



Numerical inversion of a characteristic function: An alternative tool to form the probability distribution of output quantity in linear measurement models

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ABSTRACT

Measurement uncertainty analysis based on combining the state-of-knowledge distributions requires evaluation of the probability density function (PDF), the cumulative distribution function (CDF), and/or the quantile function (QF) of a random variable reasonably associated with the measurand. This can be derived from the characteristic function (CF), which is defined as a Fourier transform of its probability distribution function. Working with CFs provides an alternative and frequently much simpler route than working directly with PDFs and/or CDFs. In particular, derivation of the CF of a weighted sum of independent random variables is a simple and trivial task. However, the analytical derivation of the PDF and/or CDF by using the inverse Fourier transform is available only in special cases. Thus, in most practical situations, a numerical derivation of the PDF/CDF from the CF is an indispensable tool. In metrological applications, such approach can be used to form the probability distribution for the output quantity of a measurement model of additive, linear or generalized linear form. In this paper we propose new original algorithmic implementations of methods for numerical inversion of the characteristic function which are especially suitable for typical metrological applications. The suggested numerical approaches are based on the Gil-Pelaez inverse formulae and on using the approximation by discrete Fourier transform and the fast Fourier transform (FFT) algorithm for computing PDF/CDF of the univariate continuous random variables. As illustrated here, for typical metrological applications based on linear measurement models the suggested methods are an efficient alternative to the standard Monte Carlo methods.

Section: RESEARCH PAPER

Keywords: GUM; linear measurement model; probability density function; characteristic function; numerical inversion; Gil-Pelaez inversion formulae; FFT algorithm

Citation: Viktor Witkovský, Numerical inversion of a characteristic function: An alternative tool to form the probability distribution of output quantity in linear measurement models, Acta IMEKO, vol. 5, no. 3, article 6, November 2016, identifier: IMEKO-ACTA-05 (2016)-03-06

Section Editor: Franco Pavese, Italy

Received April 27, 2016; **In final form** April 27, 2016; **Published** November 2016

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Funding: The work was supported by the Slovak Research and Development Agency, project APVV-15-0295, and by the Scientific Grant Agency VEGA of the Ministry of Education of the Slovak Republic and the Slovak Academy of Sciences, by the projects VEGA 2/0047/15 and VEGA 2/0011/16

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1. INTRODUCTION

The basic working tool in measurement uncertainty analysis, as advocated in the current revision (under preparation) of the *Guide to the expression of uncertainty in measurement (GUM)* [1], and consistent with its *Supplement 1 – Propagation of distributions using a Monte Carlo method* [2], is the *state-of-knowledge PDF* about the quantity (true value of measurand), based on the currently available information. The state-of-knowledge PDF quantifies the degree of belief about the values that can be assigned to the

quantity based on the available information. The expectation and the standard deviation of this PDF (if they exist) are used to report the measurement result and the associated (standard) measurement uncertainty.

Although the latest GUM development emphasizes the Bayesian view of probability in the evaluation of measurement uncertainty, it should be clearly stated and understood that this approach is not based on the strict Bayesian principles of statistical inference (i.e. straightforward application of the

Bayes' theorem). For more details and further discussion see, e.g., [3]-[5], or [6], and also [7] and [8].

In fact, the GUM approach is based on using a well-defined functional relationship between the mutually inter-related quantities for propagating the state-of-knowledge PDFs of the input quantities, represented by the random variables (RVs), into the state-of-knowledge PDF of the output quantity – which is believed to be a RV reasonably associated with the measurand. Frequently, it is suggested to use a well-known functional relationship (based, e.g., on the physical and/or geometrical laws) between the true value of the measurand and the true values of the other influencing input variables, which is typically expressed by the measurement equation of the measurement model.

Obviously, such PDF of the output quantity represents currently available knowledge (limited, but hopefully the best to date) about the measurand, i.e. it expresses probability distribution of the values being attributed to a quantity (the measurand), based on information used (which could be rather limited and/or heavily biased). This interpretation is consistent to the original GUM definition of the uncertainty in measurement (see [1], clause 2.2.3), which is defined as a parameter, associated with the result of a measurement, that characterizes the dispersion of the values that could be reasonably attributed to the measurand. However, the derived term *coverage interval* is inconsistent with this interpretation, for more details and discussion see [8].

In fact, without imposing further (well and clearly defined) model assumptions and optimality criteria for selecting and combining the information, it can be only hardly expected that the presented result shall represent the best (in what sense?) estimate of the true measurand value. On the other hand, the proposed GUM approach could be well accepted as a (simple) method for combining experimental results with the expert judgment in order to get comprehensive characterization of our knowledge about the true value of measurand, based on all currently available information, albeit without the possibility of guaranteeing the (otherwise naturally) required statistical properties and/or optimality criteria. If this is the goal, other means and/or subsequent analysis should be applied and properly used.

As already mentioned, the term *coverage interval* (introduced in [2], and defined as the interval containing the (true) value of a quantity with a stated probability (say 95 %), based on the information available) is not properly used in this context. Hence, as an alternative to the *95 % coverage interval*, here we shall use a more appropriate term – the *95 % state-of-knowledge interval*. This should read as *the interval of 95 % values that could be reasonably attributed to the unknown value of measurand based on the current state-of-knowledge* (i.e. based on the measurement model, the currently available information, and method used for combining the information). Of course, further study is necessary for characterizing the optimality properties of the used method, e.g., under repeatability conditions.

A standard approach to derive the state-of-knowledge PDF is based on the propagation of distributions using a Monte Carlo method, as suggested in Supplement 1 of the GUM, [2]. For more details and discussion on applicability of the uncertainty evaluation methods based on the GUM and its Supplement 1 see, e.g., [9]-[12].

A principal advantage of the Monte Carlo methods is their simplicity and asymptotic consistency (convergence to the true values with growing number of the Monte Carlo simulations).

A disadvantage of the Monte Carlo methods is their principal ambiguity (i.e. non-uniqueness/variability of the results under independently repeated computations with given number of simulations) and typically large demand on the computational resources. Often, to achieve the pre-selected accuracy level, a need of a very large number of simulations is required.

Alternatively, in linear measurement models, the state-of-knowledge PDF of the output quantity can be derived by inverting its characteristic function, which can be easily derived from the known characteristic functions of the input quantities.

A principal advantage of the methods based on inversion of the characteristic function is their principal exactness (as there is a theoretical one-to-one mapping between the CF and the CDF) and efficiency for all values of the computed CDF/PDF/QF. However, in real situations, the precision of the used computational methods is also subject to possible numerical errors. A typical numerical error of such results is due to particular algorithmic implementation (as e.g., the truncation error and/or the integration error), which can be and should be properly controlled. As we shall illustrate below, in typical metrological applications with linear measurement models and the well behaved probability distributions of the input quantities, the numerical precision and efficiency of the here presented simple methods and algorithms is superior to the standard Monte Carlo methods.

We notice that among other possible alternative approaches to evaluate the propagated probability distribution of the output quantity we can include the advanced methods for arithmetic computations with random variables and their distributions, see e.g. [13], [14], and also [15], [16]. However, applicability of these methods is still limited to a relatively small number of the input random variables.

2. LINEAR MEASUREMENT MODEL AND THE CHARACTERISTIC FUNCTIONS

As mentioned above, an alternative tool to form the state-of-knowledge probability distribution of the output quantity in a linear measurement model is based on the numerical inversion of its characteristic function (CF), which is defined as a Fourier transform of its PDF, see (2).

Computing the (inverse) Fourier transform numerically is a well-known problem, frequently connected with the problem of computing integrals of highly oscillatory (complex) functions. The problem was studied for a long time in general, but also with focus on specific applications, see, e.g., [17]-[22], to show just a few. In particular, the methods suggested for inverting the characteristic function for obtaining the probability distribution function include [23]-[27].

Approximations of the continuous Fourier transform by the discrete Fourier transform and by using the FFT algorithm are widely used in different fields of engineering. However, using the FFT for evaluation of the PDF/CDF from the characteristic function is not widespread in statistical applications (one important exception is the field of financial mathematics and econometrics), and in general, not well implemented in relevant software packages.

In [28], Korczyński, Cox, and Harris suggested and illustrated the use of convolution principles in metrology applications. Their suggested approach was based on consecutive replacing of the convolution integrals by the convolution sums evaluated by using the fast Fourier transform (i.e. without direct using the exact characteristic functions), to

form the probability distribution for the output quantity in the measurement model of additive, linear or generalized linear form.

If compared with the here proposed approach based on combining and inverting the exact characteristic functions, the numerical precision of their suggested approach can quickly deteriorate with the growing number of the required convolution integrals.

In fact, in metrological applications a number of measurement models used in uncertainty evaluation are, at least approximately (up to reasonable level), of the additive linear form

$$Y = c_1 X_1 + \dots + c_n X_n, \quad (1)$$

where the input quantities X_1, \dots, X_n are independent random variables with known probability distributions, $X_j \sim F_{X_j}$, for $j = 1, \dots, n$, possibly parametrized by θ_j . Here, c_1, \dots, c_n denote the known constants and Y represents the univariate output quantity (a random variable with an unknown distribution to be determined).

The characteristic function of a continuous univariate random variable $X \sim F_X$, with its probability density function $\text{pdf}_X(x)$, is defined as a Fourier transform of its PDF,

$$\text{cf}_X(t) = \int_{-\infty}^{\infty} e^{itx} \text{pdf}_X(x) dx, \quad t \in \mathbf{R} \quad (2)$$

Analytical expressions of the characteristic functions are known for many standard probability distributions, see e.g. [29]-[31], or other available sources. Otherwise, CF could be derived either analytically, expressed by using computer-based tools, e.g. by using MATHEMATICA, or evaluated numerically.

In Table 1 we present some selected characteristic functions of the univariate distributions, frequently used in metrological applications. Compare the presented distributions with those in Table 1 in [2]. Notice that the characteristic functions of the symmetric zero-mean distributions are purely real functions of the argument $t \in \mathbf{R}$.

Deriving CF of a weighted sum of independent random variable is a simple and trivial task. Let $\text{cf}_{X_j}(t)$ denote the characteristic function of X_j . The characteristic function of Y defined by (1) is

$$\text{cf}_Y(t) = \text{cf}_{X_1}(c_1 t) \dots \text{cf}_{X_n}(c_n t). \quad (3)$$

For illustration, in Figure 1 we plotted the CF of a linear combination of two independent chi-squared random variables with $\nu_1 = 1$ and $\nu_{10} = 10$ degrees of freedom, evaluated for $t \in (-1,1)$.

Here we shall assume that the considered characteristic functions of the input and/or output quantities, the random variables X_1, \dots, X_n and Y are known or can be easily derived. Then, by the Fourier inversion theorem, the PDF of the random variable Y is given by

$$\text{pdf}_Y(y) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-ity} \text{cf}_Y(t) dt, \quad y \in \mathbf{R}. \quad (4)$$

Analytical derivation of the PDF by using the (inverse) Fourier transform (4) is available only in special cases. Thus, in most practical situations, a numerical derivation of the PDF/CDF from the CF is an indispensable tool.

In the next section we present two simple but frequently very efficient approaches (approximate numerical methods) for inversion of the characteristic function together with a detailed description of their algorithmic implementations, which are suitable for typical metrological applications.

Table 1. Characteristic functions of continuous univariate distributions used in metrological applications (selected symmetric zero-mean distributions and non-negative distributions). Here, $K_\nu(z)$ denotes the modified Bessel function of the second kind, $J_\nu(z)$ is the Bessel function of the first kind, and $U(a, b, z)$ is the confluent hypergeometric function of the second kind.

| Probability distribution | Characteristic function (CF) |
|---|--|
| Gaussian $N(0,1)$ | $\text{cf}(t) = e^{-\frac{1}{2}t^2}$ |
| Student's t t_ν | $\text{cf}(t) = \frac{1}{\sqrt{2^{\nu-1}\Gamma(\frac{\nu}{2})}} \left(\frac{1}{\nu^2} t \right)^{\frac{\nu}{2}} K_{\frac{\nu}{2}}\left(\sqrt{\frac{1}{\nu^2}} t \right)$ |
| Rectangular $R(-1,1)$ | $\text{cf}(t) = \frac{\sin(t)}{t}$ |
| Triangular $T(-1,1)$ | $\text{cf}(t) = \frac{2-2\cos(t)}{t^2}$ |
| Arcsine $U(-1,1)$ | $\text{cf}(t) = J_0(t)$ |
| Exponential $Exp(\lambda)$ | $\text{cf}(t) = \frac{\lambda}{\lambda-it}$ $\lambda > 0$ rate |
| Gamma $\Gamma(\alpha, \beta)$ | $\text{cf}(t) = \left(1 - \frac{it}{\beta}\right)^{-\alpha}$ $\alpha > 0$ shape, $\beta > 0$ rate |
| Chi-squared χ_ν^2 | $\text{cf}(t) = (1 - 2it)^{-\frac{\nu}{2}}$ $\nu > 0$ degrees of freedom |
| Fisher-Snedecor's F F_{ν_1, ν_2} | $\text{cf}(t) = \frac{\Gamma(\frac{\nu_1 + \nu_2}{2})}{\Gamma(\frac{\nu_1}{2})\Gamma(\frac{\nu_2}{2})} U\left(\frac{\nu_1}{2}, 1 - \frac{\nu_2}{2}, -\frac{\nu_2}{\nu_1} it\right)$ $\nu_1 > 0, \nu_2 > 0$ degrees of freedom |

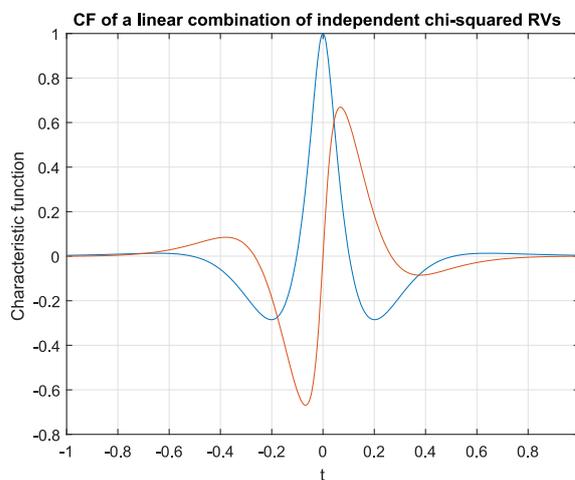


Figure 1. Real (blue) and imaginary (red) part of the characteristic function of $Y = 10 X_{\chi_1^2} + X_{\chi_{10}^2}$ — the linear combination of two independent chi-squared random variables with $\nu_1 = 1$ and $\nu_1 = 10$ degrees of freedom, evaluated for $t \in (-1,1)$.

3. NUMERICAL INVERSION OF THE CHARACTERISTIC FUNCTION

The exact inverse Fourier transform (4) can be naturally approximated by the truncated integral form,

$$\text{pdf}_Y(y) = \frac{1}{2\pi} \int_{-T}^T e^{-ity} \text{cf}_Y(t) dt, \quad (5)$$

where T is a sufficiently large (real) value, and the integrand is a complex (oscillatory) function, which is assumed to decay to zero reasonably fast for $|t| \rightarrow \infty$ (as is typical for continuous distributions used in metrological applications). Note that the selection of the integration limit T and the speed of integrand function decay contribute significantly to the truncation error of this approximation.

In general, the required integral can be evaluated by any suitable numerical quadrature method. Frequently, a simple trapezoidal rule gives fast and satisfactory results. However, caution is necessary if the integrand is a highly oscillatory function, what is the case if $\text{abs}(y)$ is a large value from the tail area of the distribution, as e.g. the 99 % quantile. In such situations a more advanced quadrature method should be used, typically in combination with efficient root-finding algorithms and algorithms for accelerated computing of the limit values of the sums of alternating series (not considered here), see e.g., [21], [32]. Note that the selection of the integration method significantly contributes to the integration error of this approximation. Figure 2 illustrates the problem of integrating the highly oscillatory integrand function.

For typical metrological applications we suggest to consider algorithms based on the Gil-Pelaez inversion formulae (6)-(7) and the approximate discrete Fourier transform (21) resp. (22), based on the simple trapezoidal rule for computing the required sub-integrals. The possible numerical error of the results (i.e. the truncation error and the integration error) can be controlled by selecting a proper truncation limit T (sufficiently large, leading to a small truncation error), and by dividing the selected integration interval $(0, T)$ to a large number, say N , of small sub-intervals, where the trapezoidal rule provides a satisfactorily good numerical approximation (with small integration error) of the true integral value. For theoretical results on how to control the truncation and integration errors in such and similar situations see, e.g., [35].

3.1. The Gil-Pelaez inversion formulae

In [33], Gil-Pelaez derived the inversion formulae, suitable for numerical evaluation of the PDF and/or the CDF, which

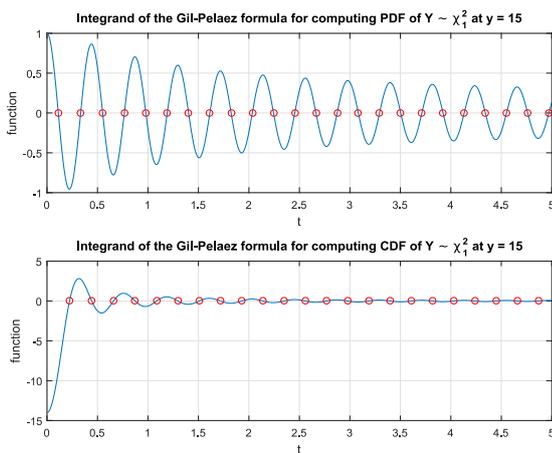


Figure 2. Integrand functions for computing the PDF/CDF of the chi-squared distributed random variable, $Y \sim \chi^2_1$, at $y = 15$, computed by the Gil-Pelaez inversion formulae of its characteristic function $cf_Y(t) = (1 - 2it)^{-\frac{1}{2}}$. The plotted integrand functions of the integrals in (6) and (7) are evaluated for $t \in (0, T)$, $T = 5$. The red circles depict the zeros (roots) of the integrand functions on $(0, T)$. The total integral can be computed as an infinite sum of sub-integrals - the limit value of the sum of alternating series.

require integration of a real-valued function, only. The PDF is given by

$$\text{pdf}_Y(y) = \frac{1}{\pi} \int_0^\infty \Re \left(e^{-ity} cf_Y(t) \right) dt. \quad (6)$$

Further, if y is a continuity point of the cumulative distribution function of Y , the CDF is given by

$$\text{cdf}_Y(y) = \frac{1}{2} - \frac{1}{\pi} \int_0^\infty \Im \left(\frac{e^{-ity} cf_Y(t)}{t} \right) dt. \quad (7)$$

By $\Re(f(t))$ and $\Im(f(t))$ we denote the real and imaginary part of the complex function $f(t)$, respectively.

Numerical inversion of the characteristic function based on (6) and (7) have been successfully implemented for evaluation of the distribution function of a linear combination of independent chi-squared RVs by Imhof in [34] and by Davies in [35]. Further, Gil-Pelaez's method has been implemented in the algorithm `tdist`, see [36] and [37], for computing the distribution of a linear combination of independent Student's t random variables and/or other symmetric zero-mean random variables, and also for computing the distribution of a linear combination of independent inverted gamma random variables suggested in [38], and the distribution of a linear combination of independent log-Lambert $W \times \chi^2_\nu$ RVs, [39]. In [40], the algorithm `tdist` has been suggested and applied for computing the 95 % state-of-knowledge interval (considered as the approximate 95 % confidence interval) for the common mean value in the inter-laboratory comparisons with systematic effects (biases).

In general, the integrals in (6) and (7) can be computed by any numerical quadrature method, possibly in combination with efficient root-finding algorithms and accelerated computing of limits of the alternating series, as considered, e.g., in [20] and [25]. Frequently, (6) and (7) can be efficiently approximated by a simple trapezoidal quadrature:

$$\begin{aligned} \text{pdf}_Y(y) &\approx \frac{\delta_t}{\pi} \sum_{j=0}^N w_j \Re \left(e^{-it_j y} cf_Y(t_j) \right) \\ &\approx \frac{\delta_t}{\pi} \left(w_0 + \sum_{j=1}^N w_j \cos(t_j y) \Re \left(cf_Y(t_j) \right) \right. \\ &\quad \left. + \sum_{j=1}^N w_j \sin(t_j y) \Im \left(cf_Y(t_j) \right) \right) \end{aligned} \quad (8)$$

$$\begin{aligned} \text{cdf}_Y(y) &\approx \frac{1}{2} - \frac{\delta_t}{\pi} \sum_{j=0}^N w_j \Im \left(\frac{e^{-it_j y} cf_Y(t_j)}{t_j} \right) \\ &\approx \frac{1}{2} - \frac{\delta_t}{\pi} \left(w_0 (\text{mean}(Y) - y) + \right. \\ &\quad \left. + \sum_{j=1}^N w_j \cos(t_j y) \Im \left(\frac{cf_Y(t_j)}{t_j} \right) \right. \\ &\quad \left. + \sum_{j=1}^N w_j \sin(t_j y) \Re \left(\frac{cf_Y(t_j)}{t_j} \right) \right), \end{aligned} \quad (9)$$

where N is a sufficiently large number of (equidistant) sub-intervals of $(0, T)$, w_j are the appropriate quadrature weights, and t_j denote the appropriate (equidistant) nodes from the interval $(0, T)$, for sufficiently large T .

In particular, for the trapezoidal quadrature rule we set

- $\delta_t = \frac{T}{N}$ or alternatively $\delta_t = \frac{2\pi}{B-A}$, which gives $T = \frac{N 2\pi}{B-A}$,
- $w_0 = w_N = \frac{1}{2}$, and $w_j = 1$ for $j = 1, \dots, N-1$,
- $t_j = j\delta_t$ for $j = 0, \dots, N$, with $T = t_N = N\delta_t$.

Here, the interval (A, B) specifies the range of typical values y , i.e. a large part of the distribution support of the random variable Y .

As a simple rule of thumb, if the (optimum) value of T is unknown we suggest to start with the application of the *six-sigma-rule*, i.e. set the typical range (A, B) as an intersection of the natural parametric space of Y with the interval (L, U) (e.g., $(A, B) = (L, U) \cap \mathbf{R}$ or $(A, B) = (L, U) \cap \mathbf{R}_+$, with

- $L = \text{mean}(Y) - 6 \text{std}(Y)$,
- $U = \text{mean}(Y) + 6 \text{std}(Y)$,

where $\text{mean}(Y)$ and $\text{std}(Y)$ represent the expectation and the standard deviation of the probability distribution of Y , and define $T = \frac{N \cdot 2\pi}{B-A}$ for some pre-selected fixed N . Note that the value of T should be kept sufficiently large, such that the characteristic function is sufficiently small for all $t > T$, i.e. $\text{abs}(\text{cf}_Y(t)) < \epsilon$ for small ϵ , say $\epsilon = 10^{-12}$. This can be effectively controlled by using a proper value (sufficiently large) of N .

Further, for computing the leading term in (9), we use the result from [36]: If the mean (expectation) of Y exists, then

$$\lim_{t \rightarrow 0} \Im \left(\frac{e^{-ity \text{cf}_Y(t)}}{t} \right) = \text{mean}(Y) - y. \quad (10)$$

The required $\text{mean}(Y)$ and $\text{std}(Y)$ can be evaluated analytically, from the moments of the input variables, or approximately, by using numerical differentiation of the characteristic function of Y , $\text{cf}_Y(t)$. In particular,

$$\text{mean}(Y) \approx \frac{1}{12ih} \left(\text{cf}_Y(-2h) - 8\text{cf}_Y(-h) + 8\text{cf}_Y(h) - \text{cf}_Y(2h) \right), \quad (11)$$

$$\text{std}(Y) \approx \left(m_2(Y) - \text{mean}^2(Y) \right)^{1/2}, \quad (12)$$

where

$$m_2(Y) \approx \frac{1}{144h^2} \begin{pmatrix} \text{cf}_Y(-4h) - 16\text{cf}_Y(-3h) \\ +64\text{cf}_Y(-2h) + 16\text{cf}_Y(-h) \\ -130 \\ +16\text{cf}_Y(h) + 64\text{cf}_Y(2h) \\ -16\text{cf}_Y(3h) + \text{cf}_Y(4h) \end{pmatrix}, \quad (13)$$

for any small $h > 0$, e.g., $h = 10^{-4}$. This numerical approach is applicable even in the cases when the theoretical moments of the considered distribution, defined by $\text{cf}_Y(t)$, do not exist (e.g., for the Student's t distribution with 1 or 2 degrees of freedom).

The truncation limit $T = N\delta_t = N \frac{2\pi}{B-A}$ depends on N and (A, B) . The trade-off between the values of $B - A$, N , δ_t and T , strongly depends on the particular distribution of Y and its CF.

For example, for a highly precise numerical inversion of the standard normal CF, $\text{cf}_Y(t) = e^{-\frac{1}{2}t^2}$, computed in double precision arithmetic with precision better than $\epsilon = 10^{-14}$, it is sufficient to set $(A, B) = (-8, 8)$ with $B - A = 16$, $N = 2^5 = 32$, leading to $\delta_t = \frac{\pi}{8}$ and $T = 4\pi$ with $\text{cf}_Y(T) = e^{-\frac{1}{2}T^2} \approx 5 \times 10^{-35}$. On the other hand, the numerical inversion of the rectangular CF given by $\text{cf}_Y(t) = \frac{\sin(t)}{t}$ requires in double precision arithmetic the value $T = 10^{14}$ to get $\text{abs}(\text{cf}(t)) \leq 10^{-14}$ for $t > T$. For the natural choice of $(A, B) = (-1, 1)$ with $B - A = 2$, this suggests to set $N \approx 10^{13}$, what is an unacceptable value, and thus it reveals that the simple trapezoidal rule is not a suitable integration method for the highly precise numerical inversion of the rectangular distribution CF. Fortunately, CF of the output quantity Y in typical metrological situations based on linear measurement models is a well behaved function, and the methods based on

simple trapezoidal quadrature are efficient to provide good numerical approximations of the true values.

In general, the pre-selected values of T and N should be checked and/or properly corrected. A simple diagnostic check is based on evaluating $\text{abs}(\text{cf}_Y(T))$. For large T this should be a small value (smaller than the accepted truncation error). This check allows to control also the level of N , given the already fixed and sufficiently large interval (A, B) .

We note that the presented quadrature method requires only one evaluation of the characteristic function $\text{cf}_Y(t_j)$ at t_j , $j = 1, \dots, N$, for any $y \in (A, B)$ in $\text{pdf}_Y(y)$ and $\text{cdf}_Y(y)$, respectively. Moreover, the computation is further simplified if Y is a continuous random variable with a symmetric zero-mean distribution, i.e. with purely real CF,

$$\text{pdf}_Y(y) \approx \frac{\delta_t}{\pi} \left(\frac{1}{2} + \sum_{j=1}^{N-1} \cos(t_j y) \text{cf}_Y(t_j) \right), \quad (14)$$

$$\text{cdf}_Y(y) \approx \frac{1}{2} - \frac{\delta_t}{\pi} \left(-\frac{y}{2} + \sum_{j=1}^{N-1} \sin(t_j y) \frac{\text{cf}_Y(t_j)}{t_j} \right). \quad (15)$$

Finally, the quantile function (QF) can be evaluated by using the iterative Newton-Raphson scheme, based on repeated evaluations of the PDF/CDF, see (8)-(9) and/or (14)-(15).

```

% EXAMPLE (MATLAB ALGORITHM CF2DISTGP)
%
% PDF and CDF of a linear combination of RVs:
% Y = c1*X1 + c2*X2 + c3*X3 + c4*X4 + c5*X5,
% where,
% X1 ~ Normal(0,1) with c1=1,
% X2 ~ Student's t with 1 df and c2=1,
% X3 ~ Rectangular on (-1,1) with c3=5,
% X4 ~ Triangular on (-1,1) with c4=1,
% X5 ~ U-distribution on (-1,1) with c5=10

cfN = @(t) exp(-t.^2/2);
cft = @(t,nu) min(1,besselk(nu/2, ...
    abs(t).*sqrt(nu),1) .* ...
    exp(-abs(t).*sqrt(nu)) .* ...
    (sqrt(nu).*abs(t)).^(nu/2) / ...
    2^(nu/2-1)/gamma(nu/2));
cfr = @(t) min(1,sin(t)./t);
cft = @(t) min(1,(2-2*cos(t))./t.^2);
cfU = @(t) besselj(0,t);
c = [1 1 5 1 10]; nu = 1;
cfY = @(t) ...
    cfN(c(1)*t) .* ...
    cft(c(2)*t,nu) .* ...
    cfr(c(3)*t) .* ...
    cft(c(4)*t) .* ...
    cfU(c(5)*t);
y = linspace(-50,50,201)';

[result,cdf,pdf] = cf2DistGP(cfY,y);

```

In particular, for a fixed probability level $p \in (0,1)$, the p -quantile of the (continuous) distribution of Y , say $q = \text{qf}_Y(p)$, is given as a solution (fixed point) of the following iterative scheme,

$$\text{qf}_Y^{k+1}(p) = \text{qf}_Y^k(p) - \frac{(\text{cdf}_Y(\text{qf}_Y^k(p)) - p)}{\text{pdf}_Y(\text{qf}_Y^k(p))}, \quad (16)$$

where $k = 0, 1, \dots$, and the starting value $\text{qf}_Y^0(p)$ is set as, e.g., $\text{qf}_Y^0(p) = \text{mean}(Y)$, defined by (11).

A working version of the MATLAB algorithm `cf2DistGP` for computing the PDF/CDF by numerical inversion of the characteristic function, based on the Gil-Pelaez inversion formulae, is presented in Appendix A.

For illustration, the MATLAB code presented above evaluates the PDF and CDF of the output variable Y , which is a linear combination of the independent random variables with a normal, Student's t , rectangular, triangular and arcsine distributions, i.e. $Y = X_N + X_{t_v} + 5X_R + X_T + 10X_U$, by using the algorithm `cf2DistGP` with its default settings of T and N .

Similarly, the PDF/CDF of the random variable $Y = X_N + X_{t_v} + 5X_R + X_T + 10X_U$ can be evaluated by using the MATLAB algorithm `tdist`, see also Figure 3:

```

% EXAMPLE (MATLAB ALGORITHM TDIST)
%
% TDIST at Matlab Central File Exchange:
% http://www.mathworks.com/matlabcentral/
% /fileexchange/4199-tdist
%
% PDF and CDF of a linear combination of RVs
% Y = c1*X1 + c2*X2 + c3*X3 + c4*X4 + c5*X5
% with:
% X1 ~ Normal(0,1) [we set df1=Inf] with c1=1,
% X2 ~ Student's t with 1 df [set df2=1], c2=1,
% X3 ~ Rectangular on (-1,1) [set df3=-1], c3=5,
% X4 ~ Triangular on (-1,1) [set df4=-2], c4=1,
% X5 ~ U-distribution on (-1,1) [df5=-3], c5=10

df      = [Inf 1 -1 -2 -3];
coefs   = [1 1 5 1 10];
[pdf,y] = tdist([],df,coefs,'PDF');
cdf      = tdist(y,df,coefs,'CDF');

figure; plot(y,pdf); grid
figure; plot(y,cdf); grid

```

3.2. Numerical inversion of the characteristic function by using the FFT algorithm

This approach for computing the PDF by numerical inversion of the characteristic function by using the FFT algorithm is based on the results by Hürlimann in [41]. Alternatively, for other applications based on using the

fractional fast Fourier transform (FRFT), see [42] and also [43]-[46].

Here we shall approximate the continuous Fourier transform (CFT), say

$$F(y) = \int_{-\infty}^{\infty} e^{-i2\pi uy} f(u) du, \quad (17)$$

by a discrete Fourier transform (DFT). The DFT can be efficiently evaluated by using the FFT algorithm that computes the same result as the DFT, but much faster.

For complex numbers f_0, \dots, f_{N-1} the DFT is defined as

$$F_k = \sum_{j=0}^{N-1} e^{-i2\pi k \frac{j}{N}} f_j, \quad k = 0, \dots, N-1. \quad (18)$$

Formally, here we shall use the following notation,

$$\mathbf{F}_N = FFT(\mathbf{f}_N), \quad (19)$$

where $\mathbf{f}_N = (f_0, \dots, f_{N-1})$ and $\mathbf{F}_N = (F_0, \dots, F_{N-1})$.

The relationship between the CF and the PDF is given by the (inverse) continuous Fourier transform defined by (4). For a sufficiently large interval $(-T, T)$, it is possible to approximate a PDF by (5). Here we shall consider the integral approximation, based on the mid-point integration rule, $\int_a^b f(x) dx \approx \frac{f(a)+f(b)}{2} (b-a)$, which corresponds to the trapezoidal quadrature. For more alternative approaches based on more sophisticated integration rules see, e.g., [39].

Similarly as before, let (A, B) denote a sufficiently large interval, where the distribution of Y is concentrated. A reasonable rule for determining (A, B) can be based, for example, on the six-sigma-rule, or its modifications, by using an altered multiplication coefficient (e.g., use 10 instead of 6).

Let $y_k = A + k\delta_y$, with $\delta_y = \frac{B-A}{N}$, and $k = 0, \dots, N-1$. For N large, $T = \pi/\delta_y$ is also large, and from (5), by using $t = 2\pi u$, $dt = 2\pi du$, and $du = \frac{1}{B-A}$, we get

$$pdf_Y(y_k) \approx \frac{1}{2\pi} \int_{-\frac{1}{2\delta_y}}^{\frac{1}{2\delta_y}} e^{-i2\pi u y_k} cf_Y(2\pi u) du. \quad (20)$$

Now, we shall approximate the integral (19) by using the approximate trapezoidal quadrature rule, for each of the N sub-intervals. Thus,

$$pdf_Y(y_k) \approx \frac{1}{B-A} \sum_{j=0}^{N-1} e^{-i2\pi u_j y_k} cf_Y(2\pi u_j), \quad (21)$$

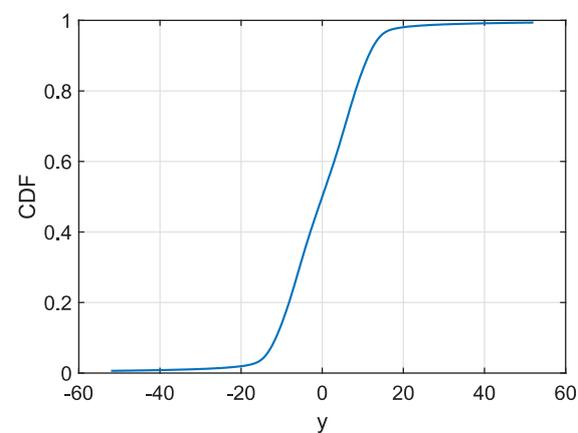
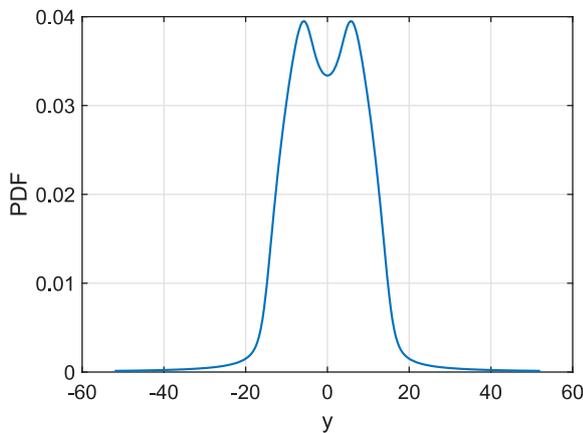


Figure 3. The probability density function (PDF) and the cumulative distribution function (CDF) of a random variable $Y = \sum_{j=1}^5 c_j X_j$, with $X_1 \sim N(0,1)$, $X_2 \sim t_{v=1}$, $X_3 \sim R(-1,1)$, $X_4 \sim T(-1,1)$, $X_5 \sim U(-1,1)$, and coefficients $c = (c_1, \dots, c_5) = (1,1,5,1,10)$, evaluated by numerical inversion of its characteristic function by the MATLAB algorithm `tdist`, see also the Examples.

where $u_j = \frac{1+j-N}{2(B-A)}$, $j = 0, \dots, N-1$.

From that, by using $e^{i\pi} = -1$, the expressions for u_j and y_k , and the DFT defined by (17), we finally get the formal relationship

$$\mathbf{pdf} = \mathbf{C} \odot FFT(\mathbf{D} \odot \mathbf{cf}), \quad (22)$$

where \odot denotes the dot product (element wise multiplication),

- $\mathbf{pdf} = (\text{pdf}_Y(y_0), \dots, \text{pdf}_Y(y_{N-1}))$,
- $\mathbf{C} = (C_0, \dots, C_{N-1})$, with
- $C_k = \frac{1}{B-A} (-1)^{\left(\left(1-\frac{1}{N}\right)\left(\frac{NA}{B-A}+k\right)\right)}$, $k = 0, \dots, N-1$,
- $\mathbf{D} = (D_0, \dots, D_{N-1})$, with
- $D_k = (-1)^{\frac{2A}{B-A}k}$, $k = 0, \dots, N-1$,
- $\mathbf{cf} = (\text{cf}_Y(t_0), \dots, \text{cf}_Y(t_{N-1}))$, with
- $t_k = \frac{2\pi}{B-A} \left(\frac{1}{2} + k - \frac{N}{2}\right)$, $k = 0, \dots, N-1$.

Further, CDF is evaluated here by simple cumulative sum from the evaluated PDF values, and QF is evaluated by interpolation from the CDF.

A working version of the MATLAB algorithm cf2DistFFT for computing the PDF/CDF/QF by numerical inversion of the characteristic function, based on the FFT algorithm, is presented in Appendix B.

For illustration, the MATLAB code presented below evaluates the PDF/CDF of the output variable $Y = 10 X_{\chi_1^2} + X_{\chi_{10}^2}$, by using the algorithm cf2DistFFT with its default settings of (A, B) and N .

```

% EXAMPLE (MATLAB ALGORITHM CF2DISTFFT)
%
% Distribution of a linear combination of RVs
% (chi-squared RVs with 1 and 10 DFs)
% Y = 10*X_{\chi^2_1} + X_{\chi^2_{10}}

df1 = 1;
df2 = 10;
cfChi2_1 = @(t) (1-2i*t).^(-df1/2);
cfChi2_10 = @(t) (1-2i*t).^(-df2/2);
cfY = @(t) cfChi2_1(10*t) .* cfChi2_10(t);

clear options
options.isPositiveSupport = true;
result = cf2DistFFT(cfY,[],[],options);

% PLOT THE CF OF Y
t = linspace(-1,1,501);
figure
plot(t,real(cfY(t)),t,imag(cfY(t)));grid
xlabel('t');
ylabel('Characteristic function');
title('Y = 10*X_{\chi^2_1}+X_{\chi^2_{10}}')

```

Other specific versions of the algorithm for computing the PDF/CDF/QF of a linear combination of independent random variables with the Fisher-Snedecor's F-distributions and the log-normal distributions, by numerical inversion of the characteristic function by using the FFT algorithm, are available at the MATLAB CENTRAL FILE EXCHANGE as the algorithm [Fdist](#), file ID: 56262, and the algorithm [logNdist](#), file ID: 56512, respectively.

4. COMPARISON OF THE CF APPROACH AND THE MONTE CARLO METHOD

The main advantage of the Monte Carlo methods lies in their simplicity and asymptotic consistency. A disadvantage of the Monte Carlo methods lies in the large computational demands, typically required in order to achieve the pre-specified accuracy level. On the other hand, application of the CF approach offers principal theoretical exactness which could be, however, influenced by unacceptable numerical errors (i.e. the truncation and the integration errors), if not properly used.

For illustration, here we consider the linear measurement model for calibration of a coaxial step attenuator as considered in [47], a model typical for metrological applications.

We consider this example in order to compare results based on the CF approach and the Monte Carlo method and to illustrate the applicability and/or advantage of the suggested methods for potential users in metrology applications. For more details about this specific example see [47], example S7, and/or [48].

The linear measurement model of the attenuation L_X of the attenuator to be calibrated is given by

$$L_X = const + L_S + \delta L_S + \delta L_D + \delta L_M + \delta L_K + \delta L_{ib} - \delta L_{ia} + \delta L_{ob} - \delta L_{oa}, \quad (23)$$

with the following information about the distributions of the input quantities (available from the given uncertainty budget, see S7.12 in [47] with the correction as presented in [48]):

- $const = 30.04 + 0.003 = 30.043$,
- $L_S \sim 0.0090 \times N(0,1)$,
- $\delta L_S \sim (0.0025/\sqrt{\frac{1}{3}}) \times R(-1,1)$,
- $\delta L_D \sim (0.0011/\sqrt{\frac{1}{2}}) \times U(-1,1)$,
- $\delta L_M \sim (0.0200/\sqrt{\frac{1}{2}}) \times U(-1,1)$,
- $\delta L_K \sim (0.0017/\sqrt{\frac{1}{2}}) \times U(-1,1)$,
- $\delta L_{ib} \sim (0.0003/\sqrt{\frac{1}{3}}) \times R(-1,1)$,
- $\delta L_{ia} \sim (0.0003/\sqrt{\frac{1}{3}}) \times R(-1,1)$,
- $\delta L_{ob} \sim 0.0020 \times N(0,1)$,
- $\delta L_{oa} \sim 0.0020 \times N(0,1)$.

The algorithms cf2DistGP, with default option parameters based on the six-sigma-rule and pre-selected $N = 2^{10} = 1024$, evaluated the support interval $(A, B) = (-0.1341, 0.1341)$, and hence $T = 23989$, with $\delta_t = \frac{T}{N} = 23.4$.

Then, the 97.5 %-quantile of $Y = L_X - const$ was calculated as $q = 0.03900448275179$. Thus, the calculated 95 % state-of-knowledge interval for the attenuation L_X is given as 30.043 ∓ 0.039 .

The basic diagnostic check ensures the highest precision of the presented calculations in double precision arithmetic, as $\text{abs}(\text{cf}_Y(T))=0$ (i.e. the value equals to the machine zero, which is here defined as 4.94×10^{-324}). The used computer time was $t = 3.9 \times 10^{-4}$ s.

Further, here we also present the estimated values of the required 97.5 % quantile computed by the Monte Carlo method for sample sizes M , with $M = 10^4, 10^5, 10^6, 10^7$, and 10^8 .

```

%% COMPARISON / CF APPROACH & MONTE CARLO METHOD

% CF APPROACH:

% Distribution and quantile of the output
% quantity in linear measurement model
%  $Y = L_S + \delta L_S + \delta L_D + \delta L_M + \delta L_K +$ 
%  $\delta L_{ib} - \delta L_{ia} + \delta L_{0b} - \delta L_{0a}$ 
%
const = 30.043;
prob = 0.975;
c = [0.009 0.0025/sqrt(1/3) ...
     0.0011/sqrt(1/2) 0.0200/sqrt(1/2) ...
     0.0017/sqrt(1/2) 0.0003/sqrt(1/3) ...
     -0.0003/sqrt(1/3) 0.0020 -0.0020 ];
cfN = @(t) exp(-t.^2/2);
cfR = @(t) min(1,sin(t)./t);
cfU = @(t) besselj(0,t);
cfY = @(t) cfN(c(1)*t) .* cfR(c(2)*t) .* ...
     cfU(c(3)*t) .* cfU(c(4)*t) .* ...
     cfU(c(5)*t) .* cfR(c(6)*t) .* ...
     cfR(c(7)*t) .* cfN(c(8)*t) .* ...
     cfN(c(9)*t);
[result,cdf,pdf,q_CF] = cf2DistGP(cfY,[],prob)

% 95% state-of-knowledge interval / CF APPROACH:
I_CF = const + [-q_CF,q_CF]

% MONTE CARLO METHOD:

M = [10^4 10^5 10^6 10^7 10^8];
q_MC = zeros(5,1);
time = zeros(5,1);
rng;
for m = 1:5
    tic;
    N = randn(M(m),3);
    R = 2*rand(M(m),3)-1;
    U = 2*betarnd(0.5,0.5,M(m),3)-1;
    Y = c(1)*N(:,1) + c(2)*R(:,1) ...
        + c(3)*U(:,1) + ...
        + c(4)*U(:,2) + c(5)*U(:,3) ...
        + c(6)*R(:,2) + c(7)*R(:,3) ...
        + c(8)*N(:,2) + c(9)*N(:,3);
    Y = sort(Y);
    q_MC(m) = Y(ceil(M(m)*prob));
    time(m) = toc;
end

% 95% state-of-knowledge interval / MC METHOD:
q = q_MC(5);
I_MC = const + [-q,q]

```

The estimated values of the 97.5 % quantile q , and the computer time t (in seconds), used for the sample size M :

- $M = 10^4$, $q = 0.039343812021804$, $t = 0.07$,
- $M = 10^5$, $q = 0.038985244853524$, $t = 0.08$,
- $M = 10^6$, $q = 0.038952503603421$, $t = 0.75$,
- $M = 10^7$, $q = 0.038998144396413$, $t = 7.49$,
- $M = 10^8$, $q = 0.039003626106614$, $t = 153.2$.

This clearly illustrates the advantages and computational efficiency of the proposed approach over the standard Monte Carlo methods, especially if high precision of the computed (estimated) quantiles is required.

5. CONCLUSIONS

We suggest to consider numerical methods for derivation of the state-of-knowledge PDF/CDF of the output quantity in linear measurement models from its characteristic function.

Such approach can be used to form the probability distribution for the output quantity of a measurement model of additive, linear or generalized linear form, and can be considered as an alternative tool to the uncertainty evaluation based on the Monte Carlo methods.

Here we have presented two simple but efficient approaches for numerical inversion of the characteristic function, which are especially suitable for metrological applications.

The suggested numerical approaches are based on the Gil-Pelaez inverse formula and on the approximation by discrete Fourier transform (DFT) and the FFT algorithm for computing the PDF/CDF of (univariate) continuous random variables.

As we have explained and illustrated, the suggested CF approach should be considered as an alternative to the standard approach based on the Monte Carlo methods (as considered e.g. in *Supplement 1 – Propagation of distributions using a Monte Carlo method* [2]) in specific situations, i.e. for evaluating the state-of-knowledge probability distributions of the output quantity in a linear measurement model, especially if the highest precision of the reported distribution quantiles is required. However, numerical errors of such results should be properly controlled.

For illustration purposes, here we present working versions of the MATLAB codes of the suggested algorithms (cf2DistGP and cf2DistFFT), as well as some simple examples in order to illustrate the applicability of the suggested methods.

Although the methods for inverting characteristic functions for obtaining the probability distribution functions have been studied for long time, especially in statistical literature, and the possible applications are much more general than those motivated by metrology, surprisingly, such methods are still not widespread and used in engineering applications and only rarely used among statisticians. One possible reason might be that the characteristic functions and the algorithms for numerical inversions are not directly available in standard (statistical) software packages, like e.g., R or MATLAB.

Systematic development of the methods, algorithms and the software toolbox (developed for R and/or MATLAB) for computing, combining and inverting the characteristic functions is our highly desirable goal for the next future.

ACKNOWLEDGEMENT

The work was supported by the Slovak Research and Development Agency, project APVV-15-0295, and by the Scientific Grant Agency VEGA of the Ministry of Education of the Slovak Republic and the Slovak Academy of Sciences, by the projects VEGA 2/0047/15 and VEGA 2/0011/16.

**APPENDIX A. MATLAB ALGORITHM CF2DISTGP FOR
NUMERICAL INVERSION OF THE CHARACTERISTIC
FUNCTION BASED ON THE GIL-PELAEZ INVERSION
FORMULAE**

```
function [result,cdf,pdf,qf] = ...
    cf2DistGP(cf,x,prob,options)
% Calculates CDF/PDF/QF from the characteristic
% function by the Gil-Pelaez inversion formulae,
% integrated by a simple trapezoidal quadrature.
%
% SYNTAX:
% [result,cdf,pdf,qf] = ...
%   cf2DistGP(cf,x,prob,options)

%% CHECK THE INPUT PARAMETERS

tic;
narginchk(1, 4);

if nargin < 4, options = []; end
if nargin < 3, prob = []; end
if nargin < 2, x = []; end

if ~isfield(options, 'N')
    options.N = 2^10;
end
if ~isfield(options, 'T')
    options.T = [];
end
if ~isfield(options, 'SixSigmaRule')
    options.SixSigmaRule = 6;
end
if ~isfield(options, 'xMean')
    options.xMean = [];
end
if ~isfield(options, 'xStd')
    options.xStd = [];
end

if ~isfield(options, 'tolDiff')
    options.tolDiff = 1e-4;
end

if ~isfield(options, 'qf0')
    options.qf0 = (cf(1e-4)-cf(-1e-4))/(2e-4*1i);
end

if ~isfield(options, 'crit')
    options.crit = 1e-13;
end

if ~isfield(options, 'maxiter')
    options.maxiter = 1000;
end

if ~isfield(options, 'isPlot')
    options.isPlot = true;
end

if ~isfield(options, 'DIST')
    options.DIST = [];
end

if ~isempty(options.DIST)
    xMean      = options.DIST.xMean;
    cft        = options.DIST.cft;
    dt         = options.DIST.dt;
    N          = length(cft);
    t          = (1:N)' * dt;
    range      = 2*pi / dt;
    xMin       = xMean - range/2;
    xMax       = xMean + range/2;
    xStd       = [];

```

```
else
    N          = options.N;
    T          = options.T;
    SixSigmaRule = options.SixSigmaRule;
    xMean      = options.xMean;
    xStd       = options.xStd;
    h          = options.tolDiff;
    cft        = cf(h*(1:4));
    if isempty(xMean)
        xMean = real((-cft(2) ...
            + 8*cft(1)-8*conj(cft(1)) ...
            + conj(cft(2)))/(1i*12*h));
    end
    if isempty(xStd)
        xM2 = real(-(conj(cft(4)) ...
            - 16*conj(cft(3)) ...
            + 64*conj(cft(2)) ...
            + 16*conj(cft(1)) ...
            - 130 + 16*cft(1) ...
            + 64*cft(2) ...
            - 16*cft(3)+cft(4))/(144*h^2));
        xStd = sqrt(xM2 - xMean^2);
    end
    if ~isempty(T)
        dt      = T / N;
        t       = (1:N)' * dt;
        cft     = cf(t);
        cft(N)  = cft(N)/2;
        range   = 2*pi / dt;
        xMin    = xMean - range/2;
        xMax    = xMean + range/2;
        xStd    = [];
    else
        xMin    = xMean - SixSigmaRule * xStd;
        xMax    = xMean + SixSigmaRule * xStd;
        range   = xMax - xMin;
        dt      = 2*pi / range;
        t       = (1:N)' * dt;
        cft     = cf(t);
        cft(N)  = cft(N)/2;
    end
    options.DIST.xMean = xMean;
    options.DIST.cft   = cft;
    options.DIST.dt    = dt;
end

%% ALGORITHM

if isempty(x)
    x = linspace(xMin,xMax,101)';
end

if any(x < xMin) || any(x > xMax)
    warning(['x out-of-range (the support): ', ...
        '[xMin, xMax] = [',num2str(xMin),...
        ', ',num2str(xMax),'] !']);
end

[n,m] = size(x);
x      = x(:);
E      = exp(-1i*x*t');

% CDF
cdf    = (xMean - x)/2 + imag(E * (cft ./ t));
cdf    = 0.5 - (cdf * dt) / pi;
cdf    = reshape(max(0,min(1,cdf)),n,m);

% PDF
pdf    = 0.5 + real(E * cft);
pdf    = (pdf * dt) / pi;
pdf    = reshape(max(0,pdf),n,m);

```

```

% QF
if ~isempty(prob)
    isPlot = options.isPlot;
    options.isPlot = false;
    [n,m] = size(prob);
    prob = prob(:);
    maxiter = options.maxiter;
    crit = options.crit;
    qf = options.qf0;
    criterion = true;
    count = 0;
    [res,cdfQ,pdfQ] = ...
    cf2DistGP([],qf,[],options);
    options = res.options;
    while criterion
        count = count + 1;
        correction = (cdfQ - prob) ./ pdfQ;
        qf = qf - correction;
        [~,cdfQ,pdfQ] = ...
        cf2DistGP([],qf,[],options);
        criterion = any(abs(correction) ...
            > crit * abs(qf)) ...
            && max(abs(correction)) ...
            > crit && count < maxiter;
    end
    qf = reshape(qf,n,m);
    prob = reshape(prob,n,m);
    options.isPlot = isPlot;
else
    qf = [];
    count = [];
    correction = [];
end

%% RESULT
result.cdf = cdf;
result.pdf = pdf;
result.qf = qf;
result.x = x;
result.xMean = xMean;
result.xStd = xStd;
result.xMin = xMin;
result.xMax = xMax;
result.prob = prob;
result.SixSigmaRule = options.SixSigmaRule;
result.t = t;
result.T = t(end);
result.dt = dt;
result.cf = cf;
result.N = N;
result.count = count;
result.correction = correction;
result.options = options;
result.tictoc = toc;

%% PLOT the PDF / CDF
if length(x)==1,
    options.isPlot = false;
end
if options.isPlot
    figure
    plot(x,pdf,'.-')
    grid
    title('PDF Specified by the CF')
    xlabel('x')
    ylabel('pdf')
    %
    figure
    plot(x,cdf,'.-')
    grid
    title('CDF Specified by the CF')
    xlabel('x')
    ylabel('cdf')
end
end

```

APPENDIX B. MATLAB ALGORITHM CF2DISTFFT FOR NUMERICAL INVERSION OF THE CHARACTERISTIC FUNCTION BASED ON THE FFT ALGORITHM

```

function [result,cdf,pdf,qf] = ...
    cf2DistFFT(cfFun,y,prob,options)
%cf2DistFFT calculates the approximate values
% of CDF, PDF, and QF by numerical inversion of
% the characteristic function CF by using the
% FFT algorithm.
%
% SYNTAX:
% [result,cdf,pdf,qf] = ...
%     cf2DistFFT2(cfFun,y,prob,options)
%
% Viktor Witkovsky (witkovsky@savba.sk)
% Ver.: 24-Apr-2016 17:12:15
%% CHECK THE INPUT PARAMETERS
if nargin < 1
    error('Too few inputs');
end
if nargin < 4, options = []; end
if nargin < 3, prob = []; end
if nargin < 2, y = []; end
if ~isfield(options,'N')
    options.N = 2^10;
end
N = options.N;
if ~isfield(options,'SixSigmaRule')
    options.SixSigmaRule = 6;
end
if ~isfield(options,'minY')
    options.minY = [];
end
if ~isfield(options,'maxY')
    options.maxY = [];
end
if ~isfield(options,'isForcedSymmetric')
    options.isForcedSymmetric = [];
end
if isempty(options.isForcedSymmetric)
    isForcedSymmetric = false;
else
    isForcedSymmetric = ...
    options.isForcedSymmetric;
end
if ~isfield(options,'isZeroSymmetric')
    options.isZeroSymmetric = [];
end
if isempty(options.isZeroSymmetric)
    if isForcedSymmetric
        isZeroSymmetric = true;
    else
        isZeroSymmetric = false;
    end
else
    isZeroSymmetric = options.isZeroSymmetric;
end
if ~isfield(options,'isPositiveSupport')
    options.isPositiveSupport = [];
end

```

```

if isempty(options.isPositiveSupport)
    isPositiveSupport = false;
else
    isPositiveSupport = ...
    options.isPositiveSupport;
end

if ~isfield(options,'isPlot')
    options.isPlot = true;
end

if ~isfield(options,'delta')
    options.tolDiff = 1e-4;
end

%% MOMENTS AND SUPPORT
h = options.tolDiff;
t = h*(1:4);
cf = cfFun(t);
meanY = real((-cf(2) + 8*cf(1) - ...
    8*conj(cf(1))+ conj(cf(2)))/(1i*12*h));
m2 = real(-(conj(cf(4)) - 16*conj(cf(3)) + ...
    64*conj(cf(2)) + 16*conj(cf(1)) - 130 + ...
    16*cf(1) + 64*cf(2) - 16*cf(3) + ...
    cf(4))/(144*h^2));
stdY = sqrt(m2 - meanY^2);
A = meanY - options.SixSigmaRule * stdY;
B = meanY + options.SixSigmaRule * stdY;

if isPositiveSupport
    if A <= 0 && ...
        isempty(options.isForcedSymmetric)
        A = max(0,A);
        isForcedSymmetric = true;
    elseif A > 0 && ...
        isempty(options.isForcedSymmetric)
        isForcedSymmetric = false;
    end
end

% Use the specified values (if available)
if ~isempty(options.minY), A = options.minY; end
if ~isempty(options.maxY), B = options.maxY; end

% Symmetric support [-B,B] ?
if isForcedSymmetric || isZeroSymmetric
    B = options.SixSigmaRule * ...
        sqrt(stdY^2 + meanY^2);
    if ~isempty(options.maxY)
        B = options.maxY;
    end
    A = -B;
end

%% CHARACTERISTIC FUNCTION CF
k = (0:(N-1))';
t = 2*pi * (0.5-N/2+k) / (B-A);
cf = cfFun(t(N/2+1:end));
cf = [conj(cf(end:-1:1));cf];

% CF of the 'SYMETRIZED' distribution
if isForcedSymmetric
    cf = real(cf);
end

%% PDF BY the FFT algorithm
dy = (B-A)/N;
C = (-1).^((1-1/N)*(A/dy+k))/(B-A);
D = (-1).^(-2*(A/(B-A))*k);

pdfFFT = real(C.*fft(D.*cf));
cdfFFT = cumsum(pdfFFT*dy);
yFFT = A + k * dy;

```

```

if options.isZeroSymmetric
    cdfFFT = cdfFFT + 0.5 - ...
        (cdfFFT(N/2+1)+cdfFFT(N/2))/2;
end
% SPECIAL TREATMENT for symmetrized distribution
if isForcedSymmetric
    pdfFFT = max(0,2*pdfFFT(N/2+1:end));
    cdfFFT = cdfFFT + 0.5 - ...
        (cdfFFT(N/2+1)+cdfFFT(N/2))/2;
    cdfFFT = min(1, ...
        max(0,2*cdfFFT(N/2+1:end)-1));
    yFFT = yFFT(N/2+1:end);
else
    pdfFFT = max(0,pdfFFT);
    cdfFFT = min(1,max(0,cdfFFT));
end
yMin = min(yFFT);
yMax = max(yFFT);

% INTERPOLATE QUANTILE FUNCTION : QF(prob)
if isempty(prob)
    prob = [0.9,0.95,0.975,0.99,0.995,0.999];
end

[cdfU,id] = unique(cdfFFT);
yyU = yFFT(id);
szp = size(prob);
qfFun = @(prob) interp1([-eps;cdfU],...
    [-eps;yyU+dy/2],prob);
qf = reshape(qfFun(prob),szp);

% INTERPOLATE CDF/QF/PDF
if isempty(y)
    y = linspace(A,A+(N-1)*dy,100);
end

szy = size(y);
cdfFun = @(x) interp1([-eps;yyU+dy/2],...
    [-eps;cdfU],x(:));
cdf = reshape(cdfFun(y),szy);

try
    pdfFun = @(x) interp1(yFFT,pdfFFT,y(:));
    pdf = reshape(pdfFun(y),szy);
catch
    warning('Unable to interpolate')
    pdf = NaN*y;
    pdfFun = [];
end

%% RESULT
result.y = y;
result.cdf = cdf;
result.pdf = pdf;
result.prob = prob;
result.quant = qf;
result.cdfFun = cdfFun;
result.pdfFun = pdfFun;
result.qfFun = qfFun;
result.yMin = yMin;
result.yMax = yMax;
result.cdfMin = min(cdfFFT);
result.cdfMax = max(cdfFFT);
result.N = N;
result.Details.yFFT = yFFT;
result.Details.pdfFFT = pdfFFT;
result.Details.cdfFFT = cdfFFT;
result.Details.meanY = meanY;
result.Details.stdY = stdY;
result.Details.A = A;
result.Details.B = B;
result.Details.dy = dy;
result.Details.dt = 2*pi/(B-A);
result.Details.t = t;
result.Details.cf = cf;
result.Details.cfFun = cfFun;
result.options = options;

```

```

%% PLOT THE PDF/CDF, if required
if options.isPlot
    figure
    plot(yFFT,pdfFFT,'-','LineWidth',2)
    grid
    title('PDF Specified by the CF')
    xlabel('y')
    ylabel('pdf')
    figure
    plot(yFFT,cdfFFT,'-','LineWidth',2)
    grid
    title('CDF Specified by the CF')
    xlabel('y')
    ylabel('cdf')
end
end

```

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