

A MULTIMEASURAND ISO GUM SUPPLEMENT IS URGENT

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ABSTRACT

A critical overview of the current doubtful practice on presentation of correlated data in the physics literature and in the scientific and technological databases is presented. The simple rules to calculate the rounding thresholds to preserve the positive definiteness of the covariance and correlation matrices as well as the rounding thresholds for the components of the mean vector to keep them inside the “non-rounded” scatter region are formulated. Evidence that in the multivariate case there are severe limitations on the applicability of the linear differential law of uncertainty propagation is presented. The explicit relation of the number of input random variables \mathbf{I} , the number of output variables \mathbf{D} , and the order \mathbf{T} of Taylor polynomials sufficient to preserve the self-consistent numerical presentation of the mean value of the vector function and its covariance matrix under nonlinear differential propagation procedure is obtained. It is stressed that the rounding thresholds for the safe rounding of correlated data impose the severe requirements on the storage and exchange formats of the correlated data that could not be met in the traditional publications on the paper but could be realized in the electronic media.

Keywords: Uncertainty Propagation Laws, Safe rounding of correlated data, Data quality, Measurement uncertainty

1 INTRODUCTION

Eleven years ago the famous ISO *Guide to Expression of Uncertainty in Measurement* (GUM) [1], [2], [3] appeared as the first official international document to focus metrologists and all practitioners working with measured data on the creation of an exhaustive and internationally acceptable standard on the expression of uncertainty in measurement. Unfortunately the ISO GUM is applicable only to the case of one measurand and is self-contradictory in some places because of this limitation. Existing international and national standards on the numerical expression of the estimates of physical quantities also are relatively well elaborated only for one measurand.

Historically, metrologists move slowly in creating the long awaited guidelines and standards for numerical presentations of the results on jointly measured quantities in scientific and technical documents¹. The absence of common procedures on the “expression of uncertainties” for multivariate cases leads to a proliferation of bad practices of presenting incorrect numbers in scientific and technical publications, in scientific and technological databases, and even in the authoritative numerical resources recommended by ICSU and CODATA (see examples of old and recent discussions of that “doubtful practice” in [9], [11], [12], [13], [14],[15], [29]).

Additional critical notes will be presented in the sections to follow. In some cases (unfortunately too often) the absence of presentation standards makes it impossible to compare the results of different measurements of the same set of quantities, even qualitatively.

Let us recall that for the correct numerical expression of the estimate of some random quantity one needs, at least, the following data structure: mean values and their confidence region (or scatter region). For a scalar quantity the mean value and one standard deviation interval are necessary. For a random vector, we need a mean vector and

¹It should be noted that some activity to improve the ISO GUM was started just after its first release (see [4]). Set of contemporary, informative, and instructive documents were created by SSfM group [5], [6].

multi-dimensional scatter region defined by the joint probability distribution. For example, for the m-dimensional normal distribution, the confidence region is the m-dimensional ellipsoid defined by the $m \times m$ covariance matrix. For $m = 2$, the corresponding data structure is:

$$\left(\begin{bmatrix} \zeta \\ \eta \end{bmatrix}, \begin{bmatrix} \sigma_\zeta^2 & \sigma_\zeta \sigma_\eta \cdot r_{\zeta\eta} \\ \sigma_\zeta \sigma_\eta \cdot r_{\zeta\eta} & \sigma_\eta^2 \end{bmatrix} \right) \Rightarrow \left(\begin{bmatrix} \zeta \pm \sigma_\zeta \\ \eta \pm \sigma_\eta \end{bmatrix}, \begin{bmatrix} 1 & r_{\zeta\eta} \\ r_{\zeta\eta} & 1 \end{bmatrix} \right) \quad (1)$$

To work with the above structure correctly in computations and data exchanges, one cannot use procedures developed and standardized for the case of “one measurand.” Indeed, for any admissible data transformations, we will have to trace the boundedness of the scatter region and inter-linkage of the transformed mean vector and the transformed scatter region. The end of the rounded mean vector should belong to the non-rounded scatter region. The simplest transformation that may destroy the correct result is independent rounding of the mean vector components and the matrix elements of the covariance matrix.

The above “quality requirements” are self evident; nevertheless, we have many examples from the scientific literature presenting results of measurements, computation, and data exchange procedures for which these requirements are badly violated: **(i)** experts report only mean vector components with corresponding “standard deviations” but not the correlation matrix, **(ii)** often estimates are “over-rounded” in such a way that the rounded matrix is non-positive semi-definite, and **(iii)** the end of the over-rounded mean vector is outside of the non-rounded (original) scatter region for many “standard deviations.”

To elucidate the above statements, let us consider a simple example of how one can destroy correct estimates by unjustified implementation of the procedures recommended only for the scalar case. We rotate the estimates (ζ, η) of a two-dimensional vector to obtain vector (x, y) by rotation by the angle $\pi/4$:

$$\begin{pmatrix} \zeta \\ \eta \end{pmatrix} = \begin{pmatrix} \sqrt{2}(1.500 \pm 0.100) \\ \sqrt{2}(0.345 \pm 0.001) \end{pmatrix}, \quad r(\zeta, \eta) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \Leftrightarrow \begin{cases} x = (\zeta + \eta) / \sqrt{2} \\ y = (\zeta - \eta) / \sqrt{2} \end{cases} \Leftrightarrow$$

$$\begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} 1.845 \pm 0.100 \\ 1.155 \pm 0.100 \end{pmatrix}, \quad r(x, y) = \begin{pmatrix} 1.0000 & 0.9998 \\ 0.9998 & 1.0000 \end{pmatrix} \quad (2)$$

In this example, the calculations are produced with sufficient stipulated numerical accuracy. It is easy to see that the standard rounding rules recommended for the statistically independent quantities are not applicable in this case. If the correlation coefficients are to be rounded as recommended in ISO GUM, “. . . Correlation coefficients should be given with three digit accuracy if their absolute values are near unity,” one will get a degenerate correlation matrix.

The numerical presentations of the (x, y) components, which seem redundant for statistically independent x and y estimates, are correct indeed. The independent rounding by standard rules will move the end of the (x, y) vector out of the image of the initial scatter region. For example, after the first rounding step, we get the deviation:

$$\begin{pmatrix} \Delta x / \sigma_x \\ \Delta y / \sigma_y \end{pmatrix} = \begin{pmatrix} -0.05 \\ 0.05 \end{pmatrix}, \quad r(x, y) = \begin{pmatrix} 1.0000 & 0.9998 \\ 0.9998 & 1.0000 \end{pmatrix}$$

To characterize this deviation quantitatively, we can use the quadratic form χ^2 . The confidence region in terms of $(\Delta x, \Delta y)$ is defined by the condition:

$$\begin{bmatrix} \Delta x / \sigma_x & \Delta y / \sigma_y \end{bmatrix} \cdot \frac{1}{1 - 0.9998^2} \cdot \begin{bmatrix} 1.0000 & 0.9998 \\ 0.9998 & 1.0000 \end{bmatrix} \cdot \begin{bmatrix} \Delta x / \sigma_x \\ \Delta y / \sigma_y \end{bmatrix} = \chi^2(\Delta x, \Delta y) \leq 1$$

Inserting values of the relative deviations at the first step we get:

$$\chi^2(-0.05, 0.05) = \frac{0.0025}{1 - 0.9998^2} \cdot [-1, 1] \cdot \begin{bmatrix} 1.0000 & 0.9998 \\ 0.9998 & 1.0000 \end{bmatrix} \cdot \begin{bmatrix} -1 \\ 1 \end{bmatrix} = 25 > 1$$

This value for χ^2 corresponds to deviation of the (x, y) vector out of the scatter region by more than three standard uncertainties. If rounding is performed up to one digit to the right of decimal point, as is recommended by all textbooks: $(1.845 \pm 0.100, 1.155 \pm 0.100) \Rightarrow (1.8 \pm 0.1, 1.2 \pm 0.1)$, then

$\chi^2(-0.045, 0.045) = 2025 \gg 1$, \Rightarrow deviation is more than for 30 standard uncertainties.

In many analogous cases authors give estimates of the vector components and their uncertainties only, without any information about correlations. It is easy to see from the above calculations that this can completely destroy the results of the measurement (estimation).

2 RECENT EXAMPLES OF CORRELATED DATA PRESENTATION

In what follows we will need multiple references to some instructive statements from the basic metrology document — the ISO GUM. To simplify reading we will quote some statements here.

0.1 When reporting the result of a measurement of a physical quantity, it is obligatory that some quantitative indication of the quality of the result be given so that those who use it can assess its reliability. Without such an indication, measurement results cannot be compared, either among themselves or with reference values given in a specification or standard. It is therefore necessary that there be a readily implemented, easily understood, and generally accepted procedure for characterizing the quality of a result of a measurement, that is, for evaluating and expressing its uncertainty. . . .

0.4 The ideal method for evaluating and expressing the uncertainty of the result of a measurement should be:

universal: the method should be applicable to all kinds of measurements and to all types of input data used in measurements.

The actual quantity used to express uncertainty should be:

internally consistent: it should be directly derivable from the components that contribute to it, as well as independent of how these components are grouped and of the decomposition of the components into subcomponents;

transferable: it should be possible to use directly the uncertainty evaluated for one result as a component in evaluating the uncertainty of another measurement in which the first result is used. . . . (ISO GUM [1], p. vii)

It was expected that detailed deployment of these general requirements would focus efforts of practitioners indifferent scientific and technical areas on the creation of the standard methodology of measurements and expression the results in traditional and electronic forms. An example of such recommendations from Section 7 “Reporting uncertainty” of ISO GUM is as follows:

7.1.4 Although in practice the amount of information necessary to document a measurement result depends on its intended use, the basic principle of what is required remains unchanged: when reporting the result of a measurement and its uncertainty, it is preferable to err on the side of providing too much information rather than too little. For example, one should

- a) describe clearly the methods used to calculate the measurement result and the uncertainty from the experimental observations and input data;
- b) list all uncertainty components and document fully how they were evaluated;
- c) present data analysis in such a way that each of its important steps can be readily followed and the calculation of the reported results can be independently repeated if necessary;
- d) give all corrections and constants used in the analysis and their sources. (ISO GUM [1], p. 25)

A test of the foregoing list is to ask oneself: “Have I provided enough information in a sufficiently clear manner that my result can be updated in the future if new information or data become available?”

In spite of broad discussions of the ISO GUM in international and national metrology bodies over the past ten years, we still have no commonly accepted methodology on the numerical presentations of the estimates of the multivariate random quantities in publications and in databases, even on the level of the existing ISO GUM requirements 0.0.1–

0.0.4, 7.1.4. Presumably this is because the ISO GUM is a first generation document, especially in recommendations concerning the expression of the results on several jointly measured quantities:

7.2.5 If a measurement determines simultaneously more than one measurand, that is, if it provides two or more output estimates y_i (see H.2, H.3, and H.4), then, in addition to giving y_i and $uc(y_i)$, give the covariance matrix element $u(y_i, y_j)$ or the element $r(y_i, y_j)$ of the correlation coefficient matrix (C.3.6, note 2) (and preferably both).

7.2.6 The numerical values of the estimates y and its standard uncertainty $uc(y)$ or expanded uncertainty U should not be given with an excessive number of digits. It usually suffices to quote $uc(y)$ [as well as the standard uncertainty $u(x_i)$ of the input estimates x_i] to at most two significant digits, although in some cases it may be necessary to retain additional digits to avoid round-off errors in subsequent calculations. . . .

. . . Output and input estimates should be rounded to be consistent with their uncertainties; for example, if $y = 10.05762 \Omega$ with $uc(y) = 27m\Omega$, y should be rounded to 10.058Ω . Correlation coefficients should be given with three-digit accuracy if their absolute values are near unity. (ISO GUM [1], p. 26-27)

The above example with rotation of the two dimensional random vector clearly shows that clause 7.2.6 need to be reconsidered and probably reformulated.

2.1 Incorrect expression of the uncertainty of measurements in ISO GUM

Our simple example with rotating the estimate of the two dimensional vector has shown that clause 7.2.6 of ISO GUM can be misleading. Moreover the application of the 7.2.6 recommendation for the rounding correlations in Example H.2 of section “Annex H: Examples” of ISO GUM clearly shows the failure of that recommendation. Indeed, in Tables H.3 and H.4, correlation matrices are represented with three decimal digits to the right of decimal point in accordance with 7.2.6

$$\begin{bmatrix} 1.000 & -0.588 & -0.485 \\ -0.588 & 1.000 & 0.993 \\ -0.485 & 0.993 & 1.000 \end{bmatrix} \quad (3)$$

The eigenvalues of this matrix are [2.403 740 76, 0.596 712 77, -0.000 453 53]. This means that the correlation matrix is destroyed. The correct matrix calculated from the data in Table H.2 with 16 digits to the right of decimal point is

$$\begin{bmatrix} 1.000 & -0.5882768557970084 & -0.4850646136631822 \\ -0.5882768557970084 & 1.000 & 0.9925075421320323 \\ -0.4850646136631822 & 0.9925075421320323 & 1.000 \end{bmatrix}$$

The eigenvalues are all positive, as they should be by definition of the correlation matrix: 2.403 564 371 235 8685, 0.596 435 606 493 034, 2.227 109 758 149 771×10⁻⁸.

With our estimate of the safe rounding threshold (see further in this text) we can express this matrix in a more visible form:

$$\begin{bmatrix} 1.000 & -0.58827686 & -0.48506461 \\ -0.58827686 & 1.000 & 0.99250754 \\ -0.48506461 & 0.99250754 & 1.000 \end{bmatrix}$$

Note. There is a logical inconsistency in the ISO GUM. On the one hand there is a warning in the text that it is applicable to one measurand only, but on the other hand, when describing recommendations of how to estimate the

uncertainty of the one random function which is dependent upon several random quantities we unavoidably meet the problem of the correct numerical expression for the estimates of the random vectors².

2.2 Experiment CERN-LEP-DELPHI in the European Physical Journal

Abreu [19] has presented results of Tau topological branching ratios for the reactions:

$$B_1(\tau^- \rightarrow h^- \text{ neutrals}), B_2(\tau^- \rightarrow h^+ 2h^- \text{ neutrals}), B_3(\tau^- \rightarrow 2h^+ 3h^- \text{ neutrals})$$

presented in [19] (see p. 636 and Table 6) these data can be collected into the following data structure:

$$\begin{bmatrix} B_1 \\ B_2 \\ B_3 \end{bmatrix} = \left(\begin{bmatrix} 0.85316 \pm 0.000929^{stat} \pm 0.000492^{syst} \\ 0.14569 \pm 0.000929^{stat} \pm 0.000477^{syst} \\ 0.00115 \pm 0.000126^{stat} \pm 0.000059^{syst} \end{bmatrix}, \begin{bmatrix} 1.00 & -0.98 & -0.08 \\ -0.98 & 1.00 & -0.08 \\ -0.08 & -0.08 & 1.00 \end{bmatrix} \right) \quad (4)$$

in which the correlation matrix is the correlation matrix for the total uncertainties (combined statistical and systematic). In examples 2 and 3 above, we saw that independent rounding of correlation matrix elements is a very dangerous transformation especially when correlations are large (close to 1). The total correlator in the publication under discussion is rounded up to two digits to the right of decimal point and over-rounding is suspected.

In addition, in the text, the statistical and systematic uncertainties are quoted separately (4), but there are no descriptions of how they were combined to give the total uncertainties or how the correlation of the total uncertainties ([19] page 636) was obtained. Our attempts to make the relevant data presented in different places of the cited paper agree resulted in the following matrix (5).

$$\begin{bmatrix} 1 & -0.99241481160724 & -0.0847891616844724 \\ -0.992414811607243 & 1 & -0.03348650681292892 \\ -0.084789161684472 & -0.03348650681292892 & 1 \end{bmatrix} \quad (5)$$

Its eigenvalues are 1.993743788696688, 1.0056742957244327, and 0.0005819155788786556. In accordance with the safe rounding threshold [29] (see section 4), we can represent matrix (5) in a more visible form:

$$\begin{bmatrix} 1 & -0.9924 & -0.0848 \\ -0.9924 & 1 & -0.0335 \\ -0.0848 & -0.0335 & 1 \end{bmatrix} \quad (6)$$

It differs from that of presented in the paper and can not be rounded further. We have tried to obtain the correct numerical data from the authors of the cited paper but failed. It seems that the correct original data were lost forever.

2.3 Experiment CLEO in the Physical Review

In the paper by Anastassov [20] of the CLEO collaboration, the results of joint measurement of the five combinations of the τ -lepton branching ratios are presented. The “corrected” correlation matrix represented in the Erratum has the form:

TABLE XII. Correlation coefficients between measurements of branching fractions.

C_τ	B_e	B_μ	B_h	B_μ/B_h	B_h/B_e
B_e	1	0.50	0.48	-0.42	-0.39
B_μ		1	0.50	0.58	0.08
B_h			1	0/07	0.53
B_μ/B_h				1	0.45

² Unfortunately the erroneous recommendation 7.2.6 of ISO GUM in part concerning the rounding correlations, as well as its application in example H.2 of Annex H: Examples, were not noticed by the metrology community. Both the recommendation and example H.2 are reproduced in other metrology documents [2], in the recent “best practice guide” review [7] (see p.20,) used in publications, monographs (see further examples in the subsections to follow), and in textbooks (see for example a recent textbook [18] p.128-129)

B_h/B_e					1
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The eigenvalues of this matrix are: (2.1735, 1.7819, 1.0550, -0.0075, -0.0028), in sharp contradiction with the positive definiteness requirement. The accuracy of these data are clearly in question.

2.4 Misinformation in the presentation of the fundamental physical constants in Reviews of Modern Physics and in reprints

Let us trace the variation of estimates of a selection of derived fundamental physical constants (FPC) in the last three consecutive adjustments published in the Reviews of Modern Physics and recommended by CODATA as the unique international source of reference data on FPC.

CODATA:1986 [21]	Symbol [Units]	Value (Uncertainty)×scale	Correlations
Elementary charge	e [C]	1.602 177 33(49) ×10 ⁻¹⁹	e h m _e
Plank constant	h [J s]	6.626 075 5(40) ×10 ⁻³⁴	0.997
Electron mass	m _e [kg]	9.109 389 7(54) ×10 ⁻³¹	0.975 0.989
1/α(0)	α(0) ⁻¹	137.035 989 5(61)	-0.226 -0.154 -0.005
CODATA:1998 [22]			
Elementary charge	e [C]	1.602 176 462(63)	e h m _e
Plank constant	h [J s]	×10 ⁻¹⁹ 6.626 068 76(52)	0.999
Electron mass	m _e [kg]	×10 ⁻³⁴	0.990
1/α(0)	α(0) ⁻¹	9.109 381 88(72) ×10 ⁻³¹	-0.049 0.996
		137.035 999 76(50)	-0.002 0.092
CODATA:2002 [23]			
Elementary charge	e [C]	1.602 176 53(14) ×10 ⁻¹⁹	e h m _e
Plank constant	h [J s]	6.626 0693(11) ×10 ⁻³⁴	1.000
Electron mass	m _e [kg]	9.109 3826(16) ×10 ⁻³¹	0.998 0.999
1/α(0)	α(0) ⁻¹	137.035 999 11(46)	-0.029 -0.010 0.029

All three-correlation sub-matrices (see above table) are presented in accordance with GUM clause 7.2.6 with three digits to the right of the decimal point.

All matrices turn out to be over-rounded, each of which has a negative eigenvalue with absolute values much larger than the machine zero ~10⁻¹⁷:

CODATA: 1986 {2.99891, 1.00084, 0.000420779, -0.000172106};

CODATA: 1998 {2.99029, 1.01003, -0.000441572, 0.00012358};

CODATA: 2002 {2.99802, 1.00173, 0.000434393, -0.000183906}.

In May, 2005 on the NIST site, the new version of FPC (version 4.2) appeared. In this new version the misprints encountered in versions 4.0 and 4.1 were fixed, and for the first time the computer readable files for the basic LSA (Least Square Adjusted) FPC were released. The data in the computer readable files are free of critical issues (see [29]) and presented with sufficient precision to be safely used in high precision calculations.

Historically the maintenance of the FPC set and re-adjustments are produced only at NIST (USA). All handbooks and textbooks reprinted the over-rounded data from NIST publications without mentioning the presence of large correlations between uncertainties of some constants. The majority of authoritative issues also reprinted NIST data without any comments or warnings (see [24], [25], [26], [27], and [28]).

3 THRESHOLDS FOR SAFE ROUNDING OF CORRELATED QUANTITIES

In the above examples, we show that the rules of the numerical presentations developed for one measurand are inapplicable in multivariate cases. In this section we describe the construction of thresholds for safe uniform rounding in the multivariate case developed in [29]. These thresholds are relatively simple parameters that could be used to control the self consistency of the numerical estimates of correlated quantities or, in other words, to control the quality of the multivariate data presentation. We treat the numerical data on the estimates of the random vector as self consistent if the data structure consists at least of two obligatory items:

- (i) the mean value of the vector components and
- (ii) the scatter region for it obtained with the predefined confidence level.

In the simplest case, the scatter region is the scatter ellipsoid defined by the matrix of the second moments of the joint probability distribution. For our derivations we will need a few statements from the classical matrix theory.

Weil's theorem (see [30], [32]): Let $C = A + B$, where $A, B, C \in R^{n \times n}$ – symmetric matrices and $(\alpha_1 \leq \alpha_2 \dots \leq \alpha_n)$, $(\beta_1 \leq \beta_2 \dots \leq \beta_n)$, $(\gamma_1 \leq \gamma_2 \dots \leq \gamma_n)$ their eigenvalues correspondingly. Then $\forall i$ the following inequalities are valid

$$\alpha_i + \beta_{\min} \leq \gamma_i \leq \alpha_i + \beta_{\max} . \tag{7}$$

Gershgorin's theorem ([30], [31], [32]): Every eigenvalue α_i of the matrix A belongs to the interior of one of the circles

$$|A_{ii} - \alpha_i| \leq \sum_{j=1}^n |A_{i\#j}| . \tag{8}$$

Schur's theorem ([32]): Let matrix $B \in R^{n \times n}$ is symmetric with values of the diagonal elements $B_1 \leq B_2 \dots \leq B_n$ any order) and eigenvalues $\beta_1 \leq \beta_2 \dots \leq \beta_n$, then $\forall k \leq n$

$$\sum_{i=1}^k \beta_i \leq \sum_{i=1}^k B_i \tag{9}$$

The equality takes place only for $k = n$.

Let $\{ \langle x_i \rangle, u_i, r_{ij}, N_{dig}^r \}$, $i, j = 1, \dots, n$ be the list of decimal numbers expressing the results of n jointly measured quantities with: $\langle x_i \rangle$ - the real decimal number representing the mean value of i -th observable; u_i - its uncertainty the positive real decimal number; r_{ij} - real decimal numbers representing the matrix elements of the symmetric, positive definite matrix (correlation matrix) such that $r_{ii} = 1 \forall i \leq n, |r_{i\#j}| < 1.0$; N_{dig}^r - integer non negative number defining the unified decimal precision of the non diagonal matrix elements of the correlation matrix r_{ij} .

This list is the minimum set of parameters needed for correctness and pithiness of the quantitative description of the random vector quantity $\{x_i\}$ and its scatter region defined by the “confidence radius” $R_{g,CL}$ and the joint probability distribution function g on the confidence level CL

$$\sum_{i,j} \frac{x_i - \langle x_i \rangle}{u_i} \cdot r_{ij}^{-1} \cdot \frac{x_j - \langle x_j \rangle}{u_j} < R_{g,CL}^2 \tag{10}$$

If g is unknown but the matrix of the second moments is known, Kramer's scatter ellipsoid is used with $R^2 = n + 2$ (see [34] page 80-81, [35] page 102).

A proposed additional parameter $N_{dig}^{r,th}$ is needed to assure the quality of the data and its preservation in the processes of data transfers and in calculations. From the statements of the Weil's (7), Gershgorin's (8), and Shur's (9) theorems, it follows that the rounding threshold, i.e. the minimum number N of decimal digits to the right of the decimal point that should be preserved in rounding of the non diagonal elements of the correlation matrix r_{ij} with the minimal eigenvalue $c_l = \lambda_{\min}^r$, is defined by³

³ An analogous estimate in other terms was obtained recently in paper [33].

$$N_{dig}^{r,*} \geq N_{dig}^{r,th} = \left\lceil \log_{10} \left(\frac{n-1}{2 \cdot \lambda_{\min}^r} \right) \right\rceil \quad (11)$$

Analogous rounding thresholds $N_{dig,i}^x$ are obtained for the mean values $\langle x_i \rangle$ and $N_{dig,i}^u$ for the standard deviations u_i . They also are determined by the minimal eigenvalue of the correlation matrix.

$$N_{dig,i}^x > \left\lceil \frac{1}{2} \log_{10} \left(\frac{n}{4 \cdot (R_{g,CL}^2) \cdot \lambda_{\min}^r \cdot (u_i / [ubit_i])^2} \right) \right\rceil \quad (12)$$

$$N_{dig,i}^u = N_{dig,i}^x \quad \forall i = 1, \dots, n. \quad (13)$$

In summary, the independent uniform rounding of the decimal estimates of the results of multiple, jointly measured (estimated), random quantities is allowed only under restrictions posed by the requirements of the boundedness in the “rounded scatter region” (ellipsoid) and the confinement of the end of the rounded mean vector inside the non-rounded scatter region (ellipsoid). To safely round the accuracies of the numbers in the structure should be higher than the rounding thresholds (11), (12), (13) defined by the minimal eigenvalue of the positive definite correlation matrix of the structure to be rounded.

3.1 Criteria for self-consistent expression of the results of joint measurements

For the case of joint measurements or estimations of D quantities, to express the results correctly one has to present the following (minimal) structure $\{ \langle x_i \rangle, u_i, r_{ij}, N_{dig}^r \}$, $i, j = 1, \dots, D$.

We propose to expand it to the structure

$$\left\{ \left\{ \langle x_i \rangle, u_i(x_i), N_{dig}^x \right\}, \left\{ r(x_i, x_j), N_{dig}^{r,th} \right\} \right\}, i, j = 1, \dots, D \quad (14)$$

and advocate this view as a candidate standard for the numerical expression of the correlated measurements (estimates). Such expansion is needed to assure the quality of the measured data and to inform potential users about the critical precision needed for correct numerical computations in applications. Indeed, to form the structure proposed above (14), one needs to:

- calculate the matrix elements of the correlation matrix with enough precision to assure its positive definiteness and calculate the corresponding rounding threshold $N_{dig}^{r,th}$;
- calculate mean values and their standard deviations with precisions higher than the corresponding rounding thresholds $N_{dig,i}^x$.

4 NONLINEAR UNCERTAINTIES PROPAGATION LAW IS UNAVOIDABLE

In this section, we will show that the problem of correct multivariate rounding is tightly intertwined with the problem of multivariate uncertainty propagation. In most multivariate cases, the widely used linear differential uncertainty propagation law is inapplicable. One will have to use integral (Monte Carlo) or nonlinear differential (higher order Taylor polynomials) uncertainty propagation laws.

Let us present the problem of propagating uncertainties from I random variables $\{ \langle x_i \rangle, u_i(x_i), r(x_i, x_j) \}$ with a positive definite correlation matrix $r(x_\alpha, x_\beta)$ to the system of D functions $y_i = \{F_i(x_\alpha)\}_1^D$. This means that we have to obtain estimates to fill the minimal structure $\{ \langle y_i \rangle, u_i(y_i), r(y_i, y_j) \}$. In the general case (with nonsingular functions) when the joint probability distribution function $g(x_1, \dots, x_n)$ is known, this problem is formulated as follows:

- 1) calculate the joint probability distribution function

$$G(y_1, \dots, y_D) = \int \prod_{i=1}^D \delta(y_i - F_i(x_\alpha)) \cdot g(x_\alpha) \cdot d^I x \quad (15)$$

and then calculate any of its joint moments if needed. In reality, however, this approach often turns out to be unfeasible. The $g(x_\alpha)$ is unknown, or the reliable calculation of $G(y_i)$ is impossible because of the lack of computer power.

2) The usual way to solve the uncertainty propagation problem is with the following approximations (valid and supposedly working well for the multinormal distribution $g(x_\alpha)$):

calculate
$$\mu_i = \langle y_i \rangle = \int F_i(x_\alpha) \cdot g(x_\alpha) \cdot d^I x_\alpha, \quad (16)$$

then calculate

$$u(y_i, y_j) = \int (F_i(x_\alpha) - \langle y_i \rangle) \cdot (F_j(x_\alpha) - \langle y_j \rangle) \cdot g(x_\alpha) \cdot d^I x_\alpha \quad (17)$$

It is known in classical function analysis and linear algebra that because of the positive definiteness of $g(x_\alpha)$, the matrix (17), calculated without approximation and with sufficient accuracy, is the positive definite matrix for any linearly independent system of functions $\{F_i(x_\alpha)\}_1^D$ (see [32], theorem 7.2.10).

As previously mentioned, often the distribution function is not known, but its few first moments are known. In such cases, error propagation is carried out by the “nonlinear differential uncertainty propagation law” that is derived from the integral one (17) by the replacement of $F_i(x_\alpha) - \mu_i$ for the polynomials obtained by the cuts of the Taylor series for $F_i(x_\alpha) - \mu_i$

$$F_i(x_\alpha) - \mu_i \Rightarrow P_i^T(x_\alpha) = \sum_{k=1}^T \frac{1}{k!} \cdot \frac{\partial^k F_i}{\partial x_{\alpha_1} \dots \partial x_{\alpha_k}} \cdot \Delta x_{\alpha_1} \dots \Delta x_{\alpha_k}, \quad (18)$$

where $\Delta x_{\alpha_i} = x_{\alpha_i} - \langle x_{\alpha_i} \rangle$ and the sums over the repeated indices α_j are assumed⁴.

Let us show, however, that the requirement for positive definiteness of the correlation matrix poses clear restrictions on the powers T of Taylor’s polynomials even in cases when the approximations $\mu_i \approx F_i(\langle x_\alpha \rangle)$ are valid (the senior moments are small). Indeed, the maximal number $n(T, I)$ of the linearly independent functional vectors of the type (18) is determined by the relation

$$n(T, I) = \sum_{k=1}^T \frac{(I+k-1)!}{(I-1)!k!} = \frac{(T+I)!}{T!I!} - 1. \quad (19)$$

From this estimate, the following statement applies: if the covariance matrix of the system of D functions $\{F_i(x_\alpha)\}_1^D$ depending upon I random variables $\{x_{\alpha_j}\}_1^I$ is determined by the differential uncertainty propagation law (18) of T -th order such that $n(T, I) < D$, then it is degenerate and its numerical expression in decimal numbers will be a matrix with at least one non positive eigenvalue.

In particular the widely used linear ($T = 1$) uncertainty propagation law

$$F_i(x_\alpha) - \mu_i \Rightarrow P_i^1(x_\alpha) = \sum_{\alpha=1}^I \frac{\partial F_i}{\partial x_\alpha} \cdot (x_\alpha - \langle x_\alpha \rangle) \quad (20)$$

for $D > I$ is invalid, and for $D \leq I$ it is dangerous because of the possibility of the existence of hidden functional relationships such as $\Phi(F_1, F_2, \dots, F_D) = const$. Indeed, let $D \leq I$. Then the output matrix in the linear propagation law in the general case is non degenerate. However, if there is at least one relationship of the type $\Phi(F_1, F_2, \dots,$

⁴It should be noted that in the ISO GUM the corresponding formula for higher terms contributions to the variance are incorrect, and the crucial terms are missing. This will cause wrong results in calculations (besides rounding) and for some nonlinear cases one will even obtain negative variances (see ISO GUM: clause 5.1.2)

$F_D) = const$, then the matrix $u(F_i, F_j)$ derived by the linear uncertainty propagation is degenerate. It is easy to show this. Let us have such a relationship with $\Phi(F_1, F_2, \dots, F_D)$ that is smooth enough. Then its gradient with respect to $\{x_\alpha\}^1$ is expressible as the linear combination of the gradients F_i ,

$$\frac{\partial \Phi}{\partial \alpha_i} = \frac{\partial \Phi}{\partial F_1} \cdot \frac{\partial F_1}{\partial \alpha_i} + \frac{\partial \Phi}{\partial F_2} \cdot \frac{\partial F_2}{\partial \alpha_i} + \dots + \frac{\partial \Phi}{\partial F_D} \cdot \frac{\partial F_D}{\partial \alpha_i} \equiv 0,$$

and from the other side it is the null vector. This means that gradients of F_i are linearly dependent, and hence the covariance matrix obtained by the linear uncertainty propagation law is degenerate. However, the matrix $u(F_i, F_j)$, calculated with the integral uncertainty propagation law (17) with relationship $\Phi(F_1, F_2, \dots, F_D) = const$ (imposed via the Dirac's δ -function which is non-negative everywhere by definition), is the positive definite matrix.

$$u(F_i, F_j) = \int (F_i(x_\alpha) - \mu_i) \cdot (F_j(x_\alpha) - \mu_j) \cdot \delta(\Phi(F_1, \dots, F_D) - const) \cdot g(x_\alpha) \cdot d^I x, \quad (21)$$

Unfortunately in the majority of texts known to the author on statistical data handling, the positive definiteness of the covariance (correlation) matrix is declared but often does not checkout in applied analytical and numerical calculations. Let us present an example from the recommendations of ISO GUM:

5.1.2 The combined standard uncertainty $u_c(y)$ is the positive square root of the combined variance $u_c^2(y)$, which is given by

$$u_c^2(y) = \sum_{i=1}^N \left(\frac{\partial f}{\partial x_i} \right)^2 u^2(x_i) \quad (10)$$

where f is the function given in equation (1). Each $u(x_i)$ is a standard uncertainty evaluated as described in 4.2 (Type A evaluation) or as in 4.3 (Type B evaluation). The combined standard uncertainty $u_c(y)$ is an estimated standard deviation and characterizes the dispersion of the values that could reasonably be attributed to the measurand Y (see 2.2.3). Equation 10 and its counterpart for correlated input quantities, Equation 13, both of which are based on a first-order Taylor series approximation of $Y = f(X_1, X_2, \dots, X_N)$, express what is termed in this guide the law of propagation of uncertainty (see E.3.1 and E.3.2).

Note – When the nonlinearity of f is significant, higher-order terms in the Taylor series expansion must be included in the expression for $u_c^2(y)$, Equation 10. When the distribution of each X_i is symmetric about the mean, the most important terms of next highest order to be added to the terms of Equation 10 are

$$\sum_{i=1}^N \sum_{j=1}^N \left(\frac{1}{2} \left(\frac{\partial^2 f}{\partial x_i \partial x_j} \right)^2 + \frac{\partial f}{\partial x_i} \cdot \frac{\partial^3 f}{\partial x_i \partial^2 x_j} \right) \cdot u^2(x_i) \cdot u^2(x_j)$$

See H.1 for an example of a situation where the contribution of higher-order terms to $u_c^2(y)$ needs to be considered. (ISO GUM [1], p. 19)

In this recommendation of the formula for the fourth order contribution in $u(x_i)$ into the variance of f , the terms containing the third partial derivatives of f are included by mistake and for some nonlinear f , lead to a negative valued variance $u_c^2(y)$. This mathematical incorrectness was missed in the Russian translation of the ISO GUM [3], and is reproduced in a recent SSfM document [7] (see section 6.3 p.68-70) and in a recent metrology paper devoted to the higher-order corrections for propagating uncertainties [40]. For the correct expression for this case see, for example, the recent book [36], section 12.4.2, p. 278-280.

5 CONCLUSION

In a few examples of present practice, we have shown that the current manner to express and exchange numerical multivariate measured data is obsolete⁵ and should be modernized with urgency. It seems that the majority of the published data that are incorrectly expressed and presented were obtained by inadmissible applications to the

⁵This observation is not new. It is sufficient to quote the papers [9], [10], [11], [12], [13], [39], [41] where one can find further evidence that the multivariate data presented in scientific and technical publications, posted on the web pages, stored in handbooks and in the databases are in large portions incorrect and it is dangerous to use them for simulations of refined research or for simulations in the behavior of new high precision devices without careful input control and filtering.

multivariate case through the recommendations of ISO GUM and instructions from other metrology documents that were worked out only for the case of one measurand. We calculate that such confusion is partly inspired by the (in some cases incorrect) statements in the ISO GUM and by the absence of the analogous multivariate GUM (see, however, [4], [5], and [6]).

The problem is especially sharp and urgent for the fundamental natural sciences where the requirements for data quality are becoming more and more stringent. New measurement techniques and devices have appeared and new data handling systems have been created, but the practice of expressing and exchanging the measured data still evolves too slowly. This permanent delay is the main reason for the appearance of incomplete and incorrect multivariate measured data in publications, in scientific and technological databases, and in scientific information agencies and sites that are “constrained” by the incomplete and partly incorrect recommendations and standards of respectable international metrology organizations (see the analogous view in the editorial note of Paul De Bièvre [37]).

We hope that we have found a correct way to try to arrive at partial answers to the posed questions. We suggest as a first step that the ISO GUM should be revised. It seems more reasonable not to correct the original text incrementally (in the inconsistent and incorrect places indicated in the literature) but to make a complete revision by taking into account new methodology from the SSfM programme (see [4],[7], [15], [6]); the results of the NNDC(BNL) Cross Section Evaluation Working Group summarized in [38] (see sections 30. to 40.); critical statements and suggestions from [39], [41]; and new possibilities in data presentation and exchange provided by electronic publishing⁶.

Then the planned Gum Supplement 2 (the multivariate expansion of the ISO GUM) should be prepared and issued with urgency. We propose that work to include the following topics:

- Obligatory items in the multivariate data structure should be: mean values of random vector components with their rounding thresholds; covariance matrices and correlation matrices with their rounding thresholds; minimally sufficient, but detailed, descriptions of the procedures used to obtain estimates of all components of the structure. If directed rounding is used (instead of uniform rounding), then a detailed description of the rounding strategy should be given instead of rounding thresholds.
- If the multivariate data adopted from sources with incomplete data presentations were used, then in the reported results a detailed description of the data quality “input check-ups” of the adopted data should be obligatory presented;
- If differential uncertainty propagation procedures are used in the course of obtaining the final results, a detailed description of the uncertainty propagation procedure should be presented as well as estimates for the used higher moments of the joint distribution function of the “propagated variables.”

Having reworked ISO GUM and Gum Supplements 1 and 2, the other instructive documents, guides, handbooks, and textbooks that used the obsolete recommendations of the ISO GUM should be corrected. After the first official release of the internationally approved new edition of the ISO GUM with GUM supplements 1 and 2 it will be very useful to apply to editors of all scientific journals, scientific information agencies, and data sites, as articulated in the appeal of Paul De Bièvre

“... So, a result without reliability (uncertainty) statement cannot be published or communicated because it is not (yet) a result. I am appealing to my colleagues of all analytical journals not to accept papers anymore which do not respect this simple logic”. Paul De Bièvre [12]

Having a formalized standard for the minimal, multivariate, data structure respected by the scientific and publishing communities timely revised in the metrology community, we can hope to have all procedures of multivariate data handling clearer and reported data more reliable.

⁶Suggestion on the optimal content of the reports on the search results see in [36] (section 13.2 Desiderata for an optimal report of search results, p.286-287).

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7 REFERENCES

- [1] BIPM, IEC, IFCC, ISO, IUPAC, IUPAP, and OIML (1995) *Guide to the Expression of Uncertainty in Measurement*. ISBN 92-67-10188-9, Second Edition. [ISOGUM](#)
- [2] B. N. Taylor, B. & Kuyatt, C. (1994) *Guidelines for Evaluating and Expressing the Uncertainty of NIST Measurement Results*. NIST Technical Note 1297. [NIST-GUM](#)
- [3] Slaev, V. (ed.) (1999) *Guide to the Expression of Uncertainty in Measurement* (Russian translation of the ISO GUM) - GP, VNIIM, S.-Petersburg.
- [4] Cox, M. & Harris, P. (2003) The GUM and its planned supplemental guides. *Accred. Qual. Assur.* 8, 375.
- [5] Retrieved from the WWW, August 15, 2007: <http://www.npl.co.uk/ssfm/>.
- [6] ISO/PRF Guide 99998, (2006) *Guide to the expression of uncertainty in measurement (GUM) – Supplement 1: Numerical methods for the propagation of distributions*, under development. [GUM Supplement 1](#)
- [7] Cox, M. & Harris, P. (2006) *Uncertainty Evaluation. Best Practice Guide No. 6. Software Support for Metrology*. NPL Report, DEM-ES-11, National Physics Laboratory, Teddington, UK.
- [8] Cox, M. & Harris, P. (2004) *SSfM Best Practice Guide No 11, Numerical analysis for algorithm design in Metrology*. Technical report, NPL, Teddington, UK.
- [9] Fox, L. (1971) How to get meaningless answers in scientific computation (and what to do about it). *IMA Bulletin* 7, 296.
- [10] Smith, D. (1991) *Probability, Statistics, and Data Uncertainties in Nuclear Science and Technology*. La-Grange Park, Illinois, USA: American Nuclear Society.
- [11] Kahan, W. (1996) *The Improbability of PROBABILISTIC ERROR ANALYSES for Numerical Computations*. [improber.pdf](#).
- [12] De Bièvre, P. (1997) Measurement results without statements of reliability (uncertainty) should not be taken seriously. *Accred. Qual. Assur.* 2, 269.
- [13] Badikov, S. (1998) Statistical analysis of correlated data and evaluation of the neutron cross sections. *Atomic Energy* 84, 426 (in Russian).
- [14] Siver, A. & Ezhela, V. (2003) *On the CODATA recommended values of the fundamental*

physical constants: V3.2 (1998) and V4.0 (2002). IHEP-2003-34.

- [15] Cox, M. & Harris, P. (2004) *SSfM Best Practice Guide No 11, Numerical analysis for algorithm design in metrology*. Technical report, NPL, Teddington, UK.
- [16] Ezhela, V., Kuyanov, Y., Larin, V. & Siver, A. (2004) The Inconstancy of the Fundamental Physical Constants: Computational Status. *arXiv:physics/0409117*.
- [17] Slaev, V. *Recommendations on Application of the Document "Guide to the Expression of Uncertainty in Measurement" in Russia*. [VNIIM-2000](#).
- [18] Lira, I. (2002) *Evaluating the Measurement Uncertainty. Fundamentals and practical guidance*. IoP Publishing Ltd: Bristol and Philadelphia.
- [19] Abreu, P. et al. [DELPHI Collaboration] (2001) A measurement of the tau topological branching Ratios. *European Physical Journal C* 20, 617.
- [20] Anastassov, A. et al. [CLEO Collaboration], (1998) *Physics Review D* 55 (1997) 2559 [Erratum-ibid. **D 58**, 119904].
- [21] Cohen, E. & Taylor, B. (1987) "The 1986 adjustment of the fundamental physical constants," *Review of Modern Physics* 59, 1121. [CODATA-86](#).
- [22] Mohr, P. & Taylor, B. (2000) CODATA recommended values of the fundamental physical constants: 1998. *Review of Modern Physics* 72, 351, [CODATA-98](#).
- [23] Mohr, P. & Taylor, B. (2005) CODATA recommended values of the fundamental physical constants: 2002. *Review of Modern Physics* 77, 1. [Constants2002](#)
- [24] Grigoriev, I. & Meilikhov, E. (eds.) (1991) Physical Quantities (in Russian). *M. Energoatomizdat*.
- [25] Radtsig, A. (2003) "Fundamental Physical Constants (1998)" (Russian translation of an excerpt from Ref.[22]). *UFN* 173, 339.
- [26] Yao, W. et al. [Particle Data Group], (2006) Review of Particle Physics. *Journal of Physics G* 33, 1.
- [27] Karshenboim, S. (2005) Fundamental physical constants: their role in physics and metrology and recommended values (in Russian). *UFN* 175, 271.
- [28] Lide, D. (ed.) (2005) *Handbook of Chemistry and Physics. 85th Edition*. CRC Press.
- [29] Ezhela, V., Kuyanov, Y., Larin, V. & Siver, A. (2004) The Inconstancy of the Fundamental Physical Constants: Computational Status. *arXiv:physics/0409117*.
- [30] Wilkinson, J. (1965) *The Algebraic Eigenvalue Problem*. Clarendon Press: Oxford.
- [31] Gantmakher, F. (1988) *Matrix Theory* (in Russian). M. – Nauka.
- [32] Horn, R. & Johnson, C. (1986) *Matrix Analysis*. Cambridge University Press.
- [33] Rohn, J. (2005) Nonsingularity, Positive Definiteness, and Positive Invertibility Under Fixed-Point Data Rounding. submitted to *Applications of Mathematics, September 2005*; [MSTeP](#)
Rohn, J. (2007) Nonsingularity, Positive Definiteness, and Positive Invertibility Under Fixed-Point Data Rounding. *Applications of Mathematics* 52 (2), 105-115.
- [34] Anderson, T. (1963) *An Introduction to Multivariate Statistical Analysis*. New York: John Wiley & Sons, Inc.

- [35] Borovkov, A. (1984) *Mathematical Statistics. Parameter Estimations. Hypotheses Testing* (in Russian). M. –Nauka.
- [36] D'Agostini, G. (2003) *Bayesian Reasoning in Data Analysis*. World Scientific Publishing Co. Pte. Ltd.
- [37] De Bièvre, P. (1997) Reliability is a State-of-the-Mind. *Accred. Qual. Assur.* 2, 1.
- [38] M. Herman, M. (ed.) (2005) ENDF- 6 Formats Manual. Data Formats and Procedures for the Evaluated Nuclear Data File ENDF/B-VI and ENDF/B-VIIN. Document ENDF-102, Report BNL-NCS-44945-05-Rev. [ENDF-102](#)
- [39] Ferson, S. et al. (2004) Dependence in probabilistic modeling, Dempster-Shafer theory, and probability bounds analysis. *SAND2004-3072*. Unlimited release, Printed. Pp. 59-60,107. [SAND2004-3072](#)
- [40] Wang, C. & Iyer, H. (2005) On higher-order corrections for propagating uncertainties. *Metrologia* 42, 406.
- [41] Ferson, S. et al. (2006) Experimental uncertainty estimation and statistics for data having interval uncertainty. *SAND2006-XXXX* [review draft 2], Unlimited release, Printed XXXX 2006, [SAND2006-XXXX](#)