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Multi-measurand ISO GUM is Urgent

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What are the problems?

It is not news that in spite of the continuous progress in measuring methods and systems, data handling systems, and growing computation power we still have a rather stable tendency of improper presentation of numerical results in scientific literature and even in electronic data collections, deemed as reference resources.

In this report I speculate that most probably this tendency is due to ignorance of the existing metrology documents by scientists, and from the other side, due to very slow tuning of the data standards to the fast evolution of science and technology.

To be specific, we still have no agreed procedure how to express, present and exchange the numerical data on jointly measured quantities. The famous ISO GUM is applicable to one measurand only and it is already obsolet to some extent.

The main sources of the corrupted data are:

- **over-rounding;**
- **usage the improper uncertainty propagation laws;**
- **absence of the in/out data quality assurance programs.**

What is the over-rounding of multidimensional data

Let us transform the "greek" random vector with its scatter region

$$\begin{bmatrix}\zeta\\ \eta\end{bmatrix}=\left(\begin{bmatrix}\sqrt{2}(1.500\pm0.100)\\ \sqrt{2}(0.345\pm0.001)\end{bmatrix},\quad r(\zeta,\eta)=\begin{bmatrix}1.0 & 0.0\\ 0.0 & 1.0\end{bmatrix}\right)$$

by rotation (on 45 degrees)

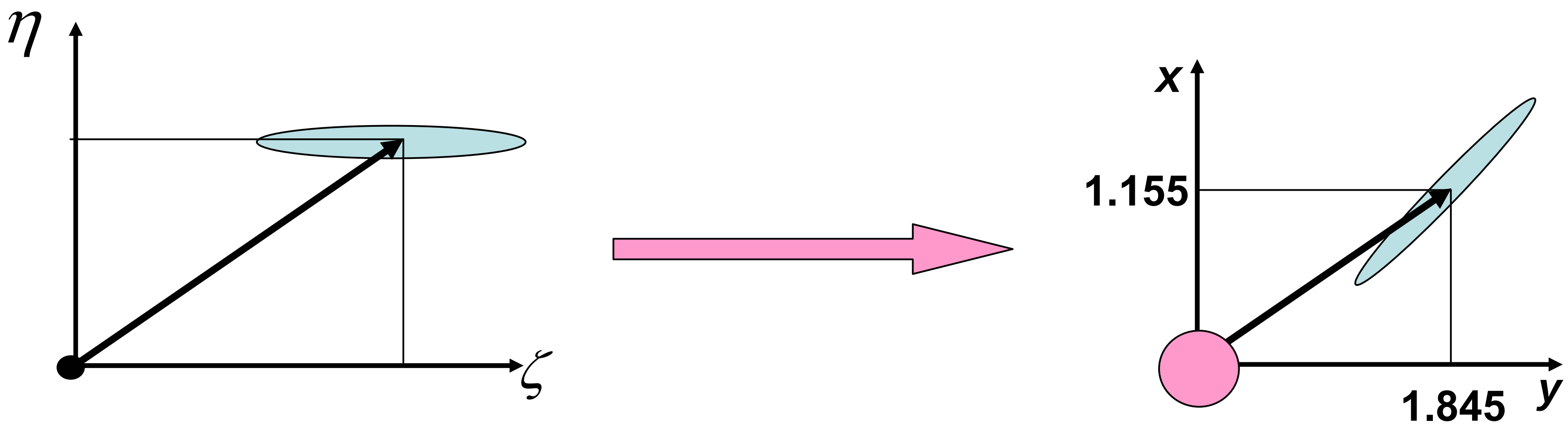
$$\begin{bmatrix}x=(\zeta+\eta)/\sqrt{2}\\ y=(\zeta-\eta)/\sqrt{2}\end{bmatrix}$$

to the "latin" vector

$$\begin{bmatrix}x\\ y\end{bmatrix}=\left(\begin{bmatrix}1.845\pm0.100\\ 1.155\pm0.100\end{bmatrix},\ r(x,y)=\begin{bmatrix}1.0000 & 0.9998\\ 0.9998 & 1.0000\end{bmatrix}\right)$$

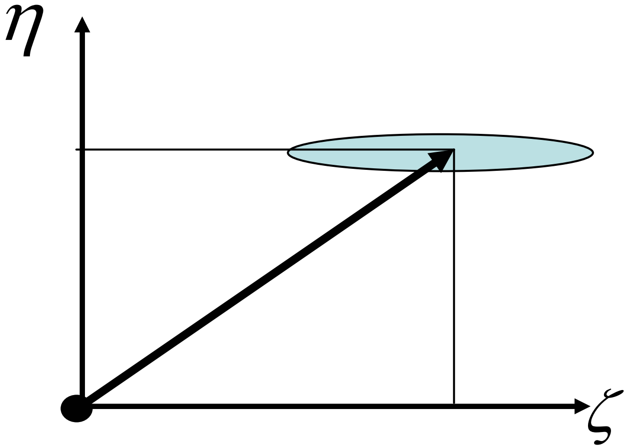
How to corrupt data in this simplest data transformation

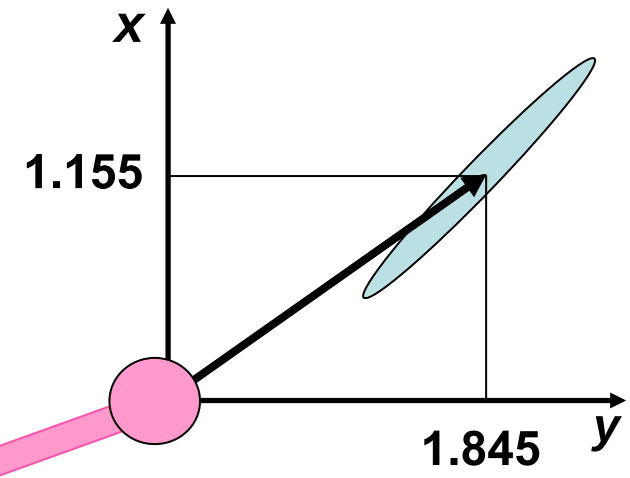
1. True calculations, true picture



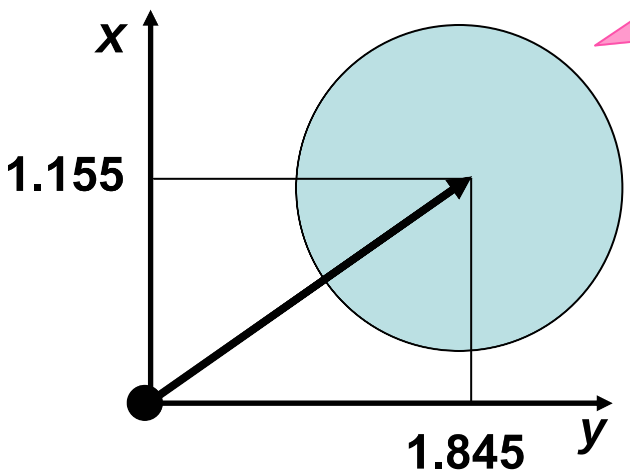
x = 1.845(100)		1.000	0.9998
y = 1.155(100)		0.9998	1.000
mean(uncertainty)		correlator	

How to corrupt data in simplest data transformation





2. Correlator ignored

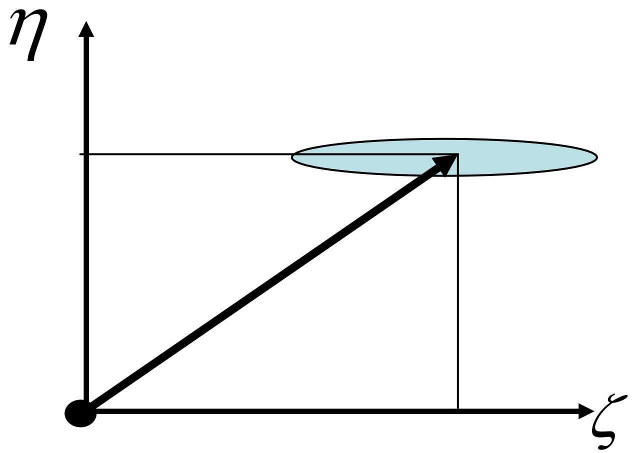


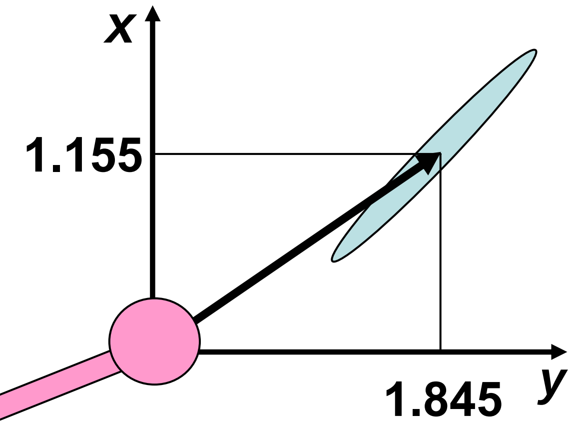
x = 1.845(100)

y = 1.155(100)

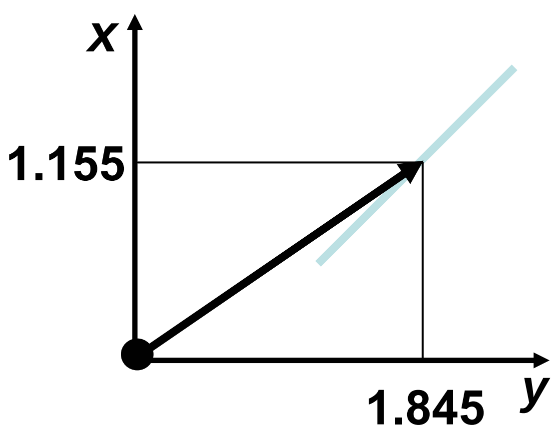
1.0	0.0
0.0	1.0

How to corrupt data in simplest data transformation





3. Correlator over-rounded

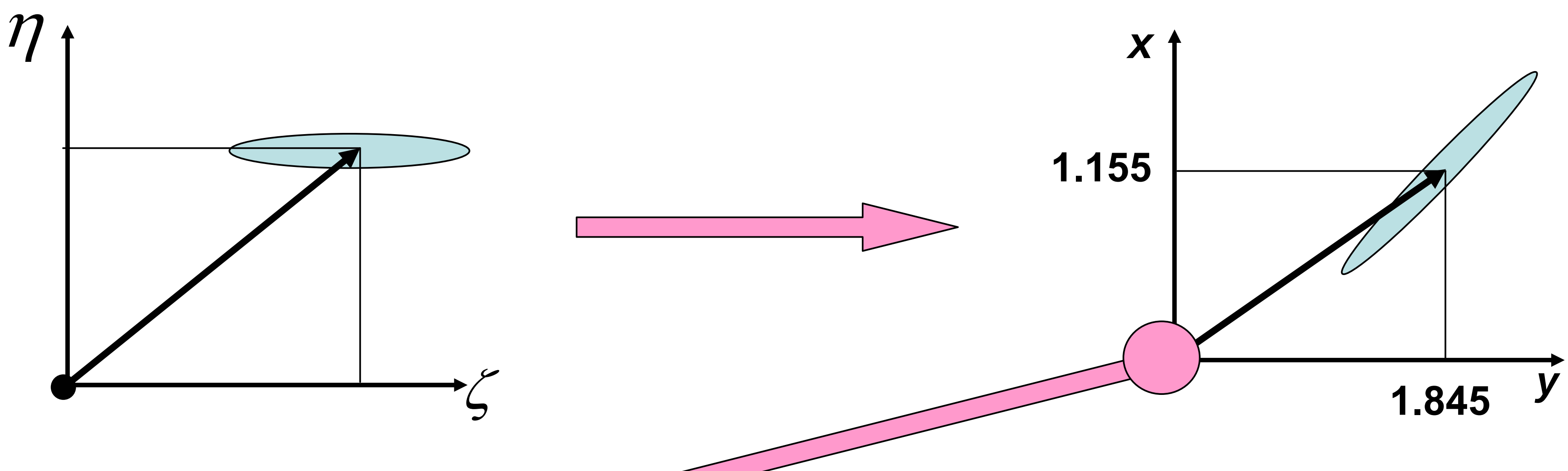


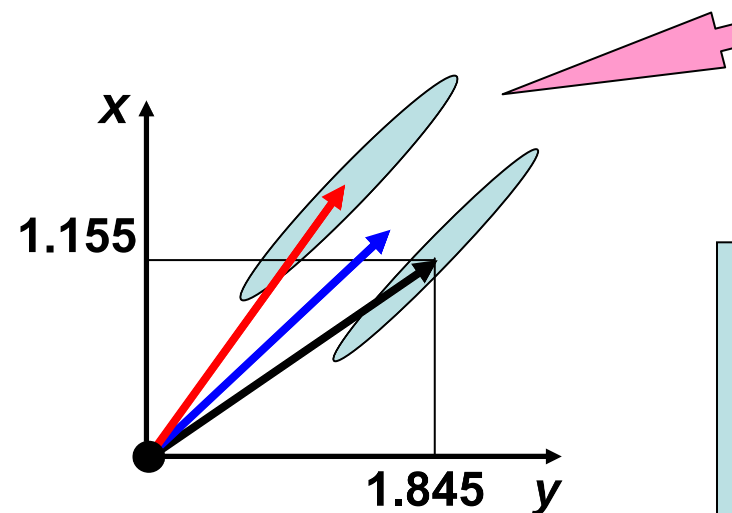
x = 1.845(100)

y = 1.155(100)

1.0	1.0
1.0	1.0

How to corrupt data in simplest data transformation





4. Mean vector over-rounded
Scatter region moved

Most harmful action

x = 1.84(10)

x = 1.8(1)

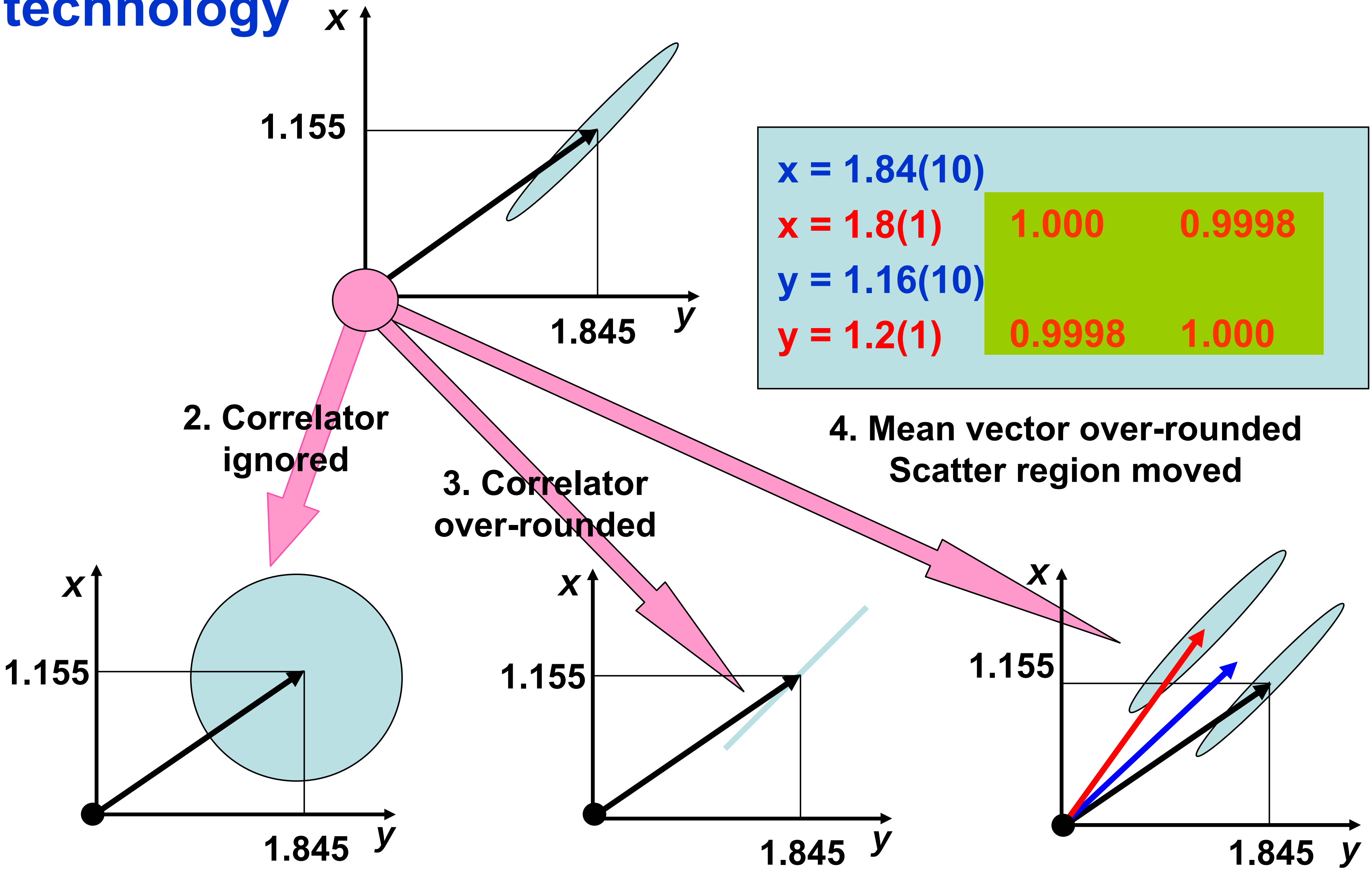
y = 1.16(10)

y = 1.2(1)

1.000	0.9998
0.9998	1.000

Data look as correct but are improbable!

All variants of correlated data corruption copiously presented in resources for science, education, and technology



Over-rounding is inspired by the ISO GUM

Quotation from the GUM

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. . . .

. . . Output and input estimates should be rounded to be consistent with their uncertainties; . . .

. . . . Correlation coefficients should be given with three-digit accuracy if their absolute values are near unity.

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

This clause should be rewrited

Biased nonlinear uncertainty propagation advocated in the 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

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

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).

Combined continuation

Biased nonlinear uncertainty propagation advocated in the 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

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

. . .

Note – When 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

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

This term sould be removed

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)

Safe rounding!

Inputs from matrix theory

Weil's theorem (see [29], [31]): Let $C = A + B$, where $A, B, C \in R^{n\times n}$ – symmetric matrices and $(\alpha_1 \leq \alpha_2 \cdots \leq \alpha_n)$, $(\beta_1 \leq \beta_2 \cdots \leq \beta_n)$, $(\gamma_1 \leq \gamma_2 \cdots \leq \gamma_n)$ their eigenvalues correspondingly.
Then $\forall i$ the following inequalities are valid

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

Gershgorin's theorem ([29], [30], [31]): Every eigenvalue α_i of the matrix A belongs to the interior of one of the circles

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

Schur's theorem ([31]): Let matrix $B \in R^{n\times n}$ is symmetric with values of the diagonal elements $b_1 \leq b_2 \leq \cdots \leq b_n$ (in any order) and eigenvalues $\beta_1 \leq \beta_2 \cdots \leq \beta_n$, then $\forall k \leq n$

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

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

On the basis of Weil, Gershgorin, and Schur spectral theorems we propose the following safe rounding threshoulds for:

Correlation coefficients

$$A \geq A_{\min}^{th} = \left\lceil \log_{10}\left(\frac{n-1}{2 \cdot \lambda_{\min}} \right) \right\rceil$$

Unitless uncertainties

$$P_U^{th} \geq \left\lceil \frac{1}{2} \log_{10}\left(\frac{n}{4 \cdot \lambda_{\min}} \right) \right\rceil$$

Unitless mean values

$$A_i \geq A_i^V = \left\lceil \frac{1}{2} \log_{10}\left(\frac{n}{4 \lambda_{\min} (U_i/[unit_i])^2} \right) \right\rceil$$

where $\lambda_{\min}$ is the minimal eigenvalue of the correlator

What is the "improper uncertainty propagation law"

The traditional way to estimate the mean value of the function depending upon *I* random variables *{c}* is just to insert their mean values into the dependence formula .

But if $\left\langle f(c_i) \right\rangle \neq f(\langle c_i \rangle)$ **we should calculate**

biases

$$\left\langle f(c_i) \right\rangle = f(\langle c_i \rangle) + \frac{1}{2} \sum_{i,j}^{I} \frac{\partial^2 f}{\partial c_i \partial c_j} \cdot cv(c_i c_j) + \ldots$$

and calculate the variance with contributioins from higher order derivatives and higher order input moments.

Two traditional ways to estimate covariances for several quantities depending upon the same set of input quantities

1. The Integral Uncertainty Propagation Law (IUPL)

$$cv(f_i, f_j) = \int (f_i - \langle f_i \rangle) \cdot (f_j - \langle f_j \rangle) \cdot g(c_\alpha) \cdot d^I c_\alpha$$

Works well (in low dimensions) if joint probability distribution function is known. But it is too expensive for high dimensional dependencies.

2. The Differential Uncertainty Propagation Law of **Order *T* -- DUPLO(*I*,*D*,*T*).**

$$cv(f_i, f_j) = \sum_{k,l=1}^{T} \frac{1}{k!l!} \frac{\partial^k f_i}{\partial c_{\alpha_1} \ldots \partial c_{\alpha_k}} \boxed{\left\langle \delta c_{\alpha_1} \ldots \delta c_{\alpha_k} \delta c_{\beta_1} \ldots \delta c_{\beta_l} \right\rangle} \frac{\partial^l f_j}{\partial c_{\beta_1} \ldots \partial c_{\beta_l}}$$

It works if joint probability distribution function is known or the set of its first higher moments (higher input covariators up to 2*T*-order) are known, and if *T* is properly chosen. Namely, covariator defined by formula will be positive definite for any dependencies if the number of input variables *I*, the number of dependent variables *D*, and the order *T* of the approximating Taylor polynomials obey the condition:

$$D \le \frac{(I+T)!}{I! \bullet T!} - 1$$

“The current doubtful practice guide”

In what follows a collection of examples of the doubtful practice is presented from the recent respectable resources :

- **Guide to the Expression of Uncertainty in Measurement** ***(ISOGUM,1995)***
- **Physical Review D55 (1997) 2259; D58 (1998) 119904,** ***CESR-CLEO Experiment***
- **European Physical Journal C20 (2001) 617,** ***CERN-LEP-DELPHI Experiment***
- **Reviews of Modern Physics, 77 (2005) 1,** ***CODATA recommended values of the fundamental physical constants 2002***
- **Journal of Physics G33 (2006) 1,** ***Review of Particle Physics***

Over-rounding in the ISO GUM

"**Annex H: Examples**" of ISO GUM clearly shows the failure of 7.2.6 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**

$$\begin{bmatrix} 1. & -0.588 & \text{[illegible]} \\ -0.588 & \text{[illegible]} & \text{[illegible]} \\ \text{[illegible]} & \text{[illegible]} & 1. \end{bmatrix}. \qquad (3)$$

Unreliable !!!

The eigenvalues of 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

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

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

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

This example should be reworked

The Physical Review D

Experiment CESR-CLEO

Over-rounding. Improper uncertainty estimation/propagation.

A. Anastassov *et al.* [CLEO Collaboration], Phys. Rev. D **55** (1997) 2559 [Erratum-ibid. D **58** (1998) 119904].

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	[illegible]
B_μ		1.00	[illegible]	[illegible]	[illegible]
B_h			[illegible]	[illegible]	0.63
[illegible]				1.00	0.45
B_h/B_e					1.00

Unreliable!!!

Eigenvalues of this matrix are as follows:

$$(2.1735,\ 1.7819,\ 1.0550,\ -0.0075,\ -0.0028)$$

So, the Erratum to the Erratum is needed

The European Physical Journal
Experiment CERN-LEP-DELPHI

Over-rounding. Improper uncertainty estimation/propagation.

P. Abreu *et al.* [DELPHI Collaboration], "A measurement of the tau topological branching ratios," Eur. Phys. J. C **20** (2001) 617.

$$\begin{bmatrix} B_1 \\ B_3 \\ B_5 \end{bmatrix} = \left(\begin{bmatrix} 0.85316 \pm 0.000929_{stat} \pm 0.000492_{syst} \\ 0.14569 \pm 0.000929_{stat} \pm 0.000477_{syst} \\ 0.00115 \pm 0.000126_{stat} \pm 0.000059_{syst} \end{bmatrix}, \begin{bmatrix} [illegible] & 0.98 & -0.08 \\ -0.9[illegible] & [illegible] & 0.08 \\ -0.08 & -0.0[illegible] & [illegible] \end{bmatrix} \right)$$

Unreliable !!!

Published correlator is incorrect and over-rounded.

Our calculations, based on data presented in the paper give the "correct" safely rounded correlator:

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

It seems that an Erratum to the paper is needed

The Reviews of Modern Physics

Over-rounding and improper incertanty propagation for derived quantities *{me, e, 1/a(0), h}*

CODATA: 1986	Symbol	Unit	Value(Uncertainty)xScale	Correlations		
Elementary charge	*e*	C	1.602 177 33(49) x 10^(-19)	*e*	*h*	*me*
Planck constant	*h*	J s	6.626 075 5(40) x 10^(-34)	0.997		
Electron mass	*me*	kg	9.109 389 7(54) x 10^(-31)	0.975	0.989	
1/(Fine strict. const.)	1/a(0)		137.035 989 5(61)	−0.226	−0.154	−0.005

CODATA: 1998	Symbol	Unit	Value(Uncertainty)xScale	Correlations		
Elementary charge	*e*	C	1.602 176 462(63) x 10^(-19)	*e*	*h*	*me*
Planck constant	*h*	J s	6.626 068 76(52) x 10^(-34)	0.999		
Electron mass	*me*	kg	9.109 381 88(72) x 10^(-31)	0.990	0.996	
1/(Fine strict. const.)	1/a(0)		137.035 999 76(50)	−0.049	−0.002	0.092

CODATA: 2002(5)	Symbol	Unit	Value(Uncertainty)xScale	Correlations		
Elementary charge	*e*	C	1.602 176 53(14) x 10^(-19)	*e*	*h*	*me*
Planck constant	*h*	J s	6.626 0693(11) x 10^(-34)	1.000		
Electron mass	*me*	kg	9.109 3826(16) x 10^(-31)	0.998	0.999	
1/(Fine strict. const.)	1/a(0)		137.035 999 11(46)	−0.029	−0.010	0.029

Eigenvalues of the selected correlation submatrices

1986: { 2.99891, 1.00084, 0.000420779, **-0.000172106** }

1998: { 2.99029, 1.01003, **-0.000441572**, 0.00012358 }

2002: { 2.99802, 1.00173, 0.000434393, **-0.000183906** }

In May 2005 the accurate data on basic FPC appeared. This gave us possibility for the further investigation of the derived FPC *{me, e, 1/a(0), h}* :

Linear Differential Uncertainty Propagation (DUP) (default machine precision)

2006: { 2.99825, 1.00175, 9.95751E-10, 9.23757E-17 }

Linear DUP (SetPrecision[exp,30])

2006: { 2.99825, 1.00175, 9.95751E-10,-6.95096E-35 }

Non- Linear DUP (second order Taylor polynomial) (SetPrecision[exp,100])

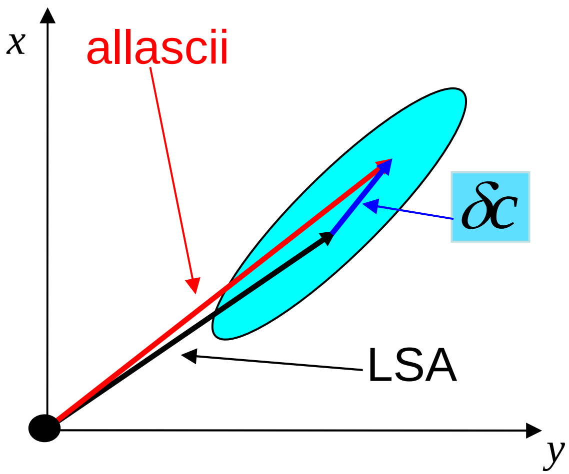
2006: { 2.99825, 1.00175, 9.95751E-10, 2.86119E-15 }

Where is the end of the rounded vector of the basic FPC?

The end of the rounded vector should belong to the non-rounded scatter region.

To characterize the deviation we use the quadratic form χ^2

$$\chi^2 = \sum_{i,j}^{n} \delta c_i \cdot [cv]_{ij}^{-1} \cdot \delta c_i$$



δc = c(allascii) –c(LSA)

$$\mu_i = \delta c_i / \sigma_i$$

Rounded vector belongs to non-rounded scatter region if:

$$\chi^2 = \sum_{i,j}^{n} \mu_i \cdot [cr]_{ij}^{-1} \cdot \mu_j < 1$$

We have 22 constants for which NIST give both allascii (rounded) and LSA “non-rounded” data for this test:

$$\chi^2 \approx 0.06 \;\; !!!$$

Comparison with CODATA recommended values of derived FPC {*me, e, 1/a(0), h*}

1. Insert values of the basic constants from LSA files into formulae

$$me = \frac{2R_\infty \cdot h}{c \cdot \alpha^2} = 9.109382551053865\text{E-}31$$

$$e = \sqrt{\frac{2 \cdot \alpha \cdot h}{\mu_0 \cdot c}} = 1.6021765328551825\text{E-}19$$

2. Biases were calculated supposing the multi-normal distribution for basic FPC. They are much less than corresponding standard deviations

	me	*e*	*1/a(0)*
bias	2.4943**E-66**	-2.6186**E-58**	1.7918**E-36**
sigma	1.5575**E-37**	1.7918**E-36**	**5.0E-7**

Comparison with CODATA recommended values for covariance matrix of derived FPC *{me, e, 1/a(0), h}*

Properties of the correlation matrix for vector *{me, e, 1/a(0), h}* calculated with DUPLO(2,4,1)

DUPLO(2,4,1)	17.06.2006
Symmetry	True
Positive definiteness	False
Is rounding correct?	False
Minimal eigenvalue	**-6.9 E-108**
Rounding threshold	**Warning!** Matrix is non positive definite

Properties of the correlation matrix for vector *{me, e, 1/a(0), h}* calculated with DUPLO(2,4,2)

DUPLO(2,4,2)	17.06.2006
Symmetry	True
Positive definiteness	True
Is rounding correct?	True
Minimal eigenvalue	**2.8 E-15**
Rounding threshold	15

But where is the end of the rounded vector for derived FPC?

FPC	Our calculations with DUPLO(2,4,2)	Allascii (NIST)
me	9.10938255105386**5**E-31	9.1093826 [illegible]
e	1.602176532855182**8**E-19	1.602[illegible] E-19
1/a(0)	137.035999105576373	[illegible]03599911
h	6.626069310828000E-34 (LSA)	6.6260693 E-34

IMPROBABLE !!!

$$\chi^2 = 2.18E+10$$

Thus, we see that the values of the derived vector components {*me,e,1/a(0)*} presented on the NIST site in allascii.txt file are

improbable!!!

The vector is out of the scatter region for the 10^10 standard deviations due to improper uncertainty propagation and over-rounding

Journal of Physics G33 (2006) 1,
Review of Particle Physics

Selected example: constraint fit of η decay rates.

Unrounded double-precision value of correlation coefficients accessible by the PDG Live constitute the non positive semi-definite correlation matrix.

The minimal eigenvalue of the correlation matrix is

-1.40*10^{-8}

and is far from the machine zero, which is ~10^{-16} I guess.

So, either the correlation matrix is badly over-rounded or fit is unstable (unreliable)

CONCLUSION

OUR PRPOSALS ARE AS FOLLOWS:

- The original GUM should be corrected in places where the rounding rules for correlated data are discussed and used;
- The GUM formula for the nonlinear uncertainty propagation should be corrected to assure the positive valued variance;
- The obligatory quotation of the rounding thresholds for correlation matrix and for the mean values and their uncertainties should be included into the GUM-Supplement-2 recommendations;
- Our rule to find the order *T* of the Taylor polynomials to assure the positive definiteness of the correlator for *D*-dimensional vector function depending upon *I*-random variables and specification of its *D*-dimensional scatter region should be included into the GUM-Supplement-2 recommendations;
- It should be indicated in some clause of GUM-Supplement-2 that the rounding thresholds for correlated data impose severe requirements on the storage and exchange formats of the correlated data.

SUMMARY

that was clearly formulated ten years ago remains relevant today

**“. . . 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 Bi`evre “Measurement results without statements of reliability (uncertainty) should not be taken seriously”
Accred. Qual. Assur. **2** (**1997**) 269

Having revised and expanded ISO GUM the analogous appeal should be addressed to the whole science, metrology, technology, and publishing communities and should be promoted by ICSU, CODATA, ISO and their national sub-commitees