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Monte-Carlo evaluation of measurement uncertainty using a new generator of pseudorandom numbers

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Abstract

The Monte Carlo method has been applied in metrology for a long time, but only recently (2008) it has been recommended by the international normative body (Joint Committee for Guides in Metrology) for evaluation of measurement uncertainty. This paper is devoted to the problem of efficient generation of pseudorandom numbers following a distribution whose probability density function is very close to the Gauss function, but it has finite-support, and – unlike the probability density function of the truncated normal distribution – is continuous. The applicability of the proposed solution for evaluation of measurement uncertainty is illustrated with an example of practical importance.

Keywords: evaluation of measurement uncertainty, Monte Carlo method, generation of pseudorandom numbers.

Ocena niepewności pomiarowej przy użyciu metody Monte Carlo i nowego generatora liczb pseudolosowych

Streszczenie

Zgodnie z Suplementem #1 do międzynarodowego przewodnika dotyczącego wyrażania niepewności pomiaru [2] metoda Monte Carlo staje się jedną ze standardowych metod oceny owej niepewności. Podstawowym narzędziem jej implementacji są generatory liczb pseudolosowych o rozkładach modelujących rozkłady błędów występujących w systemach pomiarowych. Nierzadko – np. w zastosowaniach, w których niepewność pomiaru przekłada się na ryzyko błędu w sztuce medycznej – zachodzi potrzeba oceny rozszerzonej niepewności pomiaru metodą najgorszego przypadku. Stosuje się wówczas liczby pseudolosowe o rozkładzie równomiernym (*à la limite* – dwupunktowym) lub obciętym normalnym. Ciąg tych ostatnich uzyskuje się zwykle poprzez odpowiednią transformację ciągu liczb o rozkładzie normalnym lub równomiernym. W obydwu przypadkach jest to operacja dość złożona obliczeniowo i dlatego wciąż pojawiają się nowe propozycje generatorów. Jedną z najnowszych oraz przegląd starszych znaleźć można w artykule [3]. Wspólną ich wadą – obok złożoności obliczeniowej – jest nieciągłość funkcji gęstości prawdopodobieństwa w punktach obcięcia oraz kilkuprocentowe zmniejszenie odchylenia standardowego. W artykule przedstawiono nowy, wolny od tych wad, generator liczb pseudolosowym o rozkładzie zbliżonym do obciętego normalnego (różnicę odpowiednich funkcji gęstości prawdopodobieństwa przedstawia rys. 1). Jego użyteczność zilustrowano przykładem zastosowania do analizy propagacji błędów danych metodą Monte Carlo w procedurze estymacji mezurandu metodą najmniejszych kwadratów w przypadku, gdy zarówno dane reprezentując zmienne niezależne i zmienną zależną obarczone są błędem przypadkowym.

Słowa kluczowe: szacowanie niepewności pomiarowej, metoda Monte Carlo, generatory liczb pseudolosowych.

1. Introduction

Unlike real-world (physical, chemical or biochemical) experiments, numerical experiments are on the whole neither expensive nor time consuming. Statistical simulation is, therefore, a very practical and reliable tool for evaluation of measurement uncertainty. Roughly speaking, it consists in:

- generation of many realisations of source uncertainties in the data using generators of pseudorandom numbers;
- computer simulation of a measuring system (or its part) under evaluation – for each realisation of those uncertainties;
- elaboration of the obtained results of simulation, aimed at determination of their statistical characteristics such as average, minimum and maximum values or dispersion of errors.

This method, known under the name of Monte Carlo method, has been applied in metrology for a long time (see, for example, the author's paper of 2000 [1]), but only recently (since 2008) it has been recommended by the international normative body (Joint Committee for Guides in Metrology) for everyday use in measurement practice [2]. This paper is devoted to an algorithmic problem of practical importance, *viz.* to efficient generation of pseudorandom number whose probability density function (PDF) is a finite-support approximation of the Gauss function. First, in Section 2, the Monte Carlo method is presented in a way it is introduced in the above-quoted document, called *GUM Supplement 1* hereinafter. Next, in Section 3, the proposed generator of pseudorandom numbers is developed, and in Section 4 – its applicability is illustrated with an example.

The following rules of mathematical notation are applied throughout this paper:

- $x, \mathbf{x}, \mathbf{X}$ – a scalar variable, a vector of scalar variables and a matrix of scalar variables;
- $\dot{x}, \dot{\mathbf{x}}, \dot{\mathbf{X}}$ – the exact values of $x, \mathbf{x}$ and $\mathbf{X}$;
- $\widetilde{x}, \widetilde{\mathbf{x}}, \widetilde{\mathbf{X}}$ – the values of $x, \mathbf{x}$ and $\mathbf{X}$, subject to source errors;
- $\hat{x}, \hat{\mathbf{x}}, \hat{\mathbf{X}}$ – the values of $x, \mathbf{x}$ and $\mathbf{X}$, subject to estimation errors;
- $\underline{x}, \underline{\mathbf{x}}, \underline{\mathbf{X}}$ – a scalar random variable, a vector of scalar random variables and a matrix of scalar random variables.

Moreover, the following specific symbols are used hereinafter:

- $\mathsf{N}\left(\mu, \sigma^2\right)$ – the normal distribution of a scalar random variable whose mean is μ and variance – σ^2;
- $\mathsf{U}\left(a, b\right)$ – the uniform distribution of a scalar random variable assuming the values from the interval $\left(a, b\right)$.

2. Monte Carlo method according to *GUM Supplement 1*

The Monte Carlo method is defined in *GUM Supplement 1* as *"method for the propagation of distributions by performing random sampling from probability distributions"* [2 – p. 5]. When applied for evaluation of measurement uncertainty, it comprises

three stages: formulation, propagation, and summarizing [2 – pp. 7–8]. Formulation is specified in *GUM Supplement 1* as follows:
- define the measurand (*i.e.* the quantity intended to be measured) $\underline{y}$;
- determine the vector of quantities $\underline{\mathbf{x}}$ upon which $\underline{y}$ depends;
- develop a model relating $\underline{y}$ and $\underline{\mathbf{x}}$ – $\underline{y} = f(\underline{\mathbf{x}})$;
- on the basis of available knowledge assign a PDF to $\underline{\mathbf{x}}$ taking into account possible statistical dependence of its components.

The second stage of the Monte Carlo procedure is aimed at computing the PDF for $\underline{y}$ on the basis the model. The last stage consists in using the PDF of $\underline{y}$ for obtaining:
- the expectation of $\underline{y}$ (taken as an estimate of the measurand);
- the standard deviation of $\underline{y}$ (taken as the standard uncertainty associated with the result of measurement).
- a coverage interval containing $\underline{y}$ with a specified probability (the coverage probability).

According to *GUM Supplement 1*, the above-listed operations can validly be applied under the following conditions [2 – pp. 15–16]:
- the function $f(\underline{\mathbf{x}})$ is continuous with respect to all elements of the vector $\underline{\mathbf{x}}$ in the neighbourhood of their best available estimates;
- the cumulative distribution function for $\underline{y}$ is continuous and strictly increasing;
- the PDF for $\underline{y}$ is continuous over the interval for which this PDF is strictly positive, unimodal and strictly increasing (or zero) to the left of the mode and strictly decreasing (or zero) to the right of the mode;
- the expectation and variance of $\underline{y}$ exist;
- a sufficiently large number of realisations R of $\underline{\mathbf{x}}$ is used for implementation of the Monte Carlo method.

3. Proposed generator of pseudorandom numbers

The sources of measurement uncertainty are most frequently modelled using random variables following normal distributions. The justification of this practice is twofold:
- the observed uncertainties as a rule result from superposition of numerous causes;
- analytical tools for processing this kind of distributions are well developed.

An obvious disadvantage of this practice is that it makes evaluation of limit errors impossible since the supports of corresponding probability density functions (PDFs) are infinite. For physical reasons (energetic limitations) the supports of empirical PDFs must be finite. This fact may be taken into account by truncation of distributions modelling sources of measurement uncertainty, *e.g.* at the level of their 3 standard deviations. If the random variable $\underline{x}$ follows the normal distribution $\mathsf{N}(0,1)$ whose PDF is:

$$f_x(x) \equiv \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{x^2}{2}\right) \tag{1}$$

then the PDF of the random variable $\underline{y}$ following the truncated distribution has the form:

$$f_y(y) = \begin{cases} k \cdot f_x(y) & \text{for } |y| \le 3 \\ 0 & \text{otherwise} \end{cases} \tag{2}$$

where:

$$k = \int_{-3}^{+3} f_x(x)dx \cong 1.002707 \tag{3}$$

is a coefficient normalising the integral of $f_y(y)$ over the interval $(-\infty,+\infty)$ to 1. The standard deviation of $\underline{y}$ is:

$$\sigma_y = \sqrt{\int_{-3}^{+3} y^2 f_y(y)dy} \cong 0.986578 \tag{4}$$

A numerical problem of practical importance is the transformation of the realisations of a random variable $\underline{x} \propto \mathsf{N}(0,1)$ or $\underline{u} \propto \mathsf{U}(0,1)$ into realisations of a random variable $\underline{y}$ whose PDF is close to the PDF of $\mathsf{N}(0,1)$, but has a finite support. A review of its solutions may be found in the 2011 paper by N. Chopin [3]; the detailed descriptions of several of them, including program implementations – in the papers [4–6]. The most traditional method consists in solving the following equation:

$$\int_{-\infty}^{y} \exp\left(-\frac{z^2}{2}\right)dz = \int_{-\infty}^{-3} \exp\left(-\frac{z^2}{2}\right)dz + u\int_{-3}^{+3} \exp\left(-\frac{z^2}{2}\right)dz \tag{5}$$

with respect to y for selected realisations u of $\underline{u}$.

When applied to modelling sources of measurement uncertainty, the truncated normal distribution reveals the following disadvantages:
- its standard deviation differs form 1 by *ca.* 0.027 when the truncation limits are ± 3;
- its PDF is discontinuous at the truncation limits;
- the generation of its realisations is quite complex.

It should be stressed that neither of those drawbacks is excluding this distribution from practical usage because:
- the perturbations of the PDF and standard deviation are, as a rule, within the limits of modelling accuracy;
- the normal cumulative distribution function and its inverse, which are necessary for solving Eq.(5) may be approximated using relatively simple functions [7, 8] or the dependence of y on u may be memorised as a look-up table.

A more elegant and convenient solution is, however, possible and proposed here. It consists of two steps:
- a modification of each realisation u of $\underline{u}$ according to the formula:

$$x = a \cdot u^c + b \tag{6}$$

- the transformation of x into y using the formulae usually applied to transformation of uniformly distributed numbers into normally distributed numbers, *viz.*:

$$y = \sqrt{-2\ln(x)}\sin(2\pi x) \text{ or } y = \sqrt{-2\ln(x)}\cos(2\pi x) \tag{7}$$

The parameters a and b are selected in such a way as to limit $\sqrt{-2\ln(x)}$ to the range $[0,3]$, *i.e.* they are obtained by solving the following equations:

$$\sqrt{-2\ln(a \cdot u^c + b)}\Big|_{u=0} = 3 \text{ and } \sqrt{-2\ln(a \cdot u^c + b)}\Big|_{u=1} = 0 \tag{8}$$

which yields: $b = \exp(-4.5)$ and $a = 1 - b$. The value of c is selected in such a way as to make the standard deviation of $\underline{y}$

equal to 1; hence $c \cong 1.0586$. The deviation of the PDF of $\underline{y}$ from the PDF of $\underline{x} \propto \mathsf{N}\ (0,1)$ is shown in Fig. 1.

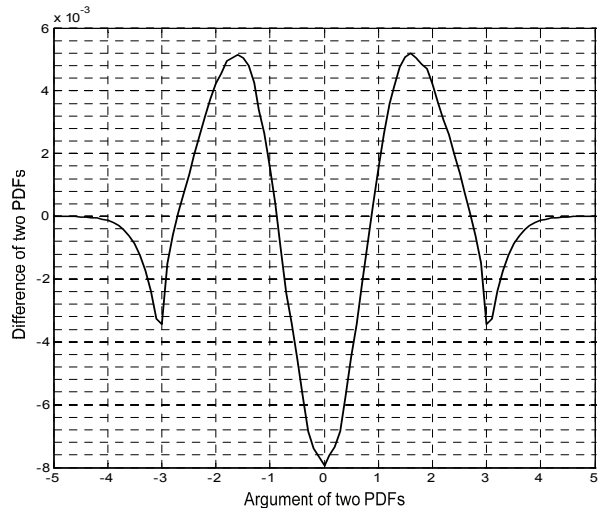


Fig. 1. The difference between the PDF of $\underline{y}$ and the PDF of $\mathsf{N}\ (0,1)$

Rys. 1. Różnica między funkcją gęstości prawdopodobieństwa zmiennej losowej $\underline{y}$ a funkcją gęstości prawdopodobieństwa rozkładu $\mathsf{N}\ (0,1)$

4. Example of application

Measurand reconstruction and calibration of measuring channels are two fundamental problems of measurement data processing. In many practically important situations, they consist in solving an overdetermined system of linear algebraic equations:

$$\dot{\mathbf{X}}\big|_{N\times M} \cdot \dot{\mathbf{p}}\big|_{M\times 1} = \dot{\mathbf{y}}\big|_{N\times 1} \quad (N > M) \tag{9}$$

with respect to $\dot{\mathbf{p}}$ on the basis of error-corrupted measurement data:

$$\underline{\widetilde{\mathbf{X}}} = \dot{\mathbf{X}} + \underline{\Delta\widetilde{\mathbf{X}}} \ \text{ and } \ \underline{\widetilde{\mathbf{y}}} = \dot{\mathbf{y}} + \underline{\Delta\widetilde{\mathbf{y}}} \tag{10}$$

The method of ordinary least squares (OLS) – more than two hundred years after its introduction by Carl Friedrich Gauss and Adrien-Marie Legendre – is still very frequently used for this purpose:

$$\underline{\hat{\mathbf{p}}} = \left(\underline{\widetilde{\mathbf{X}}}^T \cdot \underline{\widetilde{\mathbf{X}}}\right)^{-1} \cdot \underline{\widetilde{\mathbf{X}}}^T \cdot \underline{\widetilde{\mathbf{y}}} \tag{11}$$

The propagation of errors in the *y*-data in the absence of errors corrupting the *x*-data is straightforward:

$$\underline{\hat{\mathbf{p}}} - \dot{\mathbf{p}} = \left(\dot{\mathbf{X}}^T \cdot \dot{\mathbf{X}}\right)^{-1} \cdot \dot{\mathbf{X}}^T \cdot \underline{\Delta\widetilde{\mathbf{y}}} \tag{12}$$

while the propagation of errors corrupting the *x*-data, even in the absence of errors in the *y*-data, might be problematic due to the nonlinearity of the operation:

$$\Phi\left(\underline{\Delta\widetilde{\mathbf{X}}}\right) \equiv \left(\underline{\widetilde{\mathbf{X}}}^T \cdot \underline{\widetilde{\mathbf{X}}}\right)^{-1} \cdot \underline{\widetilde{\mathbf{X}}}^T \Big|_{\underline{\widetilde{\mathbf{X}}} = \dot{\mathbf{X}} + \underline{\Delta\widetilde{\mathbf{X}}}} \tag{13}$$

The analytical determination of the mean and covariance of the random vector $\underline{\hat{\mathbf{p}}} - \dot{\mathbf{p}}$ requires cumbersome approximations, even if the elements of the matrix $\underline{\Delta\widetilde{\mathbf{X}}}$ are assumed to be identical, zero-mean, statistically independent following normal distributions. The use of Monte Carlo approach seems to be a good alternative in this case. Its usefulness is here illustrated with a non-trivial example.

A family of estimation problems, differing in their numerical conditioning controlled by a parameter $\varepsilon > 0$, has been generated in the following way. The matrices $\dot{\mathbf{X}}(\varepsilon)$ have been obtained according to the formula:

$$\dot{\mathbf{X}}(\varepsilon) = \begin{bmatrix} \left.\begin{matrix} \mathbf{G}(\varepsilon) \\ \vdots \\ \mathbf{G}(\varepsilon) \end{matrix}\right\} \times \left[\frac{N}{M}\right] \\ \mathbf{g}_1^T(\varepsilon) \\ \vdots \\ \mathbf{g}_{N \bmod M}^T(\varepsilon) \end{bmatrix} \tag{14}$$

where:

$$\mathbf{G}(\varepsilon) \equiv \begin{bmatrix} 1 \\ 2 \\ \vdots \\ M \end{bmatrix} \cdot \begin{bmatrix} 1 & \frac{1}{2} & \cdots & \frac{1}{M} \end{bmatrix} + \varepsilon \cdot \mathbf{I}\big|_{M\times M} \tag{15}$$

$\mathbf{g}_m^T(\varepsilon)$ ($m = 1, ..., M$) are rows of the matrix $\mathbf{G}(\varepsilon)$, $[N/M]$ is the integer part of the result of the division N/M, and $N \bmod M$ is the reminder. All the elements of the vector $\dot{\mathbf{p}}$ have been set to 1, and the vectors $\dot{\mathbf{y}}(\varepsilon)$ have been defined as:

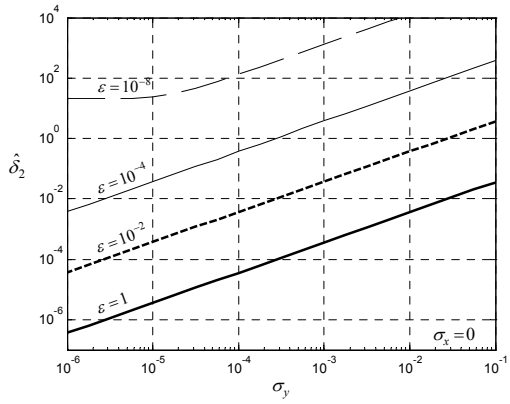
$$\dot{\mathbf{y}}(\varepsilon) = \dot{\mathbf{X}}(\varepsilon) \cdot \dot{\mathbf{p}} \tag{16}$$

The realisations of $\underline{\Delta\widetilde{\mathbf{X}}}$ and $\underline{\Delta\widetilde{\mathbf{y}}}$ have been generated using the algorithm described in the previous section. The relative aggregated error of estimation, based on $R = 1000$ realisations of errors in the data, has been used as an indicator of estimation uncertainty; it has been calculated according to the following formula:

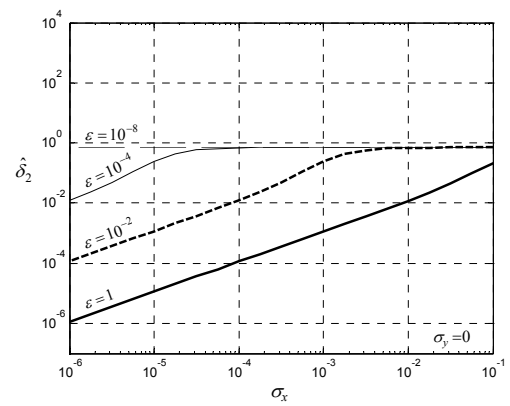
$$\hat{\delta}_2 \equiv \sqrt{\frac{1}{R}\sum_{r=1}^{R} \frac{\left\|\Delta\hat{\mathbf{p}}(r)\right\|_2^2}{\left\|\dot{\mathbf{p}}\right\|_2^2}} = \frac{1}{\left\|\dot{\mathbf{p}}\right\|_2} \sqrt{\frac{1}{R}\sum_{r=1}^{R} \left\|\Delta\hat{\mathbf{p}}(r)\right\|_2^2} \tag{17}$$

Selected results of testing, obtained for $N = 100$, $M = 10$ and $R = 1000$, are shown in Fig. 2a. For $\varepsilon = 1$, the system of normal equations is well-conditioned, and the relative aggregated error of parameter estimation $\hat{\delta}_2$ is of the same order as the standard deviation σ_y in the whole range of its values. The conditioning number is growing with decreasing ε; consequently, for $\varepsilon = 10^{-4}$ its getting greater than 100% when $\sigma_y > 3 \cdot 10^{-4}$, and is greater than 100% in the whole range of σ_y values when $\varepsilon = 10^{-8}$. In Fig. 2b and Fig. 2c, a quite surprising effect is demonstrated: a considerable improvement in the quality of estimation is caused by the presence of errors in the *x*-data. The explanation for this effect is provided in Fig. 2d: on the whole, the errors in the *x*-data are diminishing the conditioning number of the matrix $\widetilde{\mathbf{X}}(\varepsilon)$. The case of zero errors in all those data is not excluded, but its probability for the considered distribution of pseudorandom numbers is close to zero.

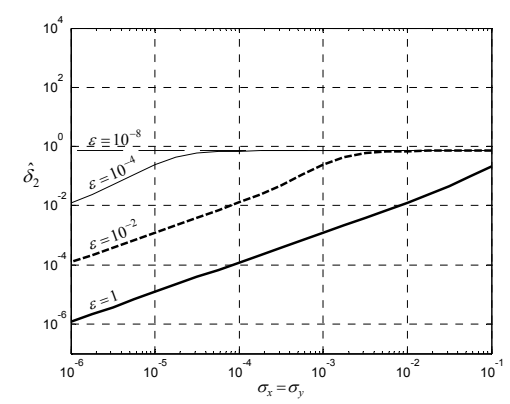
a)



b)



c)



d)

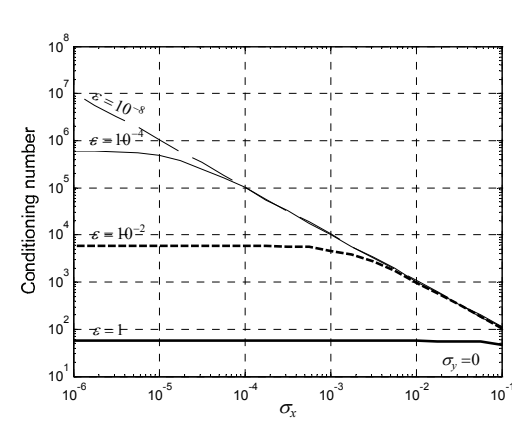


Fig. 2. The dependence of the relative aggregated error of parameter estimation on the level of errors in the data – for several values of ε

Rys. 2. Zależność względnego zagregowanego błędu estymacji parametrów od poziomu błędów danych – dla kilku wartości ε

5. Conclusion

A formula for transformation of the distribution of pseudorandom numbers from $\mathsf{N}(0,1)$ to quasi-normal has been proposed. The PDF of the latter is very close to the Gauss function, but it has finite-support $[-3,+3]$, and – unlike the probability density function of the truncated normal distribution – is continuous; moreover, its standard deviation is very close to 1. The generator of pseudorandom numbers, based on the proposed formula, seems to be an elegant and numerically efficient alternative to various generators of truncated distributions, when applied for evaluation of measurement uncertainty.

The research work reported in this paper has been supported by the Ministry of Science and Higher Education in Poland (grant No. N N505 464832).

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otrzymano / received: 27.02.2013
przyjęto do druku / accepted: 01.04.2013 *artykuł recenzowany / revised paper*