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Performance Evaluation of Monte Carlo Simulation: Case study of Monte Carlo approximation vs. analytical solution for a chi-squared distribution

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ABSTRACT

The guide to the expression of uncertainty in measurement (GUM) describes the law of propagation of uncertainty for linear models based on the first-order Taylor series approximation of $Y = f(X_1, X_2, \ldots, X_N)$. However, for non-linear models this framework leads to unreliable results while estimating the combined standard uncertainty of the model output [$u(y)$]. In such instances, it is possible to implement the method(s) described in Supplement 1 to GUM – Propagation of distributions using a Monte Carlo Method. As such, a numerical solution is essential to overcome the complexity of the analytical approach to derive the probability density functions of the output. In this paper, Monte Carlo simulations are performed with the aim of providing an insight into the analytical transformation of the probability density function (PDF) for $Y = X^2$ where X is normally distributed and a detailed comparison of analytical and Monte Carlo approach results are provided. This paper displays how the used approach enables to find PDF of Y = X^2 without the use of special functions. In addition, the singularity of the PDF and the nonsymmetric coverage interval are also discussed.

Keywords: GUM; Uncertainty estimation; Monte Carlo method; Non-central non-standard chi-squared distribution

1. Introduction to uncertainty and chi-squared distribution

Any obtained quantity as a result of observations, measurements, modelling or prediction is associated with an uncertainty that emerges from the followed procedure. The concept of errors in measurement was established in the beginning of the 20th century (Wallis & Roberts, 1956; Traub, 1997; Lane, 2011). The misconception of attributing the term 'error' on 'measurement uncertainty' was resolved with the publication of the Guide to the expression of uncertainty in measurement (GUM). GUM established a standard procedure for assessing uncertainty (GUM-1993; GUM-1995; JCGM:2008). In addition, GUM states that evaluation of uncertainty is not a routine task, but it depends on the understanding and analysis of the performed method as well as the evaluation of the practitioner itself. GUM also accepts approaches to uncertainty evaluation, including analytical methods used to derive an exact algebraic form for the probability distribution for the output Y, or a Monte Carlo method (MCM) with controlled accuracy, etc.

GUM is mainly concerned about the expression of uncertainty of the measurable quantity, called the 'measurand' – Y. The measurand is determined from N other input quantities, X_1, X_2, ..., X_N, through a multivariate functional relationship, $Y = f(X_1, X_2, X_3, \ldots, X_N)$, where x_i denote possible values of corresponding random variable X_i, respectively. Each input quantity in this relationship has its own uncertainty, expressed as $u(x_1)$, $u(x_2)$, $u(x_3)$, …, $u(x_N)$, whereby x_1, x_2,…x_N are the best estimates of input quantities X_1, X_2,…X_N. The standard uncertainties of input quantities are either evaluated as standard deviations of repeated measurement values (type-A uncertainties) or by standard deviations of the assumed probability density functions (type-B uncertainties). GUM defines the standard uncertainty of the measurand as follows:

$$u^2(y) = \sum_{i=1}^{N}\sum_{j=1}^{N}\left(\frac{\partial y}{\partial x_i}\right)\left(\frac{\partial y}{\partial x_j}\right)u\left(x_i, x_j\right) \tag{1}$$

$$= \sum_{i=1}^{N} \left(\frac{\partial y}{\partial x_i} u(x_i) \right)^2 + \sum_{\substack{i,j=1 \\ i \neq j}}^{N} \left(\frac{\partial y}{\partial x_i} \right) \left(\frac{\partial y}{\partial x_j} \right) u(x_i, x_j) \tag{2}$$

where the partial derivatives $\frac{\partial y}{\partial x_i}$ stand as the sensitivity coefficients, $u(x_i, x_i) = u(x_i) \times u(x_i) = u^2(x_i)$ as the estimated variance of x_i, and $u(x_i, x_j); i \neq j$ as the estimated covariance associated with x_i and x_j. The input quantities are often assumed to be mutually uncorrelated ($u(x_i, x_j) = 0$, when $i \neq j$), which helps simplify Eq. (2), considering only $i = j$:

$$u^2(y) = \sum_{i=1}^{N} \left(\frac{\partial y}{\partial x_i} \right)^2 u^2(x_i) \tag{3}$$

Equations (2) and (3), often called as the law of propagation of uncertainty, are based on a first-order Taylor series approximation of $Y = f\,(X_1, X_2, ..., X_N)$ and they express the basic GUM framework recommendation for evaluation of uncertainty of a multivariate system.

However, there are situations where the application of the present GUM-framework leads to unreliable results. If the model is non-linear coupled with high relative uncertainties of input quantities the present GUM framework provides unreliable estimate for the combined standard uncertainty of model output $u(y)$. Also, if the distribution of the output Y cannot be assumed to be a Gaussian or a Student's t-distribution it is not correct to use the coverage factor $k = 2$ or corresponding Student's t-coefficient to calculate the expanded uncertainty at P=95 % coverage probability. In these cases it can be recommended to use the Monte Carlo method (MCM) based on the Supplement 1 to GUM (GUM-S1, 2008). The shortcomings of the GUM are currently being dealt with a new revision of the GUM which is expected to be consistent with GUM supplements (Bich et al., 2012; Bich, 2014; Bich et al., 2016). All the distributions of input quantities will be estimated from a Bayesian point of view eliminating the need to distinguish the uncertainties as type A and type B uncertainties (Bich et al., 2016). Besides some other important changes, the new GUM will also recommend using MCM if one has little knowledge about the distribution of the model output (Bich et al., 2016). One good example about non-linear model is $Y = X^2$:

$$u^2(y) = \left(\frac{\partial y}{\partial x}\right)^2 u^2(x) \tag{4}$$

$$u(y) = \frac{\partial y}{\partial x} u(x) = 2xu(x) \tag{5}$$

$Y = X^2$ stands as the simplest nonlinear model with widespread applications, for example its use in kinematics and in fluid mechanics with velocity profiles. However, it is also implemented in different measurement systems, e.g. in remote sensing, especially in the evaluation of coverage of areas with certain specification or with cloud cover, as well as measurements of irradiation from large territories. In addition, in electrical engineering, power meters actually detect X^2 (Carobbi, 2014). A different perspective to problems of metrology in measurement systems was also presented in a very systematical manner by Danilov (2016). Moreover, another important application is for evaluating the Word Error Rate (WER) in automated measurement systems, e.g. speech recognition and Analog to Digital Converters, etc. (Catelani et al., 2010).

The probability density function (PDF) of $Y = X^2$ is asymmetric, as it cannot be negative and this leads to problems in constructing its coverage intervals. For a symmetric PDF output, symmetric coverage intervals are usually used, but in the case of an asymmetric PDF, the user must have an insight into the shape and properties of the PDF to proceed with design of coverage interval (Bich, 2014; Bich et al., 2012, 2016; Lira, 2019; Willink, 2016).

For example, when X, a priori, follows a normal distribution with non-zero mean μ_X and non-unit standard deviation σ_x, $X \sim N(\mu_X;\ \sigma_X)$, then the X^2 has non-central non-standard chi-squared distribution with one degree of freedom.

The chi-squared distribution, derived from a set of n-independent standard normal variables, $X_i \sim N(0;\ 1)$ with $i = 1, 2, \ldots, n$, is widely used for evaluating the goodness of fit of an observed distribution to a theoretical one. Unfortunately, a general case of $Y = X^2$, for a single non-central non-standard input $X \sim N(\mu_X \neq 0;\ \sigma_X \neq 1)$ is not studied in the books nor in the literature (Ventsel, 1969; Papoulis, 1990, 1991; Traub, 1997; Rice, 2007; Fornasini, 2008; Veerarajan, 2009; Lane, 2011; Suhov and Kelbert, 2014; Sahoo, 2015; Thomopoulos, 2017; Kelbert and Suhov, 2018). There is however a comparative study in the literature focusing on the random measurement errors and indirect measurement errors by Monte-Carlo method by Labutin and Pugin (2000).

The study of Kent & Hainsworth (1995) concludes that in the absence of any clear optimality criteria for choosing confidence intervals of the χ^2-distribution, a 'symmetric range' interval is the best choice. Furthermore, in the study of Attivissimo et al. (2012) where the use of frequentist and the Bayesian approach to measurement uncertainty is discussed, the authors consider an electric circuit consisting only of a battery of voltage X and a noisy unit-value resistor consuming the power $W = X^2$. A thorough uncertainty analysis of the circuit requires the computation of a number of PDFs along with expectations and variances. This study involves uniform and normal distributions for input X, Bayesian, frequentist and Monte Carlo approaches and the results are compared. An interesting result from this study is the plot from which the PDF of X^2 for normal noncentral input X can be depicted, although the analytical expression of PDF for W is given only in a general form of the Bayes' formula.

The aim of this study is to present a comprehensive analysis of the PDF in the output of $Y = X^2$ for non-central non-standard normal input X, supported with Monte Carlo simulation for extracting the PDF of the normal squared.

A literature review on the PDF of $Y = X^2$ reveals a series of publications by Cox & Harris (1999; 2003; 2006) and Cox & Siebert (2006), which show that numerical solution using MCM is an effective tool to approximate the output PDF by a frequency distribution. In addition, Cox & Siebert (2006) demonstrated that in the case of the simplest (i.e. uniform) input PDF, use of the Heaviside step function and the Markov formula allows to derive an analytic expression of the PDF of $Y = X^2$.

The aim of this study is to present a comprehensive analysis of the PDF in the output of $Y = X^2$ for a priori known non-central non-standard normal input $X \sim N(\mu_x, \sigma_x)$ determined with Monte Carlo simulation for extracting the PDF of the squared normally distributed variable. This paper improves upon the findings of the previous studies presented above. It also introduces important information to help avoid potential mistakes while obtaining results, displays the key aspects of implementation, as well as a special emphasis on a simpler PDF equation for practical calculations. This paper also covers the singularity of the PDF which is the main problem of the Monte Carlo simulation and the nonsymmetric coverage interval.

2. On the two Monte Carlo experiments

The series of works carried out by Cox et al. (1999; 2003; 2006) on the univariate model $Y = X^2$ can be considered as the basis of this problem with significant contributions to the area. Particularly, Cox & Harris (1999; 2003) considered Gaussian input $X \sim N(0.5; 0.2)$, with mean $\mu_X = 0.5$, and standard deviation $\sigma_X = 0.2$. The PDF of this input, although symmetric, is right-shifted and narrowed compared to the standard normal distribution $X \sim N(0; 1)$. The authors ran M = 10 000 MCS trials to draw a rough PDF histogram of 20 columns for output Y. Obtained set of output quantities $\{y_i\}$ enables a quick evaluation of the two main statistical output quantities, mathematical expectation μ_Y and standard deviation σ_Y, as well as the median, mode and coverage intervals. The PDF for output $Y = X^2$ is asymmetric and includes only nonnegative values which reflect its non-Gaussian origin. It is not correct to represent a coverage interval for Y in a symmetric form, $\mu_Y \pm k\sigma_Y$, where k is a coverage factor (usually, k = 1, 2 or 3). When the GUM framework cannot be applied, Monte Carlo simulation (MCS) presents itself as a good alternative (Cox & Harris, 2006; Cox & Siebert, 2006; GUM-S1; GUM-Introduction; GUM-S2). Rearrangement of $\{y_i\}$ into a non-decreasing order enables determining the quantiles to define the required expanded uncertainties through possible coverage intervals $[y_{\mathrm{low}}, y_{\mathrm{high}}]$, where the endpoints depend on the particular output PDF. For example, for the output 0.025 and 0.975 quantiles define a 95% coverage interval. Evidently, the set $\{y_i\}$ allows depicting the same value coverage interval using any another appropriate pair of quantiles such as 0.015 and 0.965, or 0.040 and 0.990, etc.

Using MCS for the statistical description of output quantities of nonlinear models presents two possible problems:

- MCS easily overlooks sharp peaks at possible singular points of an output PDF while using MCS-derived histograms for visualization of the shape of the PDF of an output quantity;
- superficial analysis of empirical cumulative distribution functions (CDF) for Y can lead to erroneous generalizations about the median value for the set of $\{y_i\}$.

For instance, a histogram of 20 columns for $Y = X^2$ with $X \sim N(0.5; 0.2)$, obtained using 10 000 MCS trials, did not reveal singularity in vicinity of $y = 0$ (Cox & Harris, 1999;

2003). However, this was solved when Cox & Harris (2006) readdressed the problem of $Y = X^2$ by inserting $X \sim N(1.2; 0.5)$, performing $M = 50\,000$ MCS trials and drawing a Y histogram of 70 columns. The enhanced resolution displayed discernible features in the histogram which was previously not evident. The more detailed PDF appeared to be bimodal with a sharp peak depicted by the first column. The authors also calculated for the output quantity the estimates of the mathematical expectation μ_Y and the associated standard uncertainty σ_Y as provided by the law of propagation of uncertainty:

$$\mu_Y = \mu_X^2 = 1.2^2 = 1.44 \tag{6}$$

$$\sigma_Y = 2\mu_X\sigma_X = 2 \times 1.2 \times 0.5 = 1.20 \tag{7}$$

The Monte Carlo experiment resulted in different values $\mu_y = 1.70$, $\sigma_Y = 1.26$. On the other hand, considered $Y = X^2$ stands out as a relatively simple non-linear model and enables analytical explanation of discrepancies in calculation of μ_Y and σ_Y as well as the appearance of a sharp peak of the PDF.

3. Expectation and variance of $Y = X^2$

In order to get the expectation of the output:

$$\mu_Y = EX^2 \tag{8}$$

the relationship for variance DX of a random variable X,

$$\sigma_X^2 = \mu_Y - \mu_X^2 \tag{9}$$

gives the expectation for output Y:

$$\mu_Y = \mu_X^2 + \sigma_X^2 \tag{10}$$

The obtained formula is universal, regardless of which PDFs are assigned to X, unconstrained by the requirement of the Gaussian distribution as input. When (10) is applied to $X \sim N(1.2; 0.5)$:

$$\mu_Y = 1.2^2 + 0.5^2 = 1.44 + 0.25 = 1.69 \tag{11}$$

which is in agreement with the Monte Carlo experiment cited above, μ_Y = 1.70, but contradicts the result of Eq. (6), μ_Y = 1.44. Derivation of a formula for variance (σ_Y^2) of the output requires the calculation of the 4th noncentral moment for input X:

$$\sigma_Y^2 = DY = E(Y - \mu_Y)^2 = EY^2 - \mu_Y^2 \tag{12}$$

considering Eq. (10) and since:

$$EY^2 = EX^4 \tag{13}$$

equation (12) can be rewritten as:

$$\sigma_Y^2 = EX^4 - (\mu_X^2 + \sigma_X^2)^2 \tag{14}$$

here the 4th non-central moment of the normal distribution:

$$EX^4 = \int_{-\infty}^{\infty} x^4 p_X(x)dx = \mu_X^4 + 6\mu_X^2\sigma_X^2 + 3\sigma_X^4 \tag{15}$$

where $p_X(x)$ is the PDF for a Gaussian input, X. Combining of Eqs. (14) and (15) gives for the variance of output, Y:

$$\sigma_Y^2 = 4\mu_X^2\sigma_X^2 + 2\sigma_X^4 \tag{16}$$

which is only valid for the Gaussian input. Applying Eq. (16) applied to a normal quantity discussed above, X ~ N(1.2; 0.5):

$$\sigma_Y^2 = 4 \times 1.2^2 \times 0.5^2 + 2\times0.5^4 = 1.565 \tag{17}$$

$$\sigma_Y = \sqrt{1.565} = 1.251 \tag{18}$$

matches the MCM result of Cox & Harris (2006), σ_Y = 1.26, and proves the use of Eq. (7) less accurate.

4. The PDF for $Y = X^2$

There are two methods to derive the PDF for $Y = X^2$. One is the PDF transformation technique which converts the input probability density function, $p_X(x)$, into output, $p_Y(y)$, and the other one is the CDF differentiation technique that starts from the cumulative distribution functions, $G_X(y)$ and $G_Y(y)$.

The equality of probability elements at both sides of the model must consider both inverse functions ($x = \pm\sqrt{y}$) and are written as:

$$p_X(-x)dx + p_X(x)dx = p_Y(y)dy \tag{19}$$

$$p_Y(y) = p_X(-\sqrt{y})\frac{dx}{dy} + p_X(\sqrt{y})\frac{dx}{dy} \tag{20}$$

$$p_Y(y) = \frac{1}{2\sqrt{y}}p_X(-\sqrt{y}) + \frac{1}{2\sqrt{y}}p_X(\sqrt{y}) \tag{21}$$

(21) is the generic form and is valid for any PDF in the input (Papoulis, 1990; 1991). In the case of normal non-standard input, $X \sim N(\mu_X; \sigma_X)$:

$$p_X(x) = \frac{1}{\sigma_X\sqrt{2\pi}}e^{-\frac{1}{2}\left(\frac{x-\mu_X}{\sigma_X}\right)^2} \tag{22}$$

the general formula (22) for the output PDF transforms into:

$$p_Y(y) = \frac{1}{2\sigma_X\sqrt{2\pi}\sqrt{y}}e^{-\frac{1}{2}\left(\frac{\sqrt{y}+\mu_X}{\sigma_X}\right)^2} + \frac{1}{2\sigma_X\sqrt{2\pi}\sqrt{y}}e^{-\frac{1}{2}\left(\frac{\sqrt{y}-\mu_X}{\sigma_X}\right)^2} \tag{23}$$

In (23) the presence of $\sqrt{y}$ in the denominators means that the obtained PDF has a singularity at $y = 0$:

$$\lim_{y\to 0} p_Y(y) = \infty \tag{24}$$

For a central but non-standard normal distribution ($\mu_X = 0$, $\sigma_X \neq 1$), (23) equals to:

(25)

and for the standard normal distribution ($\mu_X = 0$, $\sigma_X = 1$):

(26)

which is the chi-squared or χ^2-distribution with one degree of freedom.

Alternatively, the PDF for $Y = X^2$ (for a non-centered X) is by definition:

$$p_Y(y) = \frac{dG_Y(y)}{dy} \tag{27}$$

where $G_Y(y)$ is the CDF for output, defined as:

$$G_Y(y) = P(Y \le y) = P(X^2 \le y) = P(-\sqrt{y} \le X \le \sqrt{y}) \tag{28}$$

$$G_Y(y) = \int_{-\sqrt{y}}^{\sqrt{y}} p_X(x)dx \tag{29}$$

Splitting the area of integration at $x = 0$:

$$G_Y(y) = \int_{-\sqrt{y}}^{0} p_X(x)dx + \int_{0}^{\sqrt{y}} p_X(x)dx \tag{30}$$

$$G_Y(y) = -\int_{0}^{-\sqrt{y}} p_X(x)dx + \int_{0}^{\sqrt{y}} p_X(x)dx \tag{31}$$

Differentiating with respect to y gives an interim result of:

$$p_Y(y) = \frac{dG_Y(y)}{dy} = -\frac{d}{dy}\int_{0}^{-\sqrt{y}} p_X(x)dx + \frac{d}{dy}\int_{0}^{\sqrt{y}} p_X(x)dx \tag{32}$$

here we denote the first and second integral as $g_1(y)$ and $g_2(y)$, respectively. Before using the rule of differentiating with respect to the upper limit of integration, changes in variables should be performed. For the first integral:

$$\tau = -\sqrt{y};\quad \frac{d\tau(y)}{dy} = \frac{-1}{2\sqrt{y}} \tag{33}$$

$$g_1(y) = -\frac{d}{dy}\int_{0}^{-\sqrt{y}} p_X(x)dx = -(\frac{d}{d\tau}\int_{0}^{\tau} p_X(x)dx) \times \frac{-1}{2\sqrt{y}} \tag{34}$$

$$g_1(y) = p_X(\tau) \times \frac{1}{2\sqrt{y}} = \frac{1}{2\sqrt{y}} p_X(-\sqrt{y}) \tag{35}$$

using $\tau = \sqrt{y}$ for the second integral in (32):

$$g_2(y) = \frac{1}{2\sqrt{y}} p_X(\sqrt{y}) \tag{36}$$

both PDF parts, $g_1(y)$ and $g_2(y)$, given by (35) and (36), respectively, together equal again to equation (21), confirming the steps taken.

By involving modified Bessel functions of the first kind, general formula (23) for PDF of $Y = X^2$ can be represented in a form usually applied in theory of chi-squared distribution:

$$A = \frac{1}{2\sigma_X\sqrt{2\pi}\sqrt{y}} \quad \text{and} \quad a = \frac{1}{2\sigma_X^2} \tag{37}$$

Eq. (23) can be written as:

$$p_Y(y) = A\left(e^{-a(\sqrt{y}+\mu_X)^2} + e^{-a(\sqrt{y}-\mu_X)^2}\right) \tag{38}$$

$$p_Y(y) = Ae^{-a(y+\mu_X^2)}\left(e^{2a\sqrt{y}\mu_X} + e^{-2a\sqrt{y}\mu_X}\right) \tag{39}$$

using (Andras, Baricz, 2008):

$$\cosh z = \frac{e^z + e^{-z}}{2} = \sqrt{\frac{\pi z}{2}} I_{-1/2}(z) \tag{40}$$

where $I_{-1/2}$ is modified Bessel function with $-1/2$ degrees of freedom, Eq. (39) can be rewritten in a more desired form:

$$p_Y(y) = \frac{1}{2\sigma_X^2}\frac{\sqrt{\mu_X}}{\sqrt[4]{y}} exp\left(-\frac{y+\mu_X^2}{2\sigma_X^2}\right) I_{-1/2}\left(\sqrt{y}\frac{\mu_X}{\sigma_X^2}\right) \tag{41}$$

which, compared to (23), is not so convenient for practical calculations.

The interpretation of the PDF for $Y = X^2$ can be better understood by analyzing the two examples presented in the previous section. For both cases, it is assumed the input X is normally distributed, according to the two Monte Carlo experiments, $X \sim N(0.5; 0.2)$ and

X ~ N(1.2; 0.5), respectively (Cox & Harris, 1999; 2003; 2006). The general formula for output PDF (24) transforms respectively into:

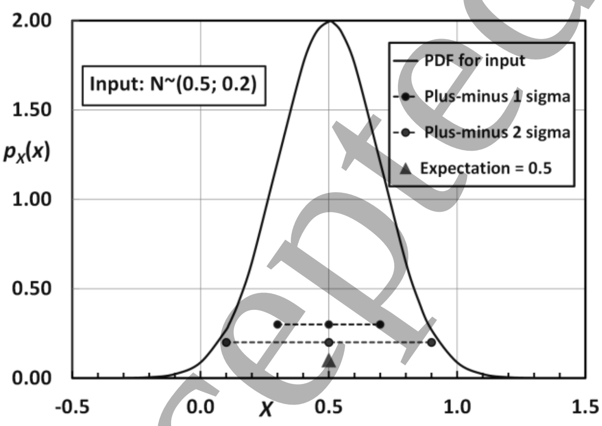
$$p_Y(y) = \frac{2.5}{\sqrt{2\pi}}\frac{1}{\sqrt{y}}e^{-12.5(\sqrt{y}+0.5)^2} + \frac{2.5}{\sqrt{2\pi}}\frac{1}{\sqrt{y}}e^{-12.5(\sqrt{y}-0.5)^2} \tag{42}$$

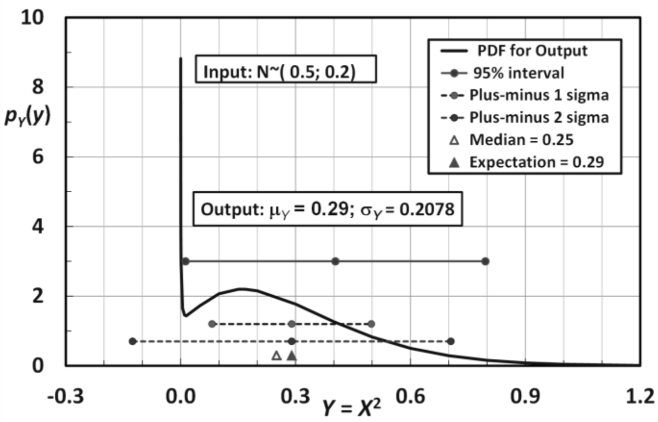
$$p_Y(y) = \frac{1}{\sqrt{2\pi}}\frac{1}{\sqrt{y}}e^{-2(\sqrt{y}+1.2)^2} + \frac{1}{\sqrt{2\pi}}\frac{1}{\sqrt{y}}e^{-2(\sqrt{y}-1.2)^2} \tag{43}$$

Plots of the two input PDFs, and their outputs, $Y = X^2$, according to (42) and (43), are presented in Fig. 1. Symmetric coverage intervals, μ ± σ and μ ± 2σ, can be seen for the input and the output, but since Y is neither symmetrically distributed nor have any negative values, symmetric coverage intervals with respect to the expectation of the output do not present any valuable information. However, the output coverage intervals can be calculated by appropriate integration of a particular $p_Y(y)$ both for the analytical approach and the MCS.

Input: normal, X~N(0.5; 0.2)

Output: $Y = X^2$, $\mu_Y = 0.29, \sigma_Y = 0.2078$





Input: normal, X~N(1.2; 0.5)

Output: $Y = X^2$, $\mu_Y = 1.69, \sigma_Y = 1.251$

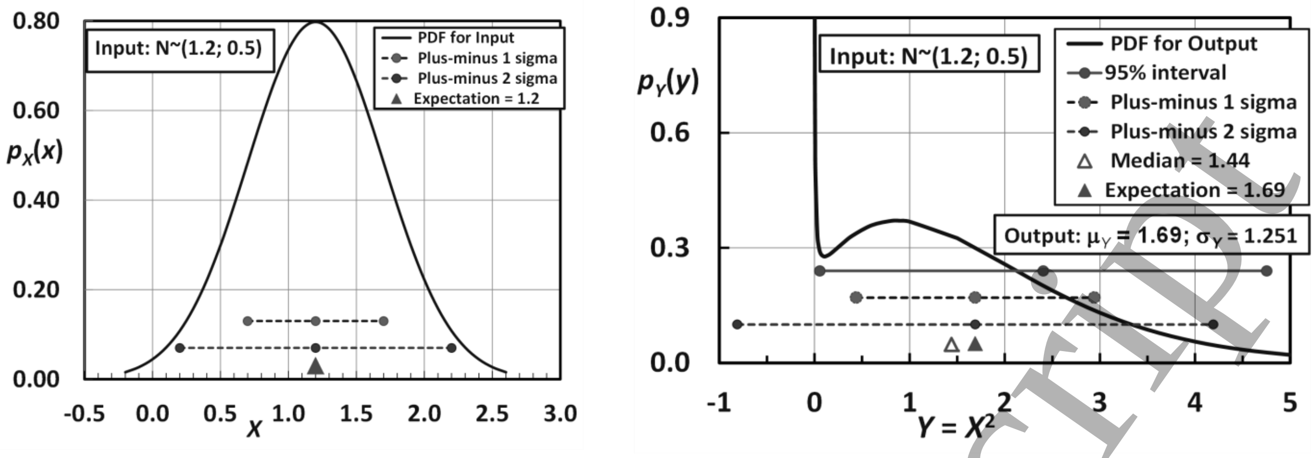


Fig. 1. On the left: probability density functions for two Gaussian input quantities, X ~ N(0.5; 0.2), and X ~ N(1.2; 0.5) respectively. On the right: probability density functions for corresponding output quantities, $Y = X^2$. The dashed horizontal lines indicate the coverage intervals (±σ and ± 2σ). For Y the ± 2σ intervals include infeasible negative X^2 values. The filled triangles indicate locations of mathematical expectations at the horizontal axes and the empty triangles of the medians for outputs. The continuous horizontal lines seen on the graphs on the right show the 95% coverage intervals, plotted according to 2.5% and 97.5% quantiles.

5. The CDF for $Y = X^2$

The cumulative distribution functions (CDF) are essential for evaluating the normalization condition of the PDF for a random quantity, as well as for a rapid assessment of median and quantile values, peak-event probabilities and the coverage intervals. For $Y = X^2$, in the case of a normal non-standard input, $X \sim N(\mu_X; \sigma_X)$, the CDF is defined as:

$$G_Y(z) = \int_0^z p_Y(y)\,dy == \frac{1}{2\sigma_X\sqrt{2\pi}} \int_0^z e^{-\frac{1}{2}\left(\frac{\sqrt{y}+\mu_X}{\sigma_X}\right)^2} \frac{dy}{\sqrt{y}} \tag{44}$$

where the first and second parts of the equation are denoted as Part I, $G_1(z)$, and Part II, $G_2(z)$, respectively. Applying the change in variables, from y to t, for Part I and Part II:

$$t = \frac{1}{\sqrt{2}\sigma_X}(\sqrt{y} + \mu_X) \tag{45}$$

$$t = \frac{1}{\sqrt{2}\sigma_X}(\sqrt{y} - \mu_X) \tag{46}$$

$G_1(z)$ and $G_2(z)$ are obtained as:

$$G_1(z) = \frac{1}{\sqrt{\pi}}\int_{A}^{B_1(z)} e^{-t^2}\,dt = \frac{1}{2}\mathrm{erf}(B_1) - \frac{1}{2}\mathrm{erf}(A) \tag{47}$$

$$G_2(z) = \frac{1}{\sqrt{\pi}}\int_{-A}^{B_2(z)} e^{-t^2}\,dt = \frac{1}{2}\mathrm{erf}(B_2) + \frac{1}{2}\mathrm{erf}(A) \tag{48}$$

where the new limits of integration:

$$A = \frac{\mu_X}{\sqrt{2}\sigma_X} \tag{49}$$

$$B_1(z) = \frac{\sqrt{z} + \mu_X}{\sqrt{2}\sigma_X} \tag{50}$$

$$B_2(z) = \frac{\sqrt{z} - \mu_X}{\sqrt{2}\sigma_X} \tag{51}$$

and the error function:

$$\mathrm{erf}(x) = \frac{2}{\pi}\int_{0}^{x} e^{-t^2}\,dt \tag{52}$$

The sum of (47) and (48) gives (after returning from z to y):

$$G_Y(y) = \frac{1}{2}\mathrm{erf}(B_1) + \frac{1}{2}\mathrm{erf}\,(B_2) \tag{53}$$

where the coefficients B_1 and B_2 depend on y, μ_X and σ_X. If the first particular input is considered again, X ~ N(0.5; 0.2), from Cox & Harris (1999; 2003), B_1 and B_2 become:

$$B_1(y) = \frac{\sqrt{y} + \mu_X}{\sqrt{2}\sigma_X} = \sqrt{12.5y} + \sqrt{3.125} \tag{54}$$

$$B_2(y) = \frac{\sqrt{y} - \mu_X}{\sqrt{2}\sigma_X} = \sqrt{12.5y} - \sqrt{3.125} \tag{55}$$

For the second input, X ~ N(1.2; 0.5), following Cox & Harris (2006), the CDF is:

$$G_Y(y) = \frac{1}{2}\mathrm{erf}(B_3) + \frac{1}{2}\mathrm{erf}(B_4) \tag{56}$$

where:

$$B_3(y) = \frac{\sqrt{y} + \mu_X}{\sqrt{2}\sigma_X} = \sqrt{2y} + 1.2\sqrt{2} \tag{57}$$

$$B_4(y) = \frac{\sqrt{y} - \mu_X}{\sqrt{2}\sigma_X} = \sqrt{2y} - 1.2\sqrt{2} \tag{58}$$

The two obtained CDFs $G_Y(y)$ are plotted in Fig. 2 and denoted as "Cumulative 1" and "Cumulative 2", respectively.

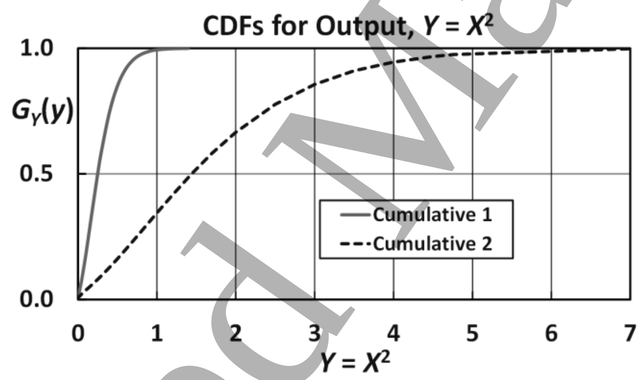


Fig. 2. Two examples of the cumulative distribution function of $Y = X^2$:

Cumulative 1 for X ~ N(0.5; 0.2); Cumulative 2 for X ~ N(1.2; 0.5).

6. Width of narrow peaks in the $Y = X^2$ PDF curves

In this section, the obtained CDFs are used for evaluating the contribution of a peak near the origin of the PDF $Y = X^2$ (as seen on the right of the Fig. 1). The area under the peak is calculated for both cases. For the first input, X ~ N(0.5; 0.2) the local minimum is located at y = 0.0145, which defines the range of the narrow peak as an interval, $0 < y \leq 0.0145$. Contribution of this peak to the whole PDF is equal to $G_Y(0.0145)$. Before performing (53), limits of integration, B_1 and B_2 are calculated:

$$B_1(y = 0.0145) = \frac{\sqrt{0.0145} + 0.5}{\sqrt{2} \times 0.2} = 2.19350 \tag{59}$$

$$B_2(y = 0.0145) = \frac{\sqrt{0.0145} - 0.5}{\sqrt{2} \times 0.2} = -1.34203 \tag{60}$$

$$G_Y(0.0145) = \frac{1}{2}\mathrm{erf}(2.19350) \text{ - } \frac{1}{2}\mathrm{erf}(1.34203) = 0.02789 \tag{61}$$

The result indicates that a narrow peak near the origin covers approximately 2.8% of the area under the PDF curve of $Y = X^2$ for the input condition of $X \sim$ N(0.5; 0.2). For the second input, $X \sim$ N(1.2; 0.5), the extension of the narrow peak is, $0 < y \leq 0.100$. The limits of integration, B_3 and B_4:

$$B_3(y = 0.100) = \frac{\sqrt{0.100} + 1.2}{\sqrt{2} \times 0.5} = 2.14427 \tag{62}$$

$$B_4(y = 0.100) = \frac{\sqrt{0.100} - 1.2}{\sqrt{2} \times 0.5} = -1.24984 \tag{63}$$

substitution of these into (49):

$$G_Y(0.100) = \frac{1}{2}\mathrm{erf}(2.14427) \text{ - } \frac{1}{2}\mathrm{erf}(1.24984) = 0.03736 \tag{64}$$

indicating that the contribution of the narrow peak covers approximately 3.7% of the area under the PDF curve of $Y = X^2$ for $X \sim$ N(1.2; 0.5).

7. Quantiles and coverage intervals for $Y = X^2$

Analytical presentation of the cumulative distribution function enables calculation for Y of quantiles and coverage intervals. Often the 95% coverage interval is defined between the 0.025 and 0.975 quantiles of the PDF for Y. These quantiles for the first example, $X \sim \mathrm{N}(0.5; 0.2)$, using (49), (50) and (51) are found as:

$$G_Y(0.0125) = 0.025 \tag{65}$$

$$G_Y(0.7957) = 0.975 \tag{66}$$

which means that the lower and upper quantiles are, $y_{2.5\%} = 0.0125$ and $y_{97.5\%} = 0.7957$, respectively.

Quantiles for the second input, $X \sim \mathrm{N}(1.2; 0.5)$:

$$G_Y(0.0561) = 0.025 \tag{67}$$

$$G_Y(4.7524) = 0.975 \tag{68}$$

which means that $y_{2.5\%} = 0.0561$ and $y_{97.5\%} = 4.7524$. These 95% of coverage intervals are displayed as continuous horizontal lines in Fig. 1 (on the right). The same coverage interval of 95% may be also given by any other appropriate pair of quantiles such as $y_{1.5\%}$ and $y_{96.5\%}$, etc.

8. About the median of $Y = X^2$

The cumulative distribution function is a useful visual aid to understanding the nature of a random quantity. The most important characteristic of a CDF itself is the median. A detailed examination of tabulated values for the cumulative distribution functions $G_Y(y)$ gives the following results:

$$G_Y(y = 0.25) = 0.499999713, \text{ for the input } X \sim \mathrm{N}(0.5; 0.2) \tag{69}$$

$$G_Y(y = 1.44) = 0.499999207, \text{ for the input } X \sim \mathrm{N}(1.2; 0.5) \tag{70}$$

from here, it appears that with a very high rate of accuracy the following statement can be written:

$$\text{median } (Y = X^2) = \mu_X^2 \tag{71}$$

However, this statement cannot present the entirety of the variability of $Y = X^2$ as the median should depend on both of the input quantities, μ_X and σ_X, not solely on μ_X. Equation (53) clarifies this situation. With the substitution of:

$$y = \mu_X^2 \tag{72}$$

into (53), the coefficients B_1, B_2 and the CDF, $G_Y(y = \mu_x^2)$, take the following values:

$$B_1(y) = \frac{\sqrt{y}+\mu_X}{\sqrt{2}\sigma_X} = \frac{\sqrt{2}\mu_X}{\sigma_X} \qquad B_2(y) = \frac{\sqrt{y}-\mu_X}{\sqrt{2}\sigma_X} = 0 \tag{73}$$

$$G_Y(y = \mu_X^2) = \frac{1}{2}\text{erf}(B_1) = \frac{1}{2}\text{erf}(\frac{\sqrt{2}\mu_X}{\sigma_X}) \tag{74}$$

which means that the CDF, $G_Y(\mu_x^2)$, actually depends on the ratio, μ_X/σ_X, and tends to the value 0.5 with μ_X over σ_X (Fig. 3). For $\mu_X/\sigma_X = 1.6$, the CDF already becomes equal to 0.499.

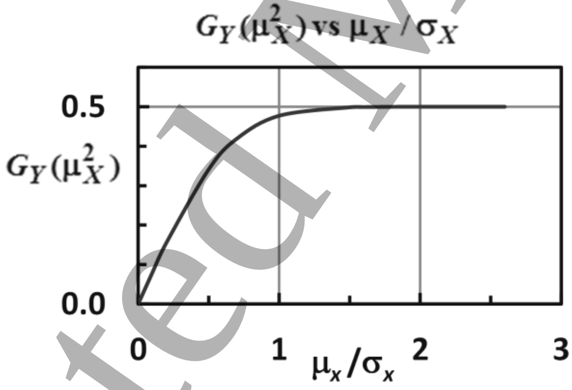


Fig. 3. Cumulative distribution function $G_Y(y)$ at $y = \mu_x^2$, as a function of the ratio of two input quantities, μ_X/σ_X.

The validity of (71) can approximated from $\mu_X/\sigma_X = 1.6$ towards larger values and the median $Y = X^2$ as μ_x^2 can be calculated. The results of medians obtained with (71) can be explained by considering the same inputs, $X \sim N(0.5; 0.2)$, and $X \sim N(1.2; 0.5)$, for which the ratios μ_X/σ_X are 2.5 and 2.4 respectively.

9. Readdressing a Monte Carlo experiment

As mentioned previously, MCS method is relatively easy to implement and therefore presents itself as a good alternative to the analytical derivation of output statistical quantities. However, MCS easily overlooks possible sharp narrow peaks in the shape of a PDF. The proper comprehension of PDF shape obtained with MCS can be achieved by considerably increasing the number of Monte Carlo trials and the number of histogram columns. In this study, for the first input, X ~ N(0.5; 0.2), a series of M = 1 000 000 Monte Carlo trials has been performed.

The Monte Carlo run for $Y = X^2$ resulted in the output mean of $\mu_Y = 0.2902$, and a standard deviation of $\sigma_Y = 0.2079$. Both results stand close to the ones obtained from analytical method $\mu_Y = 0.29$ and $\sigma_Y = 0.2078$. Additionally, the probabilistically symmetric coverage interval corresponding to 95 % coverage probability was found to lie between 0.0126 and 0.7962 while the corresponding analytically calculated coverage interval lies between 0.0125 and 0.7957 indicating a good match between the coverage intervals found by the two methods. The said-one million sets of $\{x_i\}$ and $\{y_i\}$ were reassembled into histograms of 50, 100, 300 and 1000 columns, and displayed in Fig. 4, respectively. It is obvious that 50 columns are not enough for proper visualization of the output PDF whereas 100 could be used but the output PDF is still not clearly evident. However, the histogram of 300 columns reveals the singularity near the origin while the histogram of 1000 columns only sharpens it.

Input: normal, X ~ N(0.5; 0.2)

Output: $Y = X^2$, $\mu_Y = 0.2902$, σ_Y = 0.2079

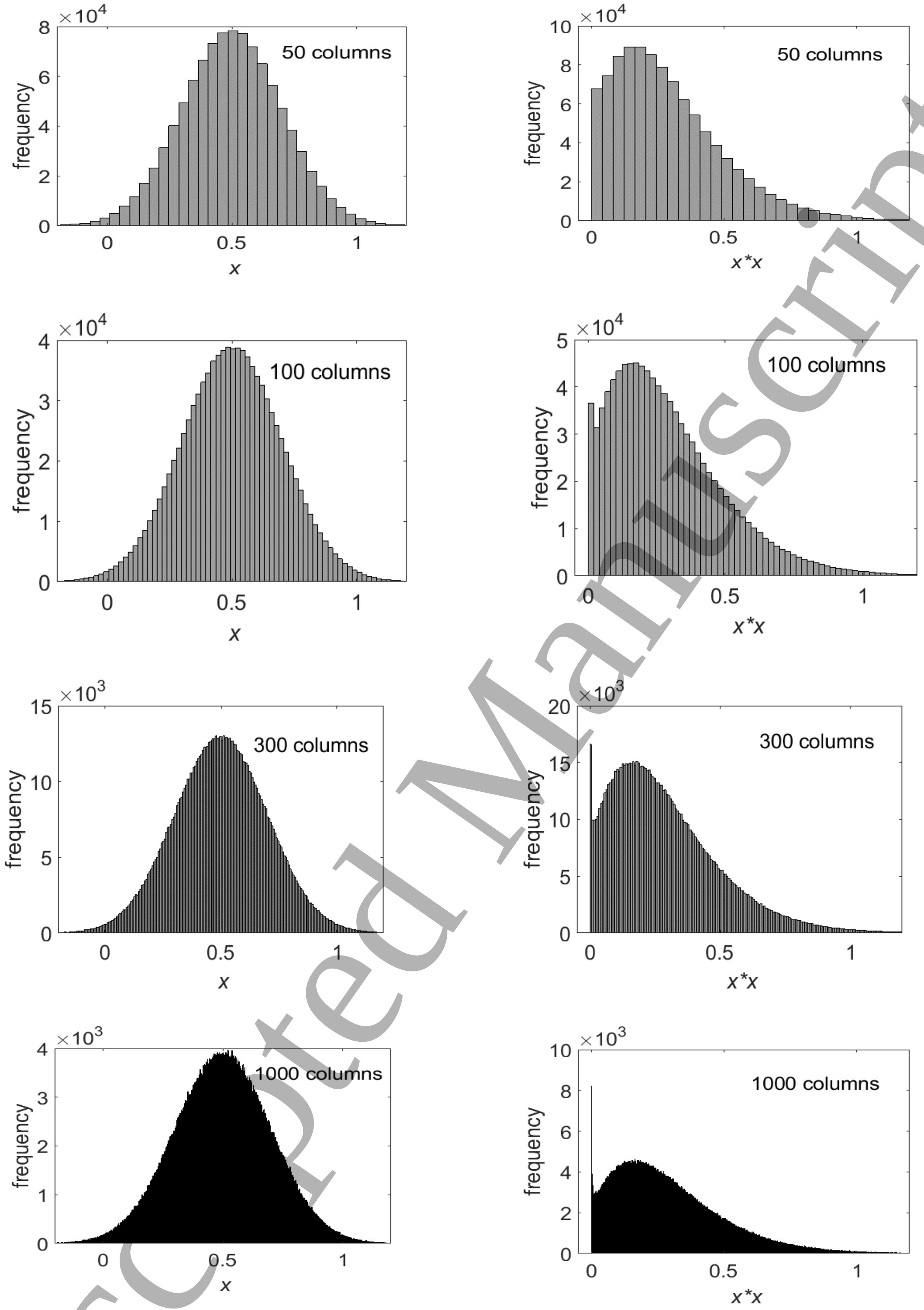


Fig. 4. Results of a series of 1000000 MC trials as histograms of 50, 100, 300 and 1000 columns.

10. Conclusions

For reliable estimation of the model output uncertainty, the model input quantities should be specified in terms of probability density functions (PDFs). In order to determine the output PDF, the practitioner must choose between analytical and numerical methods. Analytical methods ask the user to have calculus and probability and statistics knowledge as prerequisites (Rice, 2007; Fornasini, 2008; Thomopoulos, 2017), but the user can always use certain softwares to help derive the analytical solutions.

In this study, an analytic approach is described for a simple univariate model $Y = X^2$ where X is the Gaussian input with non-zero expectation and non-unit standard deviation. The analytic approach enabled a detailed description of singularity in Y near the origin as well as to reveal a peculiarity in calculation of the median for Y. However, for example in some cases of environmental modelling, either the set of input quantities (e.g. photons of solar rays, ionizing radiation from polluted territories, etc.) or the model itself (e.g. processes of light scattering on a single plant or in the entire plant cover, propagation of pollution in an environment, etc.) may be too complicated for an analytical representation. In these situations, Monte Carlo simulations (MCS) appear to be the only alternative method.

This study also demonstrated that for a relatively simple model, $Y = X^2$, there can be unexpected results, such as overlooking narrow peaks, and recommends that a sufficiently large number of trials should be chosen to obtain an adequate plot of the output histogram. For $Y = X^2$, a plot with the sufficient details that enables detection of singularity in the output, was achieved using 300 histogram columns on the basis of 1 million MC trials.

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