The Extended-Least-Squares Treatment of Correlated Data

E. Richard Cohen and Valentin S. Tuninsky

***Abstract*—A generalization of the extended-least-squares algorithms for the case of correlated discrepant data is given. The expressions for linear, unbiased, minimum-variance estimators previously derived are reformulated. *A posteriori* estimates of the variance taking into account the inconsistency of *all* the experimental data have the same form as in the case of noncorrelated data. These estimates extend the previous improvement on the "traditional" Birge-ratio procedure to the case of correlated input data.**

I. Introduction

THE mathematical analysis of measurements of the fundamental constants is generally based on the concepts of the least-squares method of data adjustment [1]. An important aspect of the least-squares technique is the proper treatment of discrepant data. In addition to the simple deletion of the more inconsistent data, several algorithms have been introduced to account for inconsistencies by expanding the *a priori* variances of the input data. Among these have been the Birge Ratio [2] for homogeneous data (data of a single 'type'), an analysis of variance with separate Birge ratios for each group of homogeneous data [3], the LCU (least change of the uncertainties) approach [4], and extended-least-squares estimates [5]. A numerical comparison of these algorithms was performed [6] on the data of several adjustments of fundamental constants. These approaches deal with information giving different levels of detail of the experimental data, and some of these approaches require more experimental detail than others. Following the recommendation of the Bureau International des Poids et Mesures [7] measurements should include, besides the measured value and an estimate s_i^2 of its variance σ_i^2, also the components $s_{i,k}^2$ of the estimate ($s_i^2 = \Sigma s_{i,k}^2$) and the degrees of freedom $\nu_{i,k}$ of those components.

The extended-least-squares (ELS) estimators [5] previously derived define *a posteriori* estimates of the unknown variables of the adjustment $\hat{x}_\alpha$ as well as the uncertainties $\hat{\sigma}_i^2$ to be assigned to the measured input quantities. Here we shall extend that discussion to include the case of correlated discrepant input data.

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E. R. Cohen is with Rockwell International Science Center, Thousand Oaks, CA 91360 USA.

V. S. Tuninsky is with the D. I. Mendeleyev Institute of Metrology, St. Petersburg, 198005, Russia.

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II. Basic Model

The operational equations for the measurements are assumed to be reducible, by an appropriate choice of variables, to the form

$$y_i = Y_i + \varepsilon_i = y_i^\circ + \sum_{\alpha=1}^{M} A_{i\alpha}\xi_\alpha + \varepsilon_i, \quad i = 1, \cdots, N \tag{1}$$

where Y_i are the 'true' values (the expectations, $Ey_i = Y_i$), $\xi_\alpha = x_\alpha - x_\alpha^\circ$ are the deviations of the unknowns from a set of initial values $x_\alpha^\circ, y_i^\circ = Y(\cdots, x_\alpha^\circ, \cdots)$, and the matrix $\boldsymbol{A} = (A_{i\alpha})$ is a constant. The errors ϵ_i are assumed to be correlated, with a variance-covariance matrix (or more succinctly, a "covariance matrix") $\boldsymbol{v} = (v_{ik})$

$$\begin{aligned}\langle \varepsilon_i \rangle &= 0\\ \langle \varepsilon_i \varepsilon_k \rangle &= v_{ik}\\ \langle \varepsilon_i \varepsilon_j \varepsilon_k \rangle &= 0\\ \langle \varepsilon_i \varepsilon_j \varepsilon_k \varepsilon_l \rangle &= v_{ij}v_{kl} + v_{ik}v_{jl} + v_{il}v_{jk}.\end{aligned} \tag{2}$$

Correlations between input data of an adjustment arise, for example, when different input data are obtained using shared instrumentation, or using the same measurement standards or the same auxiliary constants having nonnegligible uncertainties [8]. A covariance matrix may be constructed in the form

$$v_{ik} = \sum_{p=1}^{L} f_{ik}^p \sigma_p^2 \tag{3}$$

where f_{ik}^p are fixed coefficients and σ_p^2 are independent contributions for which estimates s_p^2 and the confidence parameters ν_p are known

$$\langle s_p^2 \rangle = \sigma_p^2, \quad \langle s_p^2 \varepsilon_i \rangle = 0, \tag{4}$$

$$\langle s_p^2 s_q^2 \rangle = \left(1 + \frac{2\delta_{pq}}{\nu_p}\right)\sigma_p^2 \sigma_q^2.$$

$$D(s_p^2) \equiv \langle (s_p^2 - \langle s_p^2 \rangle)^2 \rangle = 2\sigma_p^4/\nu_p. \tag{5}$$

When the *a priori* variance estimate s_p^2 is based on the observed variance of a sample drawn from a normal distribution, the variance of that estimate is inversely proportional to the degrees of freedom ν_p; this may be generalized, and ν_p may be considered to be a parameter that defines the variance of the estimate. It therefore need not necessarily be restricted to integral values.

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In the case of uncorrelated data the covariance matrix is diagonal; the uncertainty of each measured value can be associated with a distinct component σ_p^2 and we have

$$f_{ik}^p = \delta_{pi}\delta_{pk}, \quad v_{ij} = \delta_{ij}\sigma_j^2$$

and $L = N$.

Equations (1)–(5) describe the model for which a generalization of the extended-least-squares estimators are to be obtained.

III. Maximum Likelihood Estimator

The method of maximum likelihood requires a knowledge of the distribution laws of ϵ_i and s_p^2. We assume a correlated normal distribution for ϵ_i and an independent χ^2 distribution for s_p^2 (which, when ν_p is an integer, can be considered as the "radial" part of a ν_p-dimensional normal distribution for s_p):

$$N(y_1, y_2, \cdots, y_N) = \frac{\exp(-\frac{1}{2}\varepsilon^T \boldsymbol{w}\varepsilon)}{\sqrt{(2\pi)^N \det \boldsymbol{v}}} \tag{6}$$

where ^{T} denotes the transpose, $\det \boldsymbol{v}$ is the determinant of the matrix (v_{ik}), and $\boldsymbol{w} = \boldsymbol{v}^{-1}$ is the weight matrix of the input data; and

$$f(s_p^2; \nu_p) = \frac{(\nu_p s_p^2/2)^{\nu_p/2}}{\Gamma(\nu_p/2)\sigma_p^{\nu_p} s_p^2} e^{-\nu_p s_p^2/2\sigma_p^2}. \tag{7}$$

This distribution $f(s_p^2; \nu_p)$ should be considered as simply a convenient model for the distribution of s_p^2, with ν_p as a parameter.

From (3), (6), and (7), the probability density g and the likelihood function $\mathcal{L}$ to which the maximum likelihood condition is to be applied are

$$g = N(y_i; \xi_\alpha, \boldsymbol{v}) \prod_{p=1}^{L} f(s_p^2; \sigma_p^2, \nu_p) \equiv \exp(-\mathcal{L})$$

$$\mathcal{L} = \frac{1}{2}\Bigg[\boldsymbol{\varepsilon}^T \boldsymbol{w}\boldsymbol{\varepsilon} + \ln(\det \boldsymbol{v}) + \sum_p \nu_p[s_p^2/\sigma_p^2 + \ln(\sigma_p^2/s_p^2)] + \text{const.}\Bigg]. \tag{8}$$

Because the likelihood function in (8) is not separable with respect to the unknowns (ξ_α, σ_p^2), it is impossible to obtain optimum sufficient estimators [9] and there is no uniquely "best" solution to the estimation problem.

Minimizing $\mathcal{L}$ with respect to $\xi_\alpha, \partial\mathcal{L}/\partial\xi_\alpha = 0$, gives the well known estimate $\hat{\xi}_\alpha$ of general least-squares:

$$\hat{\boldsymbol{x}} = \boldsymbol{x}^\circ + \boldsymbol{C}(\boldsymbol{y} - \boldsymbol{y}^\circ) \tag{9}$$

$$\boldsymbol{C} = (\boldsymbol{A}^T\boldsymbol{w}\boldsymbol{A})^{-1}\boldsymbol{A}^T\boldsymbol{w}$$

$$\hat{\boldsymbol{y}} = \boldsymbol{y}^\circ + \boldsymbol{A}\boldsymbol{C}(\boldsymbol{y} - \boldsymbol{y}^\circ) \tag{10}$$

$$\boldsymbol{A}\boldsymbol{C}\boldsymbol{A} = \boldsymbol{A} \quad \boldsymbol{C}\boldsymbol{A}\boldsymbol{C} = \boldsymbol{C} \tag{11}$$

while minimization with respect to $\sigma_p^2\ \partial\mathcal{L}/\partial\sigma_p^2 = 0$, using the partial derivatives relations

$$\frac{\partial v_{ij}}{\partial\sigma_p^2} = f_{ij}^p$$

$$\frac{\partial \ln(\det \boldsymbol{v})}{\partial\sigma_p^2} = \mathrm{Tr}(\boldsymbol{w}\boldsymbol{f}^p)$$

$$\frac{\partial w}{\partial\sigma_p^2} = -\boldsymbol{w}\boldsymbol{f}^p\boldsymbol{w}$$

gives

$$\boldsymbol{\varepsilon}^T\boldsymbol{w}\boldsymbol{f}^p\boldsymbol{w}\boldsymbol{\varepsilon} - \mathrm{Tr}(\boldsymbol{w}\boldsymbol{f}^p) = \frac{\nu_p}{\sigma_p^4}(\sigma_p^2 - s_p^2). \tag{12}$$

Multiplying this equation by σ_p^2, summing over all values of p, and using (3) and $\boldsymbol{v} = \boldsymbol{w}^{-1}$ gives

$$\boldsymbol{\varepsilon}^T\boldsymbol{w}\boldsymbol{\varepsilon} = N + \sum_p \nu_p(1 - s_p^2/\sigma_p^2).$$

This result is a verification of the consistency of the maximum likelihood condition: taking expectations over ϵ_j, using $\langle\epsilon_j\epsilon_k\rangle = v_{jk} = (w^{-1})_{jk}$, gives

$$\langle\boldsymbol{\varepsilon}^T\boldsymbol{w}\boldsymbol{\varepsilon}\rangle = \mathrm{Tr}(\delta_{jj}) = N \quad \text{and} \quad \sum_p \nu_p(1 - s_p^2/\sigma_p^2) = 0,$$

while taking expectations over s_p^2, gives

$$\langle s_p^2\rangle = \sigma_p^2 \quad \text{and} \quad \boldsymbol{\varepsilon}^T\boldsymbol{w}\boldsymbol{\varepsilon} = N.$$

Using the estimates $\hat{\boldsymbol{x}}$ and $\hat{\boldsymbol{y}}$ from (9) and (10) gives

$$\begin{aligned}\boldsymbol{\varepsilon} &\equiv \boldsymbol{y} - \boldsymbol{Y} = (\boldsymbol{y} - \hat{\boldsymbol{y}}) + (\hat{\boldsymbol{y}} - \boldsymbol{Y}) = \boldsymbol{r} + \hat{\boldsymbol{y}} - \boldsymbol{Y}\\ &= (\boldsymbol{I} - \boldsymbol{A}\boldsymbol{C})(\boldsymbol{y} - \boldsymbol{y}^\circ) + \boldsymbol{A}(\hat{\boldsymbol{x}} - \boldsymbol{x})\end{aligned}$$

and one obtains

$$\boldsymbol{\varepsilon}^T\boldsymbol{w}\boldsymbol{f}^p\boldsymbol{w}\boldsymbol{\varepsilon} = \boldsymbol{r}^T\boldsymbol{w}\boldsymbol{f}^p\boldsymbol{w}\boldsymbol{r} + \Delta.$$

Although the expectation of $\hat{x}_\alpha - x_\alpha$ vanishes and the "best estimate" of Y_i is $\hat{y}_i$, the expectation of Δ is not zero. If the term Δ is neglected a bias will be introduced into the evaluation. Since

$$\langle\varepsilon_j\varepsilon_k\rangle = v_{jk} \quad \text{and} \quad \langle r_j r_k\rangle = [\boldsymbol{v} - \boldsymbol{A}\boldsymbol{C}\boldsymbol{v}]_{jk},$$

we introduce the matrix R_{jk} in order to compensate for this bias

$$R_{jk} = \widetilde{r_j r_k} = \frac{r_j v_{jk} r_k}{v_{jk} - \overline{V}_{jk}} = \frac{r_j r_k}{1 - \mathrm{cov}(\hat{y}_j, \hat{y}_k)/v_{jk}}$$

where $\boldsymbol{V} = (\boldsymbol{A}^T\boldsymbol{w}\boldsymbol{A})^{-1}$ is the covariance matrix of the fitted quantities $\hat{x}_\alpha$ and $\overline{\boldsymbol{V}} = \boldsymbol{A}\boldsymbol{V}\boldsymbol{A}^T$ is the covariance matrix of the adjusted input data $\hat{\boldsymbol{y}}$:

$$\mathrm{cov}(\hat{y}_j, \hat{y}_k) = \overline{\boldsymbol{V}} = \boldsymbol{A}(\boldsymbol{A}^T\boldsymbol{w}\boldsymbol{A})^{-1}\boldsymbol{A}^T.$$

The maximum-likelihood estimate for the uncertainty component σ_p^2, from (9), (10), and (12) becomes

$$[\mathrm{Tr}(\boldsymbol{w}\boldsymbol{f}^p\boldsymbol{w}\boldsymbol{R}) - \mathrm{Tr}(\boldsymbol{w}\boldsymbol{f}^p)] + \nu_p[s_p^2 - \hat{\sigma}_p^2]/\hat{\sigma}_p^4 = 0,$$

or, in a possibly better form for iteration (since the weight matrix $\boldsymbol{w}$ must be evaluated using the estimates $\hat{\sigma}_p^2$)

$$\begin{aligned}\hat{\sigma}_p^2 &= \frac{\nu_p s_p^2 + \hat{\sigma}_p^4 \operatorname{Tr}(\boldsymbol{w f^p w R})}{\nu_p + \hat{\sigma}_p^2 \operatorname{Tr}(\boldsymbol{w f^p})} \\ \boldsymbol{v} &= \sum_p \boldsymbol{f}^p \hat{\sigma}_p^2, \quad \boldsymbol{w} = \boldsymbol{v}^{-1} \\ \boldsymbol{C} &= (\boldsymbol{A}^T \boldsymbol{w A})^{-1} \boldsymbol{A}^T \boldsymbol{w} = \boldsymbol{V A}^T \boldsymbol{w} \\ \boldsymbol{r} &= (\boldsymbol{I} - \boldsymbol{AC})(\boldsymbol{y} - \boldsymbol{y}^\circ). \end{aligned} \tag{13}$$

For uncorrelated input data (*i.e.*, for $f_{jk}^p = \delta_{jp}\delta_{kp}$) this expression reduces to the form

$$\hat{\sigma}_p^2 = \frac{1}{\nu_p + 1}\left[\nu_p s_p^2 + \frac{r_p^2}{1 - \overline{V}_{pp}/\hat{\sigma}_p^2}\right]. \tag{14}$$

The results, (13) and (14) are not the only possible ones. Instead of introducing the matrix R_{jk} to compensate for the bias caused by neglecting Δ in (12), an alternative form may be found by introducing the expectation of Δ into that equation; this yields

$$\boldsymbol{r}^T \boldsymbol{w f^p w r} + \operatorname{Tr}(\boldsymbol{w f^p w \overline{V}}) - \operatorname{Tr}(\boldsymbol{w f^p}) = \nu_p[\hat{\sigma}_p^2 - s_p^2]/\hat{\sigma}_p^4,$$

or

$$\hat{\sigma}_p^2 = \frac{\nu_p s_p^2 + \hat{\sigma}_p^4[\boldsymbol{r}^T \boldsymbol{w f^p w r} + \operatorname{Tr}(\boldsymbol{w f^p w \overline{V}})]}{\nu_p + \hat{\sigma}_p^2 \operatorname{Tr}(\boldsymbol{w f^p})}. \tag{15}$$

For uncorrelated input data this reduces to

$$\hat{\sigma}_p^2 = \frac{1}{\nu_p + 1}[\nu_p s_p^2 + r_p^2 + \overline{V}_{pp}]. \tag{16}$$

The expressions (13) and (15) are equally valid estimators in the sense that the two have the same expectation, and the same may be said also for expressions (14) and (16).

IV. Minimum Variance Estimator

The minimum variance estimator requires only the lower moments of ϵ_i and s_p^2, (2) and (5) rather than a detailed knowledge of the distributions [5].

The linear, unbiased, minimum variance estimator is to be obtained in the form of a linear combination of the available information pertaining to the estimand; this leads again to (9) and (10) for the adjusted values $\hat{x}_\alpha$ and $\hat{y}_k$ with the estimate of the uncertainty $\hat{\sigma}_p^2$ given by

$$\hat{\sigma}_p^2 = a_p s_p^2 + (\boldsymbol{y} - \hat{\boldsymbol{y}})^T \boldsymbol{B}^p (\boldsymbol{y} - \hat{\boldsymbol{y}}) = a_p s_p^2 + \boldsymbol{r}^T \boldsymbol{B}^p \boldsymbol{r} \tag{17}$$

where the coefficient a_p and the $N \otimes N$ matrix $\boldsymbol{B}^p$ are to be determined.

In order that the expectation of the estimate $\hat{\sigma}_p^2$ equals the true estimand, $<\hat{\sigma}_p^2>= \sigma_p^2$, the coefficient a_p must satisfy

$$a_p = 1 - \operatorname{Tr}/.(\boldsymbol{B}^p \boldsymbol{K})/\sigma_p^2$$

where

$$\begin{aligned}\boldsymbol{K} &= \langle \boldsymbol{r r}^T \rangle = (\boldsymbol{I} - \boldsymbol{AC})\boldsymbol{v} = \boldsymbol{v} - \overline{\boldsymbol{V}} \\ \boldsymbol{K w} &= \boldsymbol{I} - \boldsymbol{AC}, \quad \boldsymbol{K w K} = \boldsymbol{K} \\ \boldsymbol{r} &= \boldsymbol{K w}(\boldsymbol{y} - \boldsymbol{y}^\circ) \\ \boldsymbol{ACK} &= \overline{\boldsymbol{V}} \boldsymbol{w K} = 0. \end{aligned} \tag{18}$$

Introducing the notation

$$T_2 = \operatorname{Tr}(\boldsymbol{B^p K}), \quad T_4 = \operatorname{Tr}(\boldsymbol{B^p K B^p K})$$

permits the variance $D(\hat{\sigma}_p^2)$ to be written in the form

$$D(\hat{\sigma}_p^2) = \frac{2}{\nu_p}[\sigma_p^2 - T_2]^2 + 2T_4. \tag{19}$$

The condition that the variance should be minimal then leads to the equation

$$\nu_p \boldsymbol{K B^p K} = [\sigma_p^2 - T_2]\boldsymbol{K}. \tag{20}$$

Multiply (20), in turn, by $\boldsymbol{w}$ and by B^p and take the traces to obtain the two equations

$$\begin{aligned}\nu_p T_2 &= [\sigma_p^2 - T_2]\nu \\ \nu &= \operatorname{Tr}(\boldsymbol{I} - \boldsymbol{AC}) = N - M \\ \nu_p T_4 &= [\sigma_p^2 - T_2]T_2\end{aligned}$$

from which the values of T_2 and T_4 are obtained

$$T_2 = \frac{\nu\sigma_p^2}{\nu_p + \nu}, \quad T_4 = \frac{\nu\sigma_p^4}{(\nu_p + \nu)^2}. \tag{21}$$

This gives

$$a_p = \frac{\nu_p}{\nu_p + \nu}, \quad \boldsymbol{K B^p K} = \frac{\sigma_p^2}{\nu_p + \nu}\boldsymbol{K}. \tag{22}$$

The minimal variance is then given by putting the results (21) into (19),

$$D(\hat{\sigma}_p^2) = \frac{2\sigma_p^4}{\nu_p + \nu}.$$

The variance of the estimate σ_p^2 has been decreased by the factor $\nu_p/(\nu_p + \nu)$; the equivalent degrees of freedom for the estimate have been increased from ν_p to $\nu_p + \nu$, showing the full efficiency of the estimator.

Because $\boldsymbol{K}$ is singular it has no inverse, and one cannot solve (20) for $\boldsymbol{B^p}$. We can, however, evaluate the quantity $\boldsymbol{r}^T \boldsymbol{B}^p \boldsymbol{r}$ without the need to evaluate $\boldsymbol{B^p}$ explicitly

$$\begin{aligned}\boldsymbol{r}^T \boldsymbol{B}^p \boldsymbol{r} &= [(\boldsymbol{I} - \boldsymbol{AC})(\boldsymbol{y} - \boldsymbol{y}^\circ)]^T \boldsymbol{B}^p (\boldsymbol{I} - \boldsymbol{AC})(\boldsymbol{y} - \boldsymbol{y}^\circ) \\ &= (\boldsymbol{y} - \boldsymbol{y}^\circ)^T (\boldsymbol{I} - \boldsymbol{w A V A}^T) \boldsymbol{B}^p (\boldsymbol{I} - \overline{\boldsymbol{V}} \boldsymbol{w})(\boldsymbol{y} - \boldsymbol{y}^\circ).\end{aligned}$$

Using (18), (20), and (21) we have

$$\begin{aligned}\boldsymbol{r}^T \boldsymbol{B}^p \boldsymbol{r} &= (\boldsymbol{y} - \boldsymbol{y}^\circ)^T \boldsymbol{w K B^p K w}(\boldsymbol{y} - \boldsymbol{y}^\circ) \\ &= \frac{\sigma_p^2}{\nu_p + \nu}(\boldsymbol{y} - \boldsymbol{y}^\circ)^T \boldsymbol{w K w}(\boldsymbol{y} - \boldsymbol{y}^\circ) \\ &= \frac{\sigma_p^2}{\nu_p + \nu}(\boldsymbol{y} - \boldsymbol{y}^\circ)^T \boldsymbol{w K w K w}(y - y^\circ) \\ &= \frac{\sigma_p^2}{\nu_p + \nu}\boldsymbol{r}^T \boldsymbol{w r} = \frac{\sigma_p^2 \chi^2}{\nu_p + \nu}. \end{aligned} \tag{23}$$

Substituting (22) and (23) into (17) gives the final form of the estimate

$$\hat{\sigma}_p^2 = \frac{\nu_p s_p^2 + \sigma_p^2 \chi^2}{\nu_p + \nu} \tag{24}$$

and the covariance matrix of the input data is

$$v_{ij} = \sum_p f_{ij}^p \frac{\nu_p s_p^2 + \sigma_p^2 \chi^2}{\nu_p + \nu}.$$

The estimate (24) for correlated data has the same form as for uncorrelated data, but the expression

$$\chi^2 = \boldsymbol{r}^T \boldsymbol{w} \boldsymbol{r} = \sum_{j,k} (y_j - \hat{y}_j) w_{jk} (y_k - \hat{y}_k)$$

appropriately takes into account the correlations between data.

V. Realization of the Estimators

Equations (13), (15), and (24) are implicit equations for $\hat{\sigma}_p^2$ that are to be solved by iteration. Equations (14) and (24) have previously been used in the analysis of uncorrelated data [6], [10]. Since the estimator (24) has the same form as for uncorrelated data, the detailed discussion [5] of its application is valid as well for the case of correlated data.

VI. Conclusions

The importance of having available methods for the objective correction of the *a priori* estimates of variances of the input data in an analysis of their inconsistency increases when the data are correlated because of the difficulty in tracing the relations among the original independently measured quantities that define the correlated input values and their uncertainties and covariances.

The approach described has the same interpretation as given for the case of uncorrelated data [5]. Its application gives improved estimates for the contributions to the covariance matrix of (3), and the *a posteriori* estimate of correlations between input values y_i can be calculated.

The primary result is the expression (24) $\hat{\sigma}_p^2 = \nu_p s_p^2 + \sigma_p^2 \chi^2 / \nu_p + \nu$, which replaces the simple Birge ratio ($\hat{\sigma}_p = \sqrt{\chi^2 / \nu s_p}$) for both correlated and uncorrelated inhomogeneous data (data of different 'types').

The effect of the application of (24) becomes most apparent when the initial approximation of the iteration is considered ($\hat{\sigma}_p^{2\,(0)} \equiv s_p^2$) so that (24) has the form

$$\frac{\hat{\sigma}_p^2}{s_p^2} = \frac{\nu_p + \chi^2}{\nu_p + \nu}.$$

From this it can be seen that the more reliable *a priori* estimates of the set $\{s_p^2\}$ (those with large ν_p) will be changed by factors closer to 1 than will the less reliable *a priori* estimates. (low ν_p). The amount of the changes will depend on the total inconsistency of data. The more the inconsistency ($\chi^2 \gg \nu$), the more all the uncertainties will be increased. For consistent data ($\chi^2 \approx \nu$) the factor is approximately unity, and there is little change in the uncertainty, while for $\chi^2 < f$ the *a priori* uncertainties will be decreased.

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