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EVALUATION AND NUMERICAL PRESENTATION OF THE RESULTS OF MULTIVARIATE MEASUREMENTS – SELECTED PROBLEMS

A brief review of some problems arising in the correct numerical expression and evaluation of results of indirect multi-parameter measurements is given. There is included a theoretical basis for determining the estimates of values, uncertainties and correlation coefficients of the indirectly obtained multi-measurand, which are processed from data of the simultaneously measured set of variables. The algebra of random vectors is used. A numerical example illustrates the linear transformation of two variables and the types of improperly evaluated results - that may occur with over-rounding. There are given thresholds of the safe uniform rounding of mean vector and its scatter ellipsoid. There is proposed an upgrading of the GUM Example H.2 and of the uncertainty equation for nonlinear functions. It is also evidenced that correlation matrix of 2010 data of fundamental physical constants recommended by CODATA has non-negligible negative eigenvalues. In the end of this work it is argued for the urgent needs of standardization of e-publication of the experimental data in two parts: e-printed traditional narrative part, and an attached computer readable file with all numerical input data and results, to allow "fast" numerical peer review of the proposed publication reporting new measurement results. This work is a result of an inter-disciplinary cooperation of a metrologist and a nuclear physicist.

Keywords: *uncertainty, indirect measurements, multi-measurand, correlated data.*

1. Introduction

Simultaneous measurements of several statistically related quantities, i.e. correlated, are performed in science, education, technology, economy and many other disciplines. From the digitally processed on- or off-line data of m variables, directly measured on input, the n other variables (in physics called as observables) are determined indirectly on output, if their mutual relation is known. In addition to estimators of values and uncertainty the knowledge about correlation coefficients of output quantities also is of special importance for some or all of these variables to be jointly processed further.

Accuracy of evaluated output multi-measurand data depends on the statistical uncertainties of given parameters of input multi-measurand, as well as on the accuracy of their processing. Final rounding of indirectly obtained data of output multi-measurand must depend on a uncertainty of the input data [6]. The "safe rounding" of the digitally processed multi-measurand data should be done in such a way that they are not be damaged. If the accuracy of final uncertainties or number of repetitions of raw measurements are not given in publication of input data then it should not be assumed that the values of estimators of standard deviations and correlation coefficients of the initial variables are correctly found from measurement data and are as their values for whole populations.

In indirect multi-dimensional measurements there are two border types of relations of the uncertainty both components u_A and u_B [1].

First case: uncertainty $u_A \ll u_B$. In such situations it is enough to provide the necessary instrumental resolution and accuracy for measurement of input values and to determine cross-links to the output.

Second case: $u_A \gg u_B$ when all environmental effects interacting on input measurements are carefully eliminated and the uncertainty of type B is small compared to the range of random scatter of observed variables. Here one should achieve maximum accuracy in measurements and then the information obtained in the experiment is not partially lost in the processing of the random input data and in the rounding of the obtained results. The number of observations should be as large as possible to minimize the statistical type uncertainty u_A.

2. Short theoretical backgrounds

The input multi-measurand can be expressed by random vector $\mathbf{X} = [X_1, X_2,... X_m]^T$ and output one – by vector $\mathbf{Y} = [Y_1, Y_2, ... Y_n]^T$. These random vectors of dimensions m and n, respectively, can describe the multi-dimensional normal distributions of **X** and **Y**. The relation between them is given by

$$\mathbf{X} = \mathbf{F}\,\mathbf{Y}.$$

If **F** is a linear operator, then $n \le m$.

The basic structure of the numerical estimation of the multi-measurand should contain averaged components of the random vector and a description of the multidimensional scatter region and the accuracy of both these data. If this region can be defined by a model of joint n-dimensional probability distribution, then, for a given probability density $p(X_1,...,X_n)$ of n-dimensional normal distribution such region takes the form of a n-dimensional hyper-ellipsoid with its center at the end of the average vector. Relations between covariance matrices of hyper-ellipsoids of the output and input measurands (in a linear approximation of the observables in the vicinity of the end of mean vector $\overline{\mathbf{X}}$ are described analytically by

$$\mathbf{c_Y} = \mathbf{S}\ \mathbf{c_X}\ \mathbf{S}^T,$$

where $\mathbf{S}\equiv(\partial\mathbf{Y})/(\partial\mathbf{X})$ is the matrix of sensitivity coefficients.

The matrix **r** of the correlation coefficients, defined by the relation $\mathbf{r} = \mathbf{y}\,\mathbf{c}\,\mathbf{y}^T$, is called the correlator. A multidimensional distribution is normal if matrices **c** and **r** are positive definite, i.e. their eigenvalues λ_i, which are the roots of the characteristic equations $\det[\mathbf{c} - \boldsymbol{\lambda}\mathbf{1}] = \mathbf{0}$, and $\det[r - \lambda 1] = 0$, respectively should be positive [3]. This requirement was not included in GUM [1]. So, to express correctly the result of measuring or evaluating vector quantity the **minimal data structure** should contain:

Mean vector,

- *Vector of standard deviations and their uncertainties (or number of measurements in each sample),*
- *Positive definite correlation matrix* and *uncertainties of their elements,*
- *Machine precision used to compute vector parameters and eigenvalues of correlation matrix*.

With these data the user will have complete information to plan and control the safe usage of data in next computations.

In Fig 1 there is shown an example of a linear transformation of two dimension (2D) "Greek" vector $\mathbf{X} = [\eta, \zeta]^T$ to "Latin" vector $\mathbf{Y} = [x, y]^T$.

Basic equations for the processing of 2D random vectors are given in Table 1 and typical distortions of output data are shown in Fig 2.

To express difference between the center of the ellipse of transformed original raw data and the end of vector $\mathbf{Y}_i$ Mahalanobis distance χ is used, which is given by

$$\chi^2 = \Delta\mathbf{Y}\frac{1}{\sigma_x\sigma_y}\mathbf{r}(x,y)^{-1}\Delta\mathbf{Y}^T.$$

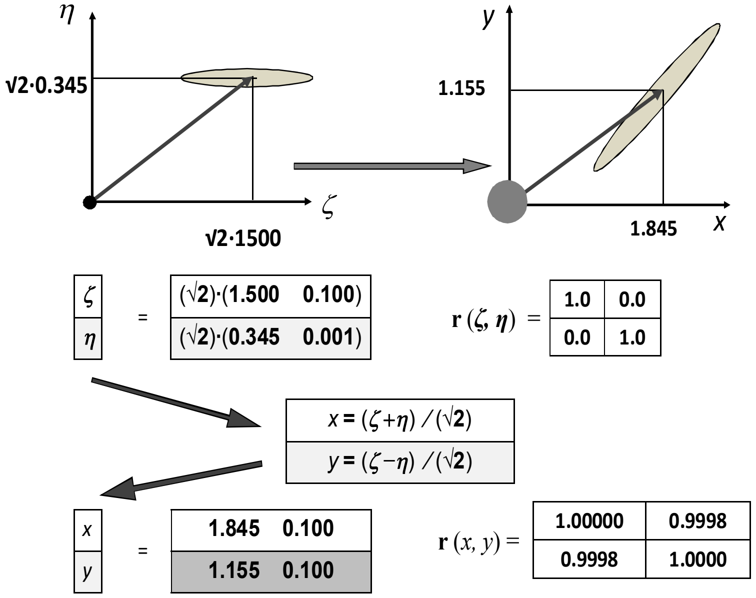

Fig. 1. Linear transformation of 2D random vector

Table 1

Basic formulas of the 2D random vector transformation of Fig 1

Transformation	Covariance matrix
$\begin{bmatrix}\bar{x}\\ \bar{y}\end{bmatrix} = \mathbf{S}\begin{bmatrix}\bar{\varsigma}\\ \bar{\eta}\end{bmatrix} = \begin{bmatrix}1 & 1\\ 1 & -1\end{bmatrix}\begin{bmatrix}\bar{\varsigma}\\ \bar{\eta}\end{bmatrix} = \begin{bmatrix}\bar{\varsigma}+\bar{\eta}\\ \bar{\varsigma}-\bar{\eta}\end{bmatrix}$	$\mathbf{c}_{xy} = \begin{bmatrix}1 & 1\\ 1 & -1\end{bmatrix}\begin{bmatrix}\sigma_\varsigma^2 & \sigma_\varsigma\sigma_\eta\rho_{\varsigma\eta}\\ \sigma_\varsigma\sigma_\eta\rho_{\varsigma\eta} & \sigma_\eta^2\end{bmatrix}\begin{bmatrix}1 & 1\\ 1 & -1\end{bmatrix} = \begin{bmatrix}\sigma_x^2 & \sigma_\varsigma^2-\sigma_\eta^2\\ \sigma_\varsigma^2-\sigma_\eta^2 & \sigma_y^2\end{bmatrix}$
Standard deviations $\sigma_x = \sqrt{\sigma_\varsigma^2+\sigma_\eta^2+2\sigma_\varsigma\sigma_\eta\rho_{\varsigma\eta}}$ $\sigma_y = \sqrt{\sigma_\varsigma^2+\sigma_\eta^2-2\sigma_\varsigma\sigma_\eta\rho_{\varsigma\eta}}$	Correlator $\mathbf{r}_{xy} = \begin{bmatrix}1 & \rho_{xy}\\ \rho_{xy} & 1\end{bmatrix}$ Where: correlation coefficient $\rho_{xy} = \frac{\sigma_\varsigma^2-\sigma_\eta^2}{\sigma_x\sigma_y}$ **c** & **r** *positive def.* $\det(\mathbf{A}-\lambda\mathbf{I}) = 0$ $\lambda_i \geq 0$

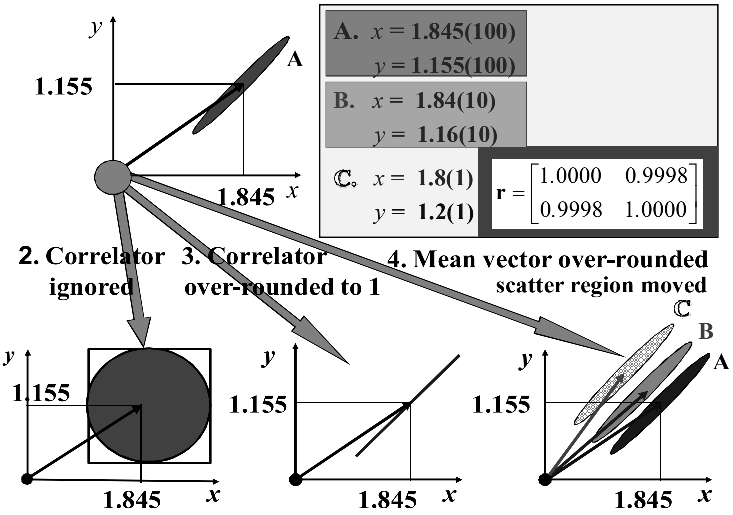

Fig. 2. Cases of improper presentation of correlated 2D data

A. Rounding of **Y** = [1,845(100); 1,155(100)] (ρ_{xy} = 0,9998),

B. Rounding to 2 digits after decimal point:

$$\mathbf{Y_1} = [1,84(10); 1,16(10)];$$

$$\Delta\mathbf{Y}_1 = \mathbf{Y_1}-\mathbf{Y} = [-0,005; 0,005];\ \chi_1^2 = 25 > 1.$$

C. Rounding to 1 digit after decimal point:

$$\mathbf{Y_2} = [1,8(10); 1,16(10)];$$

$$\Delta\mathbf{Y}_2 = \mathbf{Y_2}-\mathbf{Y} = [-0,045; 0,045];\ \chi_2^2 = 2500 >> 1.$$

For the ellipse border the distance χ = 1. Then the ends of both rounded vectors $\mathbf{Y_1}, \mathbf{Y_2}$ situated are outside of the ellipse of transformed original random input data. If the assumption proposed by V. Ezhela in [2 – 4] for safety processing of random vectors is to be satisfied, these ends has to be situated inside of this ellipse. Then in both cases the results are over-rounded. Such assumption can be valid only for the absolutely accurate input statistical data from the whole random populations of X_i or for very large – going to infinity, number of sample elements, and when instrumental errors are negligible. That condition is not fulfilled in many existing in measurement situations, where data samples of a small number of elements is only possible to obtain in a limited time of observation. All estimators of values, standard deviations and correlation coefficients obtained from the samples of limited number N of multivariate observations have their own uncertainties, which increase rapidly for small N. From above it follows that two different type of rounding procedures of multivariate data are needed:

– for safety numerical processing of random vectors, and

– for describing the accuracy of their statistical parameters.

In the second case thresholds for limiting the rounding for output data parameters have to be established as dependent on accuracy of the statistical parameters of the input samples.

3. Thresholds of the safe rounding of transformed multivariate data

From spectral theorems of matrix theory V. Ezhela obtained thresholds of the number of digits after decimal point for fully safe independent uniform rounding of the output random mean vector and its scatter ellipsoid processed from given data of input random vector [6] treated as absolutely accurate. These thresholds are valid only for digital processing itself because of the assumption that uncertainties of standard deviations and correlation coefficients of the input vector are negligible. All thresholds of such safety processing of the random vector data are expressed in terms of decimal numbers, i.e.:

− for standard deviations U_i of vector components V_i

$$A_i^U \ge A_i^{Uth} = \text{Upper Integr}\left[\frac{1}{2}\log_{10}\left(\frac{n}{4\lambda_{min}T_{CL}^2\left(\frac{U_i}{unit_i}\right)^2}\right)\right];$$

− for values of the components V_i of the average vector

$$A_i^V \ge A_i^{Vth} = A_i^{Uth};$$

− for elements of the correlation matrix

$$A^C \ge A_{i\ne j}^{Cth} = \text{Upper Integr}\left[\log_{10}\left(\frac{n-1}{2\lambda_{min}}\right)\right],$$

where λ_{min} – minimal eigenvalue of the correlation matrix; T_{CL}^2 – “tolerance” factor at defined confidence level.

Formulas looks sophisticated, but are quite easy to be used – see examples in [4], [6] and [7].

As it was noticed before, obtained experimentally measurement data have limited numbers of observations in the samples and are not absolutely accurate. Uncertainties of estimators of the most probable values of vector components and of their standard deviation have to be also taken in considerations. Then the rounding of real multi-measurements data has to be done below above thresholds given for data processing. An graphical illustration of such rounding of data from table 2 for constant correlation coefficient ρ_{xy} is shown on Fig. 3.

Table 2

Parameters	$\bar{x}$	σ_x	$\bar{y}$	σ_y
Raw results	0.3242	0.0664	0.1555	0.0256
A. rounding to 3 digits	0.324	0.067	0.156	0.026
B. rounding to 2 digits	0.32	0.07	0.16	0.03
C. rounding to 1digit	0.3	< 0.1	0.2	< 0.1

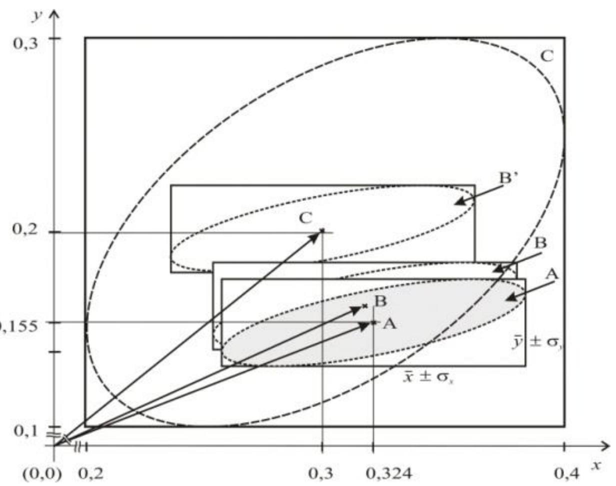

Fig . 3. Rounding with constant correlation coefficient ρ_{xy}

The largest ellipse C of rounding to 1 digit do not fully cover the primary ellipse A. Then the different rounding with changes of correlation coefficients $\rho_{ij,}$ also should be applied. Two following methods of rounding below thresholds are preliminary tested:

• **Method 1** –by truncation (omit further digits after the no changed last accepted);

• **Method 2** – to maintain a constant values of non diagonal elements of the positive covariance matrix, i.e.:

$$\rho_{RX}^{-} = \frac{\sigma_R \sigma_X}{\sigma_R^{+} \sigma_X^{+}} \rho_{RX}; \quad \rho_{RZ}^{-} = \frac{\sigma_R \sigma_Z}{\sigma_R^{+} \sigma_Z^{+}} \rho_{RZ}; \quad \rho_{XZ}^{-} = \frac{\sigma_X \sigma_Y}{\sigma_X^{+} \sigma_Z^{+}} \rho_{XZ},$$

where: signs in the upper index indicates the direction of change.

Both methods are used for rounding data of Example H.2 GUM to 3 and 2 digits after decimal point [6]. Method 1 gives a smaller values of Mahalanobis distances of vector ends from the transformed raw data ellipse center, but the smallest eigenvalue is closer to zero than in method 2. Correlator of method 1 keeps to be positive definite, but there is no the full theoretical justification of it.

Conclusion: since in multivariable measurements the rounding level of output vector **Y** depends not only on the precision of digital processing but mainly on the uncertainties of all statistical parameters of input vector **X,** then additional formulas of rounding thresholds are urgently needed.

4. Upgrading the gum proposals for multivariable measurements

All official metrological documents are applicable now to single measured quantity only. (Supplement 2 to GUM [1] – about extension it to any number of quantities is still at the draft stage.). But statements in the main text of GUM are formulated in such a manner that the reader gets the impression that a generalization to the multivariate case is straightforward. That was considered in details in Example H.2 of GUM which illustrates clauses 7.2.5 and 7.2.6.

About Example H.2 of GUM

In Table H.2 of GUM [1] there are given five raw simultaneous measurements of input vector $\mathbf{X}=[U,J,\Phi]^T$ and vector

$$\mathbf{Y} = [R = U\cos\Phi/J,\ X = U\sin\Phi/J,\ Z = U/J]^T$$

is evaluated. The results are presented there in Tables H.3 and H.4. Rounding of correlation coefficients is not properly done there, since the smallest eigenvalue of correlator matrix is negative and so the scatter region is not of the 3D-ellipsoide form. Also final output data of Example H.2 does not satisfy "physical law" of impedance of the two-terminal passive element which is: $X^2+Y^2=Z^2$ as $\boldsymbol{\sigma^2}=-71{,}5$**!?** [3, 6, 7].

For establishing requirements of safety digital processing purposes according , the input multivariate measured data of H.2 Example are treated first as absolutely accurate data of full population [6], [7]. Then, for such theoretical case, thresholds of digit numbers after decimal point are as follows: for mean values and standard uncertainty of R and Z − 5 digits, of X − 4 digits and for correlation coefficients − 8 digits! [4, 6]. So high numbers of digits cannot be accepted for describing the measurement results as they are obtained under the assumptions that: input data are treated as fully accurate, numerical results of processing are safety and uniformly rounded to maintained vector end in the scattered area of the transformed original input data. They can be used only as a reference of processing of the absolutely accurate data of the random vector of similar component values as parameter estimators of samples of the input vector **X** in H.2 Example. All these samples have only N = 5**!** measurements each and the accuracy of SD of each variable and of correlator elements is very poor. Relative uncertainty of SD of such small samples is about 36% – see Table E.1 in GUM [1].

5. Using the nonlinear uncertainty propagation

In the multivariable case the linear propagation of errors from m-dimensional vector **X** to n-dimensional vector **Y** is misleading in cases n > m. In the Notice to clause 5.1.2 of GUM [1] is determinate only the uncertainty of non-linear single function y = f(X). There is recommended that the linear propagation of variance is supplemented by higher-order components, i.e.

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

Calculations of the variance $u^2(y)$ according to this formula may give a false negative value because of the component in parentheses with the third derivative. This is illustrated below by the example of the single nonlinear polynomial function

$$F(x) = 1 - x + 2x^2 + 3x^3 + 4x^4,$$

measurand x is normally distributed around $x = 0$ with variance σ^2. Calculating the variance $u^2(F)$ according to the recommendation 5.1.2 gives

$$u^2(F) = \sigma^2 F'(0)^2 + 1/2\sigma^4 F''(0)^2 + \sigma^4 F'(0)F'''(0) =$$
$$= \sigma^2[1 + \sigma^2(16/2 - 18)] = \sigma^2[1 - 10\sigma^2].$$

For $\sigma^2 > 0.1$ is obtained $u^2(F) < 0$.

So, clause 5.1.2 of GUM should be corrected by removing the component with the third derivative.

In case of the **nonlinear processing of input vector** the widely used differential “linear uncertainty propagation law” does not work properly in more accurate calculations for highly nonlinear functions. The nonlinear uncertainty propagation should be used with the obligatory positivity constraints

$\mathbf{C}_i$, $[\delta C_a, \delta C_b]$ ⟶ $F_k(\mathbf{C}_i)$, $[\delta F_m, \delta F_n]$

COMPONENT of X (input) **COMPONENT of Y (output)**

$$[\delta F_i,\delta F_j]=\sum_{k,l=1}^{T}\frac{1}{k!\,l!}\frac{\partial^k F_i}{\partial c_{\alpha_1}\ldots\partial c_{\alpha_k}}\{\delta c_{\alpha_1}\ldots\delta c_{\alpha_k},\delta c_{\beta_1}\ldots\delta c_{\beta_l}\}\frac{\partial^l F_j}{\partial c_{\beta_1}\ldots\partial c_{\beta_l}}.$$

Covariance matrix $[\delta F_m, \delta F_n]$ is non-degenerate and positive definite if dimensions $\dim(C_i)=m$, $\dim(F_k)=n$ and the order T of component of the Taylor polynomials approximated the measuring vector function F_k obey the inequality:

$$n \le n_{th} = \frac{(m+T)!}{m!\,T!} - 1 \quad \text{Where:}$$

m	1	1	1	2	2	2	3	3	3
T	1	2	3	1	2	3	1	2	3
n_{th}	1	2	3	2	5	6	3	9	19

6. Short commentary on data of fundamental physical constants

The adjustments of the fundamental physical constants (FPC) are regularly performed by the Fundamental Constants Data Center at NIST and recommended by CODATA as the unique source of the current FPC values. There are 325 adjusted quantities, from which 79 are called basic algebraically independent constants C_α^B. As an example there are listed below in Table 3 last values of four FPC given by CODATA 2010 [9] in SI units and their correlation matrix.

Table 3

				e	h	me
Elementary charge	e	C	$1.602\,176\,565(35)\cdot 10^{-19}$			
Planck constant	h	J s	$6.626\,069\,57(29)\cdot 10^{-34}$	0.9999		
Electron mass	me	Kg	$9.109\,382\,91(40)\cdot 10^{-31}$	0.9992	0.9996	
1/fine structure const	1/α (0)	-	137.035 999 074(44)	−0.0142	−0.0005	0.0269

Eigenvalues of above correlation matrix are: [2.99942, 1.00006, 0.000719993, – 0.000202165]. The last eigenvalue is non-negligible negative. Only two of constancies FPC can be used together in joint precision calculations. More about negative eigenvalues in CODATA publications is in [3, 7, 8].

7. Application of e-publishing in multi-variable measurements

The traditional form of the scientific communication based on the paper oriented e-publications is now not the proper way to present and to exchange the multidimensional experimental data. The standardization of two-component forms of the scientific publication is unavoidable. First component will be the traditional descriptive scientific text already well formalized by publishers, but the second part should be computer readable file with all numerical input data and results to allow “fast” numerical peer review of the publication reporting new results. Some particular problems connected with that proposal are discussed in[8] and in detail in [3] together with given four dozen examples of “bad practice” of physical publications in journals of high “impact factor” and in other sources.

8. Main conclusions

Some of the presented problems of the evaluation of results and uncertainty of the indirect multivariable measurements still need farer investigations to obtain clear enough backgrounds for the common international acceptance of the rounding and digital presentation methods of multivariate data results and of the calculation uncertainty of highly nonlinear related multivariate data. Then such recommendations should be included in the Supplement 2 to the "Guide to the expression of uncertainty in measurements − Extension to any number of quantities" or included to the post-GUM documents. These problems are not yet fully included in the actual draft version of Supplement 2.

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ОЦЕНКА И ЧИСЛЕННОЕ ПРЕДСТАВЛЕНИЕ РЕЗУЛЬТАТОВ МНОГОМЕРНЫХ ИЗМЕРЕНИЙ – НЕКОТОРЫЕ ПРОБЛЕМЫ

З.Л. Варша, В.В. Эжела

Дан краткий обзор некоторых проблем, возникающих в правильном числовом выражении и оценке результатов косвенных многопараметрических измерений. Приведены теоретические основы определения оценок величин, неопределенностей и коэффициентов корреляции полученных косвенно нескольких измеряемых величин, которые обрабатываются по данным одновременно измеренного множества переменных. Используется алгебра случайных векторов. Числовой пример иллюстрирует линейное преобразование двух переменных и типы неправильно оцененных результатов, которые могут быть получены при округлении. Предложена модернизация примера GUM H.2 и уравнения неопределенности для нелинейных функций. Это доказывает, что корреляционная матрица данных фундаментальных физических констант 2010 года, рекомендованных CODATA, имеет не ничтожно малые отрицательные собственные значения. Эта работа является результатом междисциплинарного сотрудничества метролога и физика-ядерщика.

Ключевые слова: *неопределенность, косвенные измерения, мультиизмеряемые величины, коррелированные данные.*

ОЦІНКА ТА ЧИСЕЛЬНЕ ПОДАННЯ РЕЗУЛЬТАТІВ БАГАТОВИМІРНИХ ВИМІРЮВАНЬ – ДЕЯКІ ПРОБЛЕМИ

З.Л. Варша, В.В. Ежела

Надано короткий огляд деяких проблем, що виникають у правильному числовому виразі і оцінці результатів непрямих багатопараметричних вимірювань. Наведено теоретичні основи визначення оцінок величин, невизначеності і коефіцієнтів кореляції непрямо отриманих декількох вимірюваних величин, які обробляються за даними одночасно виміряної множини змінних. Використовується алгебра випадкових векторів. Числовий приклад ілюструє лінійне перетворення двох змінних і типи неправильно оцінених результатів, які можуть бути отримані при округленні. Запропоновано модернізація прикладу GUM H.2 і рівняння невизначеності для нелінійних функцій. Це доводить, що кореляційна матриця даних фундаментальних фізичних констант 2010 року, рекомендованих CODATA, має не мізерно малі негативні власні значення. Ця робота є результатом міждисциплінарного співробітництва метролога і фізика-ядерника.

Ключові слова: *невизначеність, непрямі вимірювання, мультивимірювані величини, корельовано дані.*