PROBLEMS WITH FUNDAMENTAL PHYSICAL CONSTANTS – 2005

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This note is an appeal to the physics and metrology communities to join their efforts and work out the standard on the numerical expression of the results of joint measurements. It turns out that there are no acceptable guides or rules on the numerical expression the result of jointly measured quantities.

1 Introduction

Existing standard guides on the numerical expression of the estimates of physical quantities are relatively well elaborated only for one measurand [1], [2].

Unfortunately, metrologists move too slowly with creating the long waiting guidelines and standards for numerical presentations of the results on jointly measured quantities in scientific and technical documents [1].

The absence of the common procedures on the "expression of uncertainties" in the multivariate cases leads to proliferation in the bad practice of presenting the incorrect numbers in the scientific and technical publications, in the 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 "bad practice" in [5], [6], [7], [8],[9], [25]. Additional critical notes will be presented in the sections to follow.)

In some cases (unfortunately too often) the absence of the standard on the multivariate uncertainty estimation procedure and presentation the results in publications makes it impossible comparison of different measurements of the same set of quantities, even qualitative.

Let us recall, that for the correct numerical expression the estimates of some random quantity one needs, at least, the following data structure: mean values and the confidence region (or scatter region). For the scalar quantity it is the mean value and one standard deviation interval. For the random vector we will need a mean vector and multidimensional 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 looks as:

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

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, at 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 in the computation and data exchange procedures where these requirements are badly violated: (i) experts

[1] It should be noted that some steps to improve the famous ISO GUM was started just after its first release (see [3]). Set of contemporary, informative, and instructive documents are created by SSfM programme [4].

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, (iii) the over-rounded vector of mean values of it's components moved the end of the mean vector out of unrounded (original) scatter region for many standards.

To recall, let us consider a simple example 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 two dimensional vector to obtain vector (x, y) by rotation on the angle $\pi/4$:

$$\begin{bmatrix}\zeta\\ \eta\end{bmatrix} = \left(\begin{bmatrix}\sqrt{2}(1.500 \pm 0.100)\\ \sqrt{2}(0.345 \pm 0.001)\end{bmatrix}, r(\zeta,\eta) = \begin{bmatrix}1.0 & 0.0\\ 0.0 & 1.0\end{bmatrix}\right) \Rightarrow \begin{bmatrix}x = (\zeta+\eta)/\sqrt{2}\\ y = (\zeta-\eta)/\sqrt{2}\end{bmatrix} \Rightarrow$$

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

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 correlation coefficient will 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 degenerate correlation matrix.**

- **The numerical presentations of the (x, y) components which seems 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, on the first rounding step we will get deviation

$$\begin{bmatrix}\Delta x/\sigma_x\\ \Delta y/\sigma_y\end{bmatrix} = \left(\begin{bmatrix}-0.05\\ 0.05\end{bmatrix}, r(x,y) = \begin{bmatrix}1.0000 & 0.9998\\ 0.9998 & 1.0000\end{bmatrix}\right).$$

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

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

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

$$\chi^2(-0.005, 0.005) = \frac{0.0025}{1.9998 \cdot 0.0002} \cdot [-1, 1] \cdot \begin{bmatrix}1.0000 & -0.9998\\ -0.9998 & 1.0000\end{bmatrix} \cdot \begin{bmatrix}-1\\ 1\end{bmatrix} = 25 > 1.$$

  This value for the χ^2 corresponds to deviation of the x, y vector out of scatter region by the more than 3 standard deviations. If rounding is performed up to one digit to the right of decimal point, as it is recommended in all textbooks for independent quantities: $(1.845 \pm 0.100, 1.155 \pm 0.100) \Longrightarrow (1.8 \pm 0.1, 1.2 \pm 0.1)$, then $\chi^2(-0.045, 0.045) = 2025 \gg 1$, that means that deviation is more than for 30 standard deviations.

- **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 measuring (estimation).**

2 Incorrect presentations of correlated data in physics and metrology: a few recent bad practice examples

In what follows we will need multiple references to some instructive statements from the basic metrology document — the famous 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 result 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*.
>
> **0.2** The concept of *uncertainty* as a quantifiable attribute is relatively new in the history of measurement, although *error* and *error analysis* have been long a part of the practice of measurement science or metrology. It is now widely recognized that, when all of the known or suspected components of error have been evaluated and the appropriate corrections have been applied, there still remains an uncertainty about the correctness of the stated result, that is, a doubt about how well the result of the measurement represents the value of the quantity being measured.
>
> **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 will focus efforts of practitioners from different scientific and technical areas on the creation of the standard methodology of measurements and expression the results in traditional and electronic forms.

The detailed recommendation is presented in the section **"7 Reporting uncertainty"** of the ISO GUM.

> **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.
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?"

ISO GUM [1], p. 25

In spite of broad discussions of the ISO GUM in international and national metrology bodies more than 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 the raw document especially in recommendations concerning the expression the results of 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 $u_c(y_i)$, 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 $u_c(y)$ or expanded uncertainty U should not be given with an excessive number of digits. It usually suffices to quote $u_c(y)$ [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.
In reporting final results it may sometimes be appropriate to round uncertainties up rather than to the nearest digit. For example, $u_c(y) = 10.47\ m\Omega$ might be rounded to 11 $m\Omega$. However, common sense should prevail and a value such as $u_c(y) = 28.05$ kHz should be rounded down to 28 kHz. Output and input estimates should be rounded to be consistent with their uncertainties; for example, if $y = 10.05762\ \Omega$ with $u_c(y) = 27\ m\Omega$, y should be rounded to 10.058 Ω. Correlation coefficients should be given with three-digit accuracy if their absolute values are near unity.

(ISO GUM [1], p. 26-27)

Theses statements clearly show that attempts to formulate recommendations for the multivariate case in the context entirely devoted to the univariate case are hopeless.

2.1 Incorrect expression the uncertainty of measurements in ISO GUM

On the example above with rotation the estimate of the two dimensional vector we have shown that the recommendation **7.2.6** of ISO GUM is misleading. Moreover the application of the **7.2.6** recommendation for the rounding correlations in the example **H.2** of the section **Annex H: Examples** of ISO GUM clearly shows the failure of that recommendation. Indeed, in the 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**

$$\begin{bmatrix} 1. & -0.588 & -0.485 \\ -0.588 & 1. & 0.993 \\ -0.485 & 0.993 & 1. \end{bmatrix}. \tag{3}$$

The eigenvalues this matrix are [2.403 740 76, 0.596 712 77, −0.000 453 53], that is the correlation matrix is destroyed by the recommendation **7.2.6**.

The correct matrix calculated from the data in the table **H.2** with 16 digits to the right of decimal point looks as

$$\begin{bmatrix} 1. & -0.588\,276\,855\,797\,0084 & -0.485\,064\,613\,663\,1822 \\ -0.588\,276\,855\,797\,0084 & 1. & 0.992\,507\,542\,132\,0323 \\ -0.485\,064\,613\,663\,1822 & 0.992\,507\,542\,132\,0323 & 1. \end{bmatrix},$$

their eigenvalues are all positive as it should be by definition of the correlation matrix:

$$2.403\,564\,371\,235\,8685, \quad 0.596\,435\,606\,493034, \quad 2.227\,109\,758\,149\,771 \times 10^{-8}.$$

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

$$\begin{bmatrix} 1. & -0.588\,276\,86 & -0.485\,064\,61 \\ -0.588\,276\,86 & 1. & 0.992\,507\,54 \\ -0.485\,064\,61 & 0.992\,507\,54 & 1. \end{bmatrix}.$$

Note. It should be stressed the logical inconsistency of the material organization in the ISO GUM. From the one side there is a warning in the text that it is applicable only to the one measurand case, but from the other side when describing recommendations how to estimate uncertainty of the one random function which is dependent upon several random quantities we unavoidably encountered with the problem of the correct numerical expression the estimates of the random vectors.

Unfortunately the absurdity of the recommendation **7.2.6** of ISO GUM in the part concerning the rounding correlations (as well as its application in the example H.2 of the section **Annex H: Examples**) where not noticed in the metrology community. Both, the recommendation and example H.2, are reproduced in the other metrology documents [2], used in publications, monographs (see further examples in the subsections to follow), and in the textbooks (see for example the recent textbook [14] p.128-129).

2.2 Experiment CERN-LEP-DELPHI in European Physical Journal

Presented in [15] results on the measurements of the branching ratios

$$B_1(\tau^- \to h^- \, neutrals), \quad B_3(\tau^- \to h^+ \, 2h^- \, neutrals), \quad B_5(\tau^- \to 2h^+ \, 3h^- \, neutrals)$$

one can collect into the structure (see p. 636 and Table 6.):

$$\begin{bmatrix} B_1 \\ B_3 \\ B_5 \end{bmatrix} = \left(\begin{bmatrix} 0.85316 \pm 0.000929_{stat} \pm 0.000492_{syst} \\ 0.14569 \pm 0.000929_{stat} \pm 0.000477_{syst} \\ 0.00115 \pm 0.000126_{stat} \pm 0.000059_{syst} \end{bmatrix}, \begin{bmatrix} 1.00 & -0.98 & -0.08 \\ -0.98 & 1.00 & -0.08 \\ -0.08 & -0.08 & 1.00 \end{bmatrix} \right), \tag{4}$$

in which the correlation matrix are the correlation matrix for the total uncertainties (statistical and systematic). In the examples above (2) and (3) we saw that independent rounding of correlation matrix elements is 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 the over-rounding is suspected. Besides in the text the statistical and systematic uncertainties are quoted separately (4), but there are no descriptions of how they were combined in the total uncertainties and how the correlation of the total uncertainties ([15] page 636) was obtained.

Our attempts to make agree the relevant data presented in different places in the publication turned to be successless because the lack of details in the publication concerning the data transformations for publication.

Let us present our procedures that we used to check the self-consistency of the final data presented in [15]. We use data on systematic uncertainty budget from ([15], Table 6.):

$(Source\,of\,systematic)_i$	$\sigma_i(B_1)\times 10^6$	$\sigma_i(B_3)\times 10^6$	$\sigma_i(B_5)\times 10^6$
1 Dilepton background	110	-109	-1
2 Cosmic ray background	5	-5	1
3 Four fermion background	42	-41	-1
4 $Z\to\overline{q}q$ background	25	-24	-1
5 Neural Network $\overline{q}q$ rejection	50	-48	-5
6 Tracking	157	-152	-16
7 VD efficiency	55	-60	6
8 Conversions	126	-121	-8
9 Inelastic Nucl. reinteractons	90	-80	-10
10 Elastic Nucl. reinteractions	24	-24	-2
11 Electron identification	104	-97	-7
12 δ-ray weights	8	-8	1
13 K_S regeneration	5	-5	1
14 Exclusive BRs	228	-204	-44
15 3-prong decay modelling	116	-121	10
16 Trigger	15	-15	1
17 E and p scales	19	-20	1
18 τ polarization	18	-19	1
19 Simulation statistics	310	-310	31
Total systematic	492	477	59
Statistical	929	929	126

The covariance matrix of systematic uncertainties which have the statistical origin (the uncertainties of the type A [1],[2]) is calculated as Gram matrix of the vectors $\vec{\sigma}(B_1)$,$\vec{\sigma}(B_3)$,$\vec{\sigma}(B_5)$ — contributions from different sources of the systematic uncertainties into systematic uncertainties of the observable quantity. In practice "for simplicity" the same procedure is used to combine systematic uncertainties from all sources (including the uncertainties of the type B). Following this practice we get:

$$Cov_{ij}^{syst}=\vec{\sigma}(B_i)\cdot\vec{\sigma}(B_j)=\begin{bmatrix}2.42595\times10^{-7} & -2.34695\times10^{-7} & -4.485\times10^{-9}\\ -2.34695\times10^{-7} & 2.27629\times10^{-7} & 3.065\times10^{-9}\\ -4.485\times10^{-9} & 3.065\times10^{-9} & 3.54\times10^{-9}\end{bmatrix}. \qquad (5)$$

The corresponding vector of standard deviations and correlation matrix are as follows:

$$\begin{bmatrix}0.000492539\\0.000477105\\0.000059498\end{bmatrix},\ \begin{bmatrix}1. & -0.998732 & -0.153045\\ -0.998732 & 1. & 0.107973\\ -0.153045 & 0.107973 & 1.\end{bmatrix}.$$

It should be noted that the rounding of this matrix in accordance with ISO GUM clause 7.2.6 will lead to the non positive definite rounded matrix.

From the data (4) we construct the covariance of the total uncertainties and subtracting the matrix (5), we obtain a variant of the covariance of the statistical uncertainties. This matrix has all eigenvalues positive:

$$(1.70453\times10^{-6}, 3.449919\times10^{-8}, 2.93866\times10^{-9}).$$

But the statistical matrix should be degenerate due to the used procedure to obtain estimates. The covariance matrix of the statistical uncertainties is the matrix for three observables B_1, $B_3=1-B_1-B_5$, B_5, linearly dependent upon two correlated observables B_1, B_5.

Thus, we see the sharp contradiction in the data presentations. The origin of this contradiction could be: our wrong interpretation of the paper; misprints in the journal; and distortions of the data by authors in due course of paper preparation for publication.

Fortunately we can estimate the statistical covariance matrix in the other way by using data (4) on statistical uncertainties and the constraint equation. From constraint equation $B_3=1-B_1-B_5$

we obtain the variation $\sigma_3^2 = \sigma_1^2+\sigma_5^2+2\sigma_1\sigma_5 r_{stat}(B_1, B_5)$, from which we obtain statistical correlation coefficient $r_{stat}(B_1, B_5)$ and then we can construct "the true" matrix of statistical covariances which is degenerate as it should be.

$$\begin{bmatrix} \sigma_1^2 & -(\sigma_1^2+\sigma_3^2-\sigma_5^2)/2 & (\sigma_3^2-\sigma_1^2-\sigma_5^2)/2 \\ -(\sigma_1^2+\sigma_3^2-\sigma_5^2)/2 & \sigma_3^2 & -(\sigma_3^2+\sigma_5^2-\sigma_1^2)/2 \\ (\sigma_3^2-\sigma_1^2-\sigma_5^2)/2 & -(\sigma_3^2+\sigma_5^2-\sigma_1^2)/2 & \sigma_5^2 \end{bmatrix}.$$

Its numerical expression is as follows:

$$\begin{bmatrix} 8.63041\times10^{-7} & -8.55103\times10^{-7} & -7.938\times10^{-9} \\ -8.55103\times10^{-7} & 8.63041\times10^{-7} & -7.938\times10^{-9} \\ -7.938\times10^{-9} & -7.938\times10^{-9} & 1.5876\times10^{-8} \end{bmatrix}. \tag{6}$$

The eigenvalues of this matrix are

$$(1.718144\times10^{-6}, 2.3814\times10^{-8}, 1.2\times10^{-22}),$$

the last one should be considered as zero (machine zero). Now we can obtain "the true" combined correlation matrix and compare it with that presented in the publication and with (4).

$$\begin{bmatrix} 1. & -0.9924148111607243 & -0.08478919616844724 \\ -0.9924148111607243 & 1. & -0.03348650681292892 \\ -0.08478919616844724 & -0.03348650681292892 & 1. \end{bmatrix}. \tag{7}$$

Its eigenvalues are

$$1.993743788696688, 1.0056742957244327, 0.0005819155788786556.$$

In accordance with safe rounding threshold [25] (see section 3. of this text) we can represent the matrix (7) in more visible form:

$$\begin{bmatrix} 1. & -0.9924 & -0.0848 \\ -0.9924 & 1. & -0.0335 \\ -0.0848 & -0.0335 & 1. \end{bmatrix}. \tag{8}$$

Consequently the correctly rounded branching values should have at least 5 digits to the right of the decimal point.

We have tried to obtain the correct numerical data from the authors of the cited paper but failed. The correct data were lost forever.

2.3 Experiment CLEO in Physical Review

In the paper [16] of the CLEO collaboration the result 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 branching fraction measurements.

C_τ	B_e	B_μ	B_h	B_μ/B_e	B_h/B_e
B_e	1.00	0.50	0.48	−0.42	−0.39
B_μ		1.00	0.50	0.58	0.08
B_h			1.00	0.07	0.63
B_μ/B_e				1.00	0.45
B_h/B_e					1.00

The eigenvalues of this matrix are: (2.1735, 1.7819, 1.0550, −0.0075, −0.0028) in sharp contradiction with positive definiteness requirement.

2.4 Incorrect presentation of the data on the fundamental physical constants in Reviews of Modern Physics and in other reprints

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

Table 1. Comparison of estimates of the selected FPC recommended by CODATA in 1986 [17], 1998 [18], and 2002 версия 4.0 [19].

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

All three sub-matrices are presented in accordance with the ISO GUM, clause 7.2.6 with three digits to the right of the decimal point. All matrices turned to be over-rounded, each of which has negative eigenvalue with absolute values much larger than machine zero $\sim 10^{-17}$:

$CODATA: 1986$ {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}.

Note. In May, 2005 on the NIST site the new version FPC.v.4.2 appeared. In this new version (v.4.2) the misprints discovered in versions 4.0 and 4.1 were fixed and for the first time the computer readable files for the basic (Least Square Adjusted) FPC were released. The data in the computer readable files are free of critical issues (see [25]), presented with sufficient precision to be used in high precision calculations.

WARNING

It turns out that the maintenance of the FPC set and re-adjustments are produced only in the NIST (USA). There are no other independent bodies that produce independent full-scale adjustments of the FPC system to be compared with that of produced by NIST experts. This is very strange situation in metrology where every physical and technological quantity are multiply measured in different laboratories and then results are cross-checked and corrected before unified values will be accepted for international usage.

All national metrology services unconditionally take CODATA recommendations and reprinted NIST tables without thorough critical treatments of the results and methods. For example in the USSR and now in Russia the question on the critical analysis of the CODATA recommended FPC was never raised and the CODATA FPC system was never certificated for

usage in science, technology, and education. All russian handbooks and textbooks reprinted the spoilt (over-rounded) data from NIST publications without mentioning the presence of large correlations between uncertainties of some constants. Majority of authoritative issues also reprinted incorrect NIST data without any comments or warnings (see [20], [21], [22], [23], [24]).

3 Self consistency criteria for the results of the jointly measured several physical quantities

3.1 Thresholds for the safe rounding of the correlated quantities

In the above examples we show that the rules of the numerical presentations developed for one measurand are inapplicable in multivariate case. In this section we will reproduce construction of thresholds for the safe rounding in the multivariate case, developed in [25]. These thresholds are relatively simple parameters to control the self consistency of the numerical estimates of correlated quantities. We treat the numerical data on the estimates of the random vector as self consistent if the data consist of two items: the mean values of the vector components and 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 [26], [28]): Let $C = A + B$, where $A, B, C \in R^{n\times n}$ – symmetric matrices and $(\alpha_1 \le \alpha_2 \cdots \le \alpha_n)$, $(\beta_1 \le \beta_2 \cdots \le \beta_n)$, $(\gamma_1 \le \gamma_2 \cdots \le \gamma_n)$ their eigenvalues correspondingly. Then $\forall i$ the following inequalities are valid

$$\alpha_i + \beta_{min} \le \gamma_i \le \alpha_i + \beta_{max} \ . \tag{9}$$

Gershgorin's theorem ([26], [27], [28]): Every eigenvalue α_i of the matrix A belongs to the interior of one of the circles

$$|A_{ii} - \alpha_i| \le \sum_{j=1}^{n} |A_{i\ne j}| \ . \tag{10}$$

Schur's theorem ([28]): Let matrix $B \in R^{n\times n}$ is symmetric with values of the diagonal elements $b_1 \le b_2 \le \cdots \le b_n$ (in any order) and eigenvalues $\beta_1 \le \beta_2 \cdots \le \beta_n$, then $\forall k \le n$

$$\sum_{i=1}^{k} \beta_i \le \sum_{i=1}^{k} b_i \ . \tag{11}$$

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

Let $\{\langle x_i\rangle, u_i, r_{ij}, N^r_{dig}\}$, $i, j = 1, \ldots, n$ 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 the 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

$$r_{ii} = 1 \quad \forall\, i = 1, \ldots, n, \qquad |r_{i\ne j}| < 1.0 \ ;$$

N^r_{dig} — integer non negative number defined the unified decimal precision of the non diagonal matrix elements of the correlation matrix r_{ij} .

This list is the minimal 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.

$$\sum_{ij}^{n} \frac{x_i - \langle x_i \rangle}{u_i} \cdot r_{ij}^{-1} \cdot \frac{x_j - \langle x_j \rangle}{u_j} < R^2_{g,CL} \ . \tag{12}$$

If g is unknown but the matrix of the second moments is known the Kramer's scatter ellipsoid is used with $R^2 = n + 2$ (see [30] page 80-81, [31] page 102).

Proposed additional parameter N^r_{dig} is needed to assure the quality of the data and its preservation in the processes of data transfers and in calculations. In what follows we will justify the needs and usefulness of this and other analogous parameters that follows from the requirements of the boundedness of the scatter region (positive definiteness of the correlation matrix in particular)

Let us treat two structures $D = \{\langle x_i \rangle, u_i, r_{ij}, N^r_{dig}\}$ and $D^* = \{\langle x_i \rangle^*, u^*_i, r^*_{ij}, N^{r,*}_{dig}\}$ which is obtained from D by the "uniform" rounding: $N^r_{dig} \to N^{r,*}_{dig} < N^r_{dig}$.
Let R_{ij} be the "rounder" — the real matrix addition of which to the r_{ij} will resulted in the matrix $r^*_{ij} = r_{ij} + R_{ij}$, with preservation of all general features of the original correlation matrix: the symmetry and positive definiteness but all $|r^*_{i\neq j}| < 1$ be the decimal numbers with $N^{r,*}_{dig}$ digits to the right of the decimal point. The matrix R_{ij} has the following properties:

$$R_{ii} = 0 \quad \forall i = 1, \ldots, n; \qquad |R_{i\neq j}| \leq 5.0 \times 10^{-N^{r,*}_{dig}-1}. \tag{13}$$

Now let $c_1 \leq \cdots \leq c_n$, $\rho_1 \leq \cdots \leq \rho_n$, and $c^*_1 \leq \cdots \leq c^*_n$ be the ordered sets of the eigenvalues O the r_{ij}, R_{ij}, and r^*_{ij} matrices correspondingly. Then from the Weil's theorem (9) $\forall l = 1, \ldots, n$ we will have:

$$c_l + \rho_1 \leq c^*_l \leq c_l + \rho_n.$$

Further from the Gershgorin's theorem (10)

$$\rho_1 \geq -(n-1) \cdot 5 \cdot 10^{-(N^{r,*}_{dig}+1)} = -\frac{(n-1)}{2} \cdot 10^{-N^{r,*}_{dig}}$$

and to have the positive definiteness of the r^*_{ij} matrix it is sufficient the validity of the conditions

$$0 < c_1 - \frac{(n-1)}{2} \cdot 10^{-N^{r,*}_{dig}} \leq c^*_1.$$

From the left inequality we obtain the final estimate of the minimal number of decimal digits to the right of the decimal point that should be preserved in rounding of the off diagonal elements of the correlation matrix r_{ij} with the minimal eigenvalue $c_1 = \lambda^r_{min}$.

$$\boldsymbol{N^{r,*}_{dig} \geq N^{r,th}_{dig} = \left\lceil \log_{10} \left(\frac{n-1}{2 \cdot \lambda^r_{min}} \right) \right\rceil + 1 \ .} \tag{14}$$

Note. From the statements of the Weil's (9), Gershgorin's (10), and Shur's (11) theorems it follows that any rounding of the off diagonal matrix elements of the degenerate correlation matrix (positive semi-definite) is inadmissible. The rounding of the degenerate correlation matrix will unavoidably lead to appearance of the negative eigenvalues in the rounded matrix.

Indeed, as the rounder martix is an Hermitian matrix with zero valued main diagonal from the statement of the Schur's theorem it has the negative minimal eigenvalue. Further, from the left inequality (9) of the Weil's theorem the matrix obtained by the rounding we unavoidably will have the negative eigenvalue.

In summary:

we have shown that the requirement of the positive definiteness of the correlation matrix posed firm restrictions on the rounding freedom of the matrix elements of the correlation matrix.

The minimal number of decimal digits to the right of the decimal point in the numerical expressions of the positive definite correlation matrix, or in other words the rounding threshold, is defined by the minimal eigenvalue of the unrounded matrix by the expression (14)[2].

Analogous rounding thresholds can be obtained for the mean values $\langle x_i \rangle$ and the standard deviations u_i. They also are determined by the minimal eigenvalue of the correlation matrix.

Let x_i^R be the "rounding" vector

$$|x_i^R|[unit_i] \leq 5 \cdot 10^{-(N^x_{dig,i}+1)}[unit_i] \ , \tag{15}$$

such that the end of the obtained rounded vector $\langle x_i \rangle^* = \langle x_i \rangle + x_i^R$ belongs to the interior of the "initial" scatter ellipsoid defined by the initial (non-rounded) covariance matrix (12)

$$\sum_{ij}^{n} \frac{x_i^R}{u_i} \cdot [r^{-1}]_{ij} \cdot \frac{x_j^R}{u_j} < R^2_{g,CL} \ . \tag{16}$$

In the basis of eigenvectors of the initial correlator r_{ij} the expression (16) take the form

$$\sum_{ij}^{n} \sum_{lm}^{n} \frac{x_i^R}{u_i} \cdot [L^{-1}]_{il} \cdot \frac{\delta_{lm}}{\lambda_m} \cdot [L]_{mj} \cdot \frac{x_j^R}{u_j} < R^2_{g,CL} \ , \tag{17}$$

where L is corresponding rotation matrix, and λ_m are the eigenvalues of the unrounded correlator.

As'we seek for the sufficient conditions for the end of the mean vector be in the interior of the initial (unrounded) scatter ellipsoid (17), we may demand the validity of the inequality obtained from (17) when all eigenvalues of the correlator are replaced to the minimal one, thus we obtain the followig inequality:

$$\sum_{i}^{n} \left(\frac{x_i^R}{u_i} \right)^2 < (R^2_{g,CL}) \lambda^r_{min} \ . \tag{18}$$

Inequality (18) is rather trivial and means that one can independently rounding the components of the mean vector only in the maximal hypercube imbedded into the initial scatter ellipsoid:

$$\frac{|x_i^R|}{u_i} < \sqrt{\frac{(R^2_{g,CL}) \cdot \lambda^r_{min}}{n}} \ . \tag{19}$$

Substituting bounds on the rounding vector (15) into the inequality (19) we will get after simple algebra an estimates for the rounding thresholds $N^x_{dig,i}$:

$$\boldsymbol{N^x_{dig,i} > \left\lceil \frac{1}{2} \log_{10} \left(\frac{n}{4 \cdot (R^2_{g,CL}) \cdot \lambda^r_{min} \cdot (u_i/[unit_i])^2} \right) \right\rceil} \ . \tag{20}$$

In accordance with recommendations 7.2.2, 7.2.4, ISO GUM [1] and common practice the number of decimal digits to the right of the decimal point in the mean value and in its standard deviation should be the same we put

$$N^u_{dig,i} = N^x_{dig,i}, \quad \forall i = 1, \ldots, n. \tag{21}$$

In summary, we have shown that the independent uniform rounding of the decimal estimates of numbers in the structure $\{\langle x_i \rangle, u_i, r_{ij}\}$, $i, j = 1, \ldots, n$ representing the results of jointly measured (estimated) of n random quantities is allowed only under restrictions posed by the requirements of

[2] Analogous estimate in other terms was obtained recently in the paper [29].

the boundedness the "rounded scatter region" (ellipsoid) and the confinement of the end of rounded mean vector inside the unrounded scatter region (ellipsoid).

To meet the safe rounding, the accuracies of the numbers in the structure should be higher than rounding thresholds (14), (20), (21) defined by the minimal eigenvalue of the positive definite correlation matrix of the structure to be rounded.

3.2 Criteria for self consistent expression of the results of joint measurements

In case of joint measurements or estimations, to express the results correctly one have to present the following (minimal) structure $\{\langle x_i\rangle,\ u(x_i),\ r(x_i,x_j)\},\ i,j=1,\ldots,n$.

We propose to expand it to the structure

$$\{\{\langle x_i\rangle,\ u(x_i),\ N^{x}_{dig,i}\},\ \{r(x_i,x_j),\ N^{r,th}_{dig}\}\},\quad i,j=1,\ldots,n \tag{22}$$

and advocate it as the 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 the potential users on the critical precision needed for correct numerical computations in applications.

Indeed, to form the proposed above structure (22) it is needed:

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

4 Multivariate nonlinear uncertainty propagation is unavoidable

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

Let we have the problem of the uncertainty propagation from m random variables

$$\{\langle x_\alpha\rangle,\ u(x_\alpha),\ r(x_\alpha,x_\beta)\}$$

with positive definite correlation matrix $r(x_\alpha,x_\beta)$ to the system of n functions $y_i=\{f_i(x_\alpha)\}_1^n$. This means that we have to obtain estimates to fill the minimal structure

$$\{\langle y_i\rangle,\ u(y_i),\ r(y_i,y_j)\}.$$

In general case (with nonsingular functions) when the joint probability distribution function $g(x_1,\ldots,x_m)$ is known this problem is formulated as follows:

1)Calculate the joint probability distribution function

$$F(y_1,\ldots,y_n)=\int\prod_i^n\delta(y_i-f_i(x_\alpha))\cdot g(x_\alpha)d^mx, \tag{23}$$

and then calculate all its joint moments if needed.

But in reality this way often turns to be unfeasible. The $g(x_\alpha)$ is unknown, or the reliable calculation of $F(y_i)$ is impossible due to the lack of computational power.

2) The usual way to solve the uncertainty propagation problem is the following approximations (valid and supposedly working well for the multi-normal distribution $g(x_\alpha)$).

Calculate

$$\mu_i = \langle y_i \rangle = \int f_i(x_\alpha) \cdot g(x_\alpha) d^m x \implies f_i(\langle x_\alpha \rangle). \tag{24}$$

Then calculate

$$u(y_i, y_j) = \int (f_i(x_\alpha) - \mu_i) \cdot (f_j(x_\alpha) - \mu_j) \cdot g(x_\alpha) d^m x \implies \frac{\partial f_i}{\partial x_\alpha} \cdot u(x_\alpha, x_\beta) \cdot \frac{\partial f_j}{\partial x_\beta}, \tag{25}$$

where $u(x_\alpha, x_\beta) = u(x_\alpha) \cdot r(x_\alpha, x_\beta) \cdot u(x_\beta)$, the partial derivatives calculated at $\langle x_\alpha \rangle$ with sufficient numerical accuracy, and the summation over the repeated greek indices in the rightmost part is assumed.

It is easy to show that due to the positive definiteness of $g(x_\alpha)$ the matrix (25), calculated without approximation (before the right arrow) with sufficient accuracy is the positive definite matrix for any linearly independent system of functions $\{f_i(x_\alpha)\}_1^n$ (see [28], theorem 7.2.10).

Let us show this for the functions $f_i(x_\alpha)$ from the class C^∞ and quadratically integrable with measure $g(x_\alpha)$. Indeed, the matrix (25) is $n \times n$ numerical Gram matrix of n infinite dimensional vectors $f_i(x_\alpha) - \mu_i$ from the functional space with positive definite scalar product. It is a Hermitian matrix and has the basis of eigenvectors in R^n corresponding to the real non negative eigenvalues. If the system of functional vectors $f_i(x_\alpha) - \mu_i$ is linearly independent then all eigenvalues of the matrix (25) (non approximated) are positive.

Suppose that it is not the case, and there exists nonzero vector z in R^n such that

$$\sum_1^n u(y_i, y_j) \cdot z_j = 0.$$

This means that

$$\int \left(\sum_i^n (f_i(x_\alpha) - \mu_i) \cdot z_i \right)^2 g(x_\alpha) d^m x = 0,$$

but this is possible only under condition

$$\sum_i^n (f_i(x_\alpha) - \mu_i) \cdot z_i = 0,$$

in the existence domain of the $g(x_\alpha)$. For the smooth functions f_i this condition means that

$$\sum_i^n (f_i(x_\alpha) - \mu_i) \cdot z_i \equiv 0,$$

which is the condition for the linear dependency of the functional vectors $f_i(x_\alpha) - \mu_i$. This contradiction proves the positive definiteness of the covariance matrix (25) for the system of linearly independent functions.

As it was already 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 (25) by the replacement of $f_i(x_\alpha) - \mu_i$ for the polynomials obtained by the cuts of the Taylor series for $f_i(x_\alpha) - \mu_i$ $\langle x_\alpha \rangle$

$$f_i(x_\alpha) - \mu_i \Rightarrow P_i^N(x_\alpha) = \sum_{k=1}^N \frac{1}{k!} \left. \frac{\partial^k f_i}{\partial x_{\alpha_1} \cdots \partial x_{\alpha_k}} \right|_{\langle x_\alpha \rangle} \cdot \Delta x_{\alpha_1} \cdots \Delta x_{\alpha_k}, \tag{26}$$

where $\Delta x_{\alpha_j} = x_{\alpha_j} - \langle x_{\alpha_j} \rangle$ and the sums over the repeated indices α_j are assumed [3].

[3] It should be noted that in the ISO GUM the corresponding formulae are incorrect. The crucial terms are missed. This will cause wrong results in calculations (besides rounding) and for some nonlinearity one will even obtain the negative variances (see ISO GUM: clause 5.1.2 eq. (10), clause F.1.2.3 eq.(F.2), clause H.2.3 eqs. (H.9) and (H.11)).

Let us show, however, that the requirement of the positive definiteness of the correlation matrix posed clear restrictions on the powers of the Taylor's polynomials even in the cases when the approximations $\mu_i \approx f_i(\langle x_\alpha \rangle)$ are valid (the senior moments are small).

Indeed, the maximal number $T(N,m)$ of the linearly independent functional vectors of the type (26) is determined by the relation

$$\boldsymbol{T(N,m) = \sum_{k=1}^{N} \frac{(m+k-1)!}{(m-1)! \cdot k!} = \frac{(N+m)!}{N! \cdot m!} - 1 \ .} \tag{27}$$

From this estimate the statement follows:
if the covariance matrix of the system of n functions $\{f_i(x_\alpha)\}_1^n$ depending upon m random variables $\{x_\alpha\}_1^m$ is determined by the differential uncertainty propagation law (26) of N-th order such that $T(N,m) < n$, then it is degenerate and any its numerical expression in decimal numbers will be the matrix with at least one non positive eigenvalue.

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

$$f_i(x_\alpha) - \mu_i \approx \sum_{\alpha=1}^{m} \left. \frac{\partial f_i}{\partial x_\alpha} \right|_{\langle x_\alpha \rangle} \cdot (x_\alpha - \langle x_\alpha \rangle) \tag{28}$$

for $n > m$ is invalid, and for $n \leq m$ it is dangerous because the possibility of the existence of the hidden functional relationships like $\Phi(f_1, f_2, \ldots, f_n) = const$.

Indeed, let $n \leq m$, then the output matrix in linear propagation law in the general case is non degenerate. However, if there is at least one relationship of the type $\Phi(f_1, f_2, \ldots, f_n) = const$, then the matrix $u(f_i, f_j)$ derived by the linear uncertainty propagation is degenerate.

It is easy to show this. Let we have such a relationship with $\Phi(f_1, f_2, \ldots, f_n)$ that is smooth enough. Then it's gradient with respect to $\{x_\alpha\}_1^m$ is expressible as the linear combination of the gradients f_i,

$$\frac{\partial \Phi}{\partial x_{\alpha_i}} = \frac{\partial \phi}{\partial f_1} \cdot \frac{\partial f_1}{\partial x_{\alpha_i}} + \frac{\partial \phi}{\partial f_2} \cdot \frac{\partial f_2}{\partial x_{\alpha_i}} + \cdots + \frac{\partial \phi}{\partial f_n} \cdot \frac{\partial f_n}{\partial x_{\alpha_i}} \equiv 0.$$

From the other side it is the null vector. This means that gradients of the f_i are linearly dependent, and hence the covariance matrix obtained by the linear uncertainty propagation law is degenerate.

But the matrix $u(f_i, f_j)$, calculated with the integral uncertainty propagation law (25) with relationship $\Phi(f_1, f_2, \ldots, f_n) = const$ inserted via the Dirac's δ-function which is non-negative everywhere by definition.

$$u(f_i, f_j) = \int (f_i(x_\alpha) - \mu_i) \cdot (f_j(x_\alpha) - \mu_j) \cdot g(x_\alpha) \cdot \delta(\Phi(f_i) - const) d^m x, \tag{29}$$

is the positive definite matrix.

5 Conclusion

Let us summarize the discussions of the talk. It is shown in the "bad practice examples collection" presented in above sections 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 dangerous in usage for simulations of the new fine searches, the behavior of the new high precision devices [4].

[4] It should be noted that these observations are not new, it is sufficient to quote the papers [5], [6], [7].

It seems that majority of the published data, that are incorrectly expressed and presented, where obtained by inadmissible applications to the multivariate case the recommendations of ISO GUM and instructions from other metrology documents that were worked out only for the case of one measurand.

We guess that such confusions are partly inspired by the provocative (and in some cases incorrect) statements in the ISO GUM and by the absence of the analogous multivariate GUM (see, however, [3]).

The title of the Leslie Fox 1971 paper "How to get meaningless answers in scientific computation (and what to do about it)" now may be rephrased as "How to get meaningless data from contemporary scientific data storages (and what to do about it)"

We hope that we have found a right way to try to get partial answers to the posed questions.

As a first step we propose to standardise the minimal multivariate data structure — **mean values, covariance matrix, rounding thresholds for correlation matrix and mean values** together with the minimally sufficient content of the detailed descriptions of the procedures used to obtain estimates of all components of the structure.

Having such formalised standard data structure we can hope to make all procedures of multivariate data handling more clear, reported data will became more reliable.

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