N} \frac{(y_i - kx_i)[x_i\beta_i^2 + ky_i\alpha_i^2]}{[\beta_i^2 + k^2\alpha_i^2]^2} = 0. \tag{6}$$

Note that for the model we are dealing with, the effective variance approach not only is exact, but also reduces the original $(N + 1)$-dimensional problem (the minimization of expression (2) in which all the X_i points together with k must be varied) to a one-dimensional parametric minimization of expression (4). In spite of this simplification, the remaining minimization problem has no analytical solution in the general case, essentially, because of the occurrence of k in the denominators of (6), and therefore computational methods must be used to find k. Nevertheless, several well known numerical techniques, such as Brent's method, golden section search or quasi-Newton-based methods, can be successfully applied. For details and algorithms on these and other minimization procedures see the work of Press *et al* (1992).

2.2. Evaluation of the fitted points

Once k is known, it is worthwhile to look for the fitted points X_i and Y_i. Starting with expression (2) and considering S a minimum function of X_i, we have $\partial S/\partial X_i = 0$, from which X_i results in

$$X_i = \frac{x_i\beta_i^2 + ky_i\alpha_i^2}{\beta_i^2 + k^2\alpha_i^2}.$$

Now, the Y_i variables can be found directly by the definition $Y_i = kX_i$.

As limiting cases, from these expressions it can be seen that

$$X_i = x_i \qquad \text{and} \qquad Y_i = kx_i$$

whenever $\alpha_i = 0$; whereas

$$X_i = y_i/k \qquad \text{and} \qquad Y_i = y_i$$

whenever $\beta_i = 0$, as one would expect from the classical least-squares fits with errors in only one coordinate.

3. Variance of *k*

To quantify the accuracy of the ratio estimation, it is necessary to evaluate the variance of k arising from the data uncertainties. Using the well known error propagation formula, valid for small and uncorrelated random errors, we have

$$\sigma^2(k) = \sum_{i=1}^{N} \left[\left(\frac{\partial k}{\partial x_i}\alpha_i\right)^2 + \left(\frac{\partial k}{\partial y_i}\beta_i\right)^2\right] \tag{7}$$

where the quantities $\partial k/\partial x_i$ and $\partial k/\partial y_i$ remain to be determined from the proposed model and from the experimental data set.

As we have already mentioned, it is not always possible to find an analytical expression for k from equation (6), and therefore the partial derivatives appearing in expression (7) cannot always be directly evaluated. Nevertheless, one can resort to the following implicit derivation procedure.

By differentiating expression (5) with respect to x_i, and evaluating the result for the value of k which minimizes S, we have

$$\frac{\partial}{\partial x_i}\frac{\partial S}{\partial k}+\frac{\partial^2 S}{\partial k^2}\frac{\partial k}{\partial x_i}=0 \qquad 1\le i\le N$$

which allow us to obtain

$$\frac{\partial k}{\partial x_i}=\frac{W_i(d_i-kF_i)}{\Delta} \tag{8}$$

where $W_i=(\beta_i^2+k^2\alpha_i^2)^{-1}$ is the overall weight of the ith point; $d_i=y_i-kx_i$ is the vertical separation between the ith point and the fitting line; the factor F_i is defined as $F_i=x_i+2kd_iW_i\alpha_i^2$; and

$$\Delta=\frac{1}{2}\frac{\partial^2 S}{\partial k^2}=\sum_{i=1}^{N}W_i(F_i^2-W_i d_i^2\alpha_i^2). \tag{9}$$

In the same manner, by differentiating expression (5) now with respect to y_i, we obtain

$$\frac{\partial k}{\partial y_i}=\frac{W_iF_i}{\Delta}. \tag{10}$$

Finally, the variance of k is obtained by replacing $\partial k/\partial x_i$ and $\partial k/\partial y_i$ in expression (7). Once the replacements are worked out, the following expression results for $\sigma^2(k)$

$$\sigma^2(k)=\frac{1}{\Delta^2}\sum_{i=1}^{N}W_i^2(x_i^2\beta_i^2+y_i^2\alpha_i^2). \tag{11}$$

Note that once k is obtained either by minimizing expression (4) or by solving equation (6), the variance $\sigma^2(k)$ can be obtained from a direct evaluation of expression (11). It is necessary to mention that Δ must be no-null to allow expressions (8) and (10), and consequently the variance of k as given by (11), to be defined. Since the condition $\Delta>0$ is sufficient to ensure the existence of a minimum of S, the requirement $\Delta\neq 0$ is compatible with the minimization of S.

4. Special cases

Although it is not possible to give a general analytical solution of equation (6), there are three cases of practical interest, where this equation can be explicitly solved in terms of the given data points and their uncertainties. These cases arise when α_i and β_i are proportional to one another. In fact, if $\beta_i=c\alpha_i$, c = constant, equation (4) reduces to

$$S=\frac{\sum_{i=1}^{N}\omega_{x_i}(y_i-kx_i)^2}{c^2+k^2} \tag{12}$$

and the minimum condition is expressed by

$$\sum_{i=1}^{N}\omega_{x_i}d_i(x_ic^2+ky_i)=0 \tag{13}$$

which, provided $\sum_{i=1}^{N}\omega_{x_i}x_iy_i\neq 0$, has the solutions

$$k=\frac{B\pm\sqrt{B^2+\left[2c\sum_{i=1}^{N}\omega_{x_i}x_iy_i\right]^2}}{2\sum_{i=1}^{N}\omega_{x_i}x_iy_i} \tag{14}$$

where

$$B=\sum_{i=1}^{N}\omega_{x_i}(y_i^2-c^2x_i^2).$$

If $\sum_{i=1}^{N}\omega_{x_i}x_iy_i=0$, then equation (13) leads to $k=0$, provided $B\neq 0$. If $\sum_{i=1}^{N}\omega_{x_i}x_iy_i=0$ and $B=0$ simultaneously, then k becomes indeterminate. It must be noted that if $\sum_{i=1}^{N}\omega_{x_i}x_iy_i=0$ there is zero linear correlation between x and y (Bevington 1969) and it is then inappropriate to attempt to fit the data to the line $y=kx$. Nevertheless, these two possibilities must be taken into account when programming an algorithm.

The two solutions given by equation (14) correspond to the closest and farthest fitting lines, that is, those which minimize and maximize S respectively. Let us call k_+ the solution taken with the '+' sign in equation (14) and k_- the one corresponding to the '−' sign. It can be seen that $k_+k_-<0$. Moreover, it can be verified that

$$k_+k_-=-c^2=-\left(\frac{\beta_i}{\alpha_i}\right)^2$$

which means that when neither of the two coordinates is error free, the two fitted lines are not necessarily perpendicular. Care must be taken, however, when $\alpha_i\to 0$ or $\beta_i\to 0$ in the above expression, because in these limiting cases one of the two solutions is lost. If $\alpha_i\to 0$, for example, expression (12) becomes the classical least-squares fitting for the model $y=kx$ with variable β_i errors, which has the unique solution

$$k=\frac{\sum_{i=1}^{N}\omega_{y_i}x_iy_i}{\sum_{i=1}^{N}\omega_{y_i}x_i^2} \qquad \text{when} \qquad \alpha_i=0.$$

On the other hand, if $\beta_i\to 0$, it can be seen from equation (13) that the non-trivial solution is also unique, just because it comes from a linear equation in k. In fact, it can be shown that the resulting expression for k in this limiting case is

$$k=\frac{\sum_{i=1}^{N}\omega_{x_i}y_i^2}{\sum_{i=1}^{N}\omega_{x_i}x_iy_i} \qquad \text{when} \qquad \beta_i=0.$$

Returning to the general case, when $\alpha_i\beta_i\neq 0$, the problem of selecting k remains to be solved. There are several ways to choose the correct solution among the two available ones given by expression (14). From physical insight, for instance, one frequently knows the sign of k and therefore one can select the correct slope beforehand. Another way is by computing S from equation (4) for both values of k to see which of them yields the lower value of S. In addition, it can be checked that $\Delta>0$ for the value of k which minimizes S. One further method is a direct inspection of a data plot together with the two lines to decide which is the best. This is a simple, almost trivial method, which should be viewed as a necessary qualitative complement to the quantitative alternatives expressed above.

The variance of k for the special case we are interested in is

$$\sigma^2(k) = \frac{\sum_{i=1}^{N} \omega_{x_i}(y_i^2 + c^2 x_i^2)}{\Delta^2 (c^2 + k^2)^2}$$

where Δ is evaluated from expression (9) using $W_i = \omega_{x_i}/(c^2 + k^2)$, and $F_i = x_i + (2kd_i)/(c^2 + k^2)$.

Now, let us consider the remaining two special cases. By taking $\alpha_i = \alpha$ and $\beta_i = \beta$, $\forall i$, and hence by putting $c = \beta/\alpha$ and $\omega_{x_i} = \alpha^{-2}$ in the above expressions, the case of constant errors along each axis can be handled. Finally, one can consider equal errors for all the data points in both coordinates, that is $\alpha_i = \beta_i = \sigma_o$, $\forall i$, with σ_o = constant. Perhaps this is the less general case but is also a common situation which the experimentalist must face, when dealing with voltages of similar amplitudes, for instance. All the needed formulae can be obtained by putting $c = 1$ and $\omega_{x_i} = \sigma_o^{-2}$. The resulting expressions for these two last special cases will not be displayed here for brevity.

Before passing to the next section, it is convenient to mention that all the obtained results satisfy the scaling law

$$k(ux, vy) = \frac{v}{u} k(x, y) \qquad u, v \text{ constant}, u \neq 0$$

where $k(ux, vy)$ means the value of k obtained after scaling the x and $y$axes by the factors u and v respectively.

The reversibility criterion against coordinates interchange, i.e.

$$k(x, y) = k^{-1}(y, x) \tag{15}$$

is also satisfied. This last desirable feature is not fulfilled by all the proposed data reduction methods, as we shall see at the end of the next section.

5. Comparison with the weighted average method

It is useful to compare the results obtained in sections 2–4, with those that arise from the error theory applied to a set of quotients. In fact, having a series of N points (x_i, y_i), one could attempt to estimate the ratio k by evaluating the N quotients y_i/x_i and then averaging all these partial results. Following this procedure, one gets

$$k_i = \frac{y_i}{x_i} \qquad 1 \leq i \leq N$$

and

$$\sigma^2(k_i) = \frac{y_i^2}{x_i^2}\left(\frac{\alpha_i^2}{x_i^2} + \frac{\beta_i^2}{y_i^2}\right) \qquad 1 \leq i \leq N$$

as results from the usual error propagation law.

The weighted average $\langle k \rangle$ of the k_i values is defined as (Bevington 1969)

$$\langle k \rangle = \frac{\sum_{i=1}^{N} \sigma^{-2}(k_i) k_i}{\sum_{i=1}^{N} \sigma^{-2}(k_i)} \tag{16}$$

and its variance is given by

$$\sigma^2(\langle k \rangle) = \frac{1}{\sum_{i=1}^{N} \sigma^{-2}(k_i)}.$$

It can be shown that although $\langle k \rangle$ can be a good approximation to k, it is verified that

$$\langle k \rangle \neq k$$

because $\langle k \rangle$ is not a solution of equation (6). To see this, it is sufficient to consider the particular case of two data points (a, b) and (b, a), $a \neq b$, with both a and b greater than 0, for instance. In addition, equal uncertainties for a and b can be assumed for the sake of simplicity. After some algebra, the averaging scheme yields $\langle k \rangle = (a^3 b + b^3 a)/(a^4 + b^4)$, which does not satisfy equation (6). In fact, by solving equation (6), or by following the procedure discussed in section 4, one obtains $k = 1$. This last result is what one could expect from symmetry considerations.

Only in the limiting case in which $\alpha_i = 0\ \forall i$, one gets $\langle k \rangle = k$. In fact, it can be seen from equation (6) that

$$k = \frac{\sum_{i=1}^{N} \beta_i^{-2} x_i y_i}{\sum_{i=1}^{N} \beta_i^{-2} x_i^2} \qquad \text{when} \qquad \alpha_i = 0 \forall i$$

which coincides with $\langle k \rangle$ as defined in expression (16). Moreover, it can be proven, by simple substitution, that

$$\sigma(\langle k \rangle) = \sigma(k)$$

under the hypothesis $\alpha_i = 0\ \forall i$.

To close the comparison between the results obtained in sections 2–4 and the averaging procedure we are discussing here, it is worthwhile to mention that if there are errors in both coordinates, the averaging scheme does not satisfy the reversibility criterion (15), i.e.

$$\langle k(x, y) \rangle \neq \langle k(y, x) \rangle^{-1}$$

as can be shown from expression (16). This fact makes the formalism discussed in sections 2–4 more suitable for determining the ratio between two measured quantities than the weighted average method.

6. Final remarks and conclusions

Although it is not possible to solve analytically the equation that determines k in the general case, explicit analytical solutions were given for particular cases of experimental interest. These cases were studied in some detail, ending with ready-to-use formulae. Obtaining k in the general case can be done by minimizing equation (4), which is easy to evaluate, and depends on only one parameter. Well known algorithms can be used to solve this problem.

The variance of k was analytically given for the general case, in a closed form. Closed expressions for the fitted points (X_i, Y_i) were also obtained, and limiting cases when one coordinate is error free were checked. The reversibility of the obtained results when coordinates are interchanged was also stated.

Certainly, there will be situations where k and $\langle k \rangle$ will coincide within their standard dispersions. Hence, it could be argued that all that has been discussed in this article is of little significance. Nonetheless, in the opinion of the author, an experimentalist will prefer to process a high quality data set using an adequate method, instead of losing part of that quality merely by using a poor numerical procedure. This is particularly important when the data must be processed to find a reliable calibration factor.

In this sense, when errors in both coordinates are present, the use of the weighted average should be avoided, or at least, it should be considered as an approximation susceptible to be improved using the method discussed in the current work. Within the same spirit, only those curve fitting algorithms that allow for the inclusion of overall weighting factors, which in turn depend upon the fitting parameter as stated by expression (4), should be used to obtain k.

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