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Implementation of the characteristic functions approach to measurement uncertainty evaluation

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Abstract

Probability distributions suitable for modelling measurements and determining their uncertainties are usually based on a standard approximation approach as described in GUM, i.e. the GUM uncertainty framework (GUF), using the law of uncertainty propagation (also known as the delta method) or a more accurate method based on the law of probability propagation calculated using the Monte Carlo method (MCM). As an alternative to GUF and MCM, we present a characteristic function approach (CFA), which is suitable for determining measurement uncertainties by using the exact probability distribution of a measured quantity in linear measurement models by inverting the associated characteristic function (CF), which is defined as a Fourier transform of the probability density function (PDF). In this paper, we present the current state of the MATLAB implementation of the characteristic function approach (the toolbox CharFunTool) and illustrate the use and applicability of the CFA for determining the distribution and uncertainty evaluation with a simple example. The proposed approach is compared with GUM, MCM and the kurtosis uncertainty method (KUM).

Keywords: measurement uncertainty; GUM procedure; Monte Carlo method; kurtosis method; characteristic function approach; numerical inversion.

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1. Introduction

In measurement and metrology, it is necessary to take into account a complex combination of influencing effects caused by measurement errors and the effects of systematic errors or other possible sources of uncertainty determined by type A and type B evaluation methods. These complex effects can significantly affect the accuracy of the uncertainty analysis of measurement results. Usually, probability distributions suitable for modelling measurement results and determining their uncertainties are based on a standard approach described in the Guide to the Expression of Uncertainty in Measurement (GUM) [1] using the law of uncertainty propagation or on a method based on the propagation of probability distributions calculated by Monte Carlo methods based on GUM-S1 [2] and GUM-S2 [3]. An alternative tool for forming the probability distribution of the output quantity in linear measurement models is based on the numerical inversion of its characteristic function defined as a Fourier transform of its PDF, see e.g. [4–5], here denoted as the characteristic function approach (CFA) [6]. The aim of this paper is to present to the interested reader the development and implementation of a set of suitable MATLAB algorithms, the package CharFunTool – The Characteristic Functions Toolbox, [7].

CharFunTool is a MATLAB repository of algorithms for evaluating the characteristic functions of selected probability distributions and tools for combining and numerically inverting them. It is most commonly used to evaluate the cumulative distribution function (CDF), the probability density function (PDF) and the quantile function (QF) from a given (combined or derived) characteristic function. For the current status of the toolbox, see the webpage https://github.com/witkovsky/CharFunTool. The toolbox includes the implementation of various inversion algorithms, including those based on the Gil-Pelaez inversion formulae [8] combined with the simple trapezoidal quadrature rule [9] or other more sophisticated quadratures and advanced acceleration methods used to calculate the required Fourier transform integrals of oscillatory functions, see e.g. [10–12]. The current version of CharFunTool was developed with MATLAB version 9.10 (R2021a). For installation, you can either clone the directory with the downloadable Git application or download the available archive file (ZIP). After unpacking the archive file, you have to add the CharFunTool directory to the MATLAB path.

The simplest example to illustrate the functionality of the CharFunTool package is the numerical inversion of a characteristic function of the standard

Table 1

Characteristic functions of continuous univariate distributions used in metrological applications (selected symmetric zero-mean distributions) presented together with their standard deviation, kurtosis and the coverage factor associated with the probability $P \in (0.1)$. Here, $J_\nu(z)$ is the Bessel function of the first kind and $K_\nu(z)$ denotes the modified Bessel function of the second kind

Probability distribution	Characteristic function (CF)	Standard deviation (uncertainty)	Kurtosis	Coverage factor
Gaussian $N(0,1)$	$\mathrm{cf}(t) = e^{-\frac{1}{2}t^2}$	1	0	$z_{1+\frac{P}{2}}$
Student's t t_ν	$\mathrm{cf}(t) = \frac{1}{2^{\frac{\nu}{2}-1}\Gamma\left(\frac{\nu}{2}\right)}\left(\nu^{\frac{1}{2}}\lvert t\rvert\right)^{\frac{\nu}{2}} K_{\frac{\nu}{2}}\left(\nu^{\frac{1}{2}}\lvert t\rvert\right)$	$\sqrt{\frac{\nu}{\nu-2}}$	$\frac{6}{\nu-4}$	$t_{\nu,1+\frac{P}{2}}$
Rectangular $R(-1,1)$	$\mathrm{cf}(t) = \frac{\sin(t)}{t}$	$\frac{1}{\sqrt{3}}$	$-\frac{5}{6}$	P
Triangular $T(-1,1)$	$\mathrm{cf}(t) = \frac{2-2\cos(t)}{t^2}$	$\frac{1}{\sqrt{6}}$	$-\frac{3}{5}$	$1-\sqrt{1-P}$
Arcsine $U(-1,1)$	$\mathrm{cf}(t) = J_0(t)$	$\frac{1}{\sqrt{2}}$	$-\frac{3}{2}$	$\sin\left(\frac{\pi}{2}P\right)$

normal distribution, which can be implemented in MATLAB by two simple commands. The commands cf=@(t)exp(-t.^2/2) and result=cf2DistGP(cf) evaluate the PDF and CDF of the standard normal distribution for 100 automatically specified equidistant x-values using only the specified characteristic function, and plot their graphs. The detailed results are saved in the result data structure for further use. To get started with the toolbox, we recommend you take a look at the collection of examples and the detailed help on the included characteristic functions and inversion algorithms.

This paper is structured as follows. In Section 2 we present the basic principles of combining characteristic functions and the basic methods for their numerical inversion. We present a list of the currently available characteristic functions included in the package. In Section 3, we illustrate the applicability of this implementation for the calculation of the distribution of the output quantity, based on a linear measurement model and a fully specified uncertainty budget. The exact result is compared with the results of the MCM method [13] and the KUM method, see e.g. [14].

2. Characteristic functions, their combinations, and numerical inversion

Let Y denote the continuous univariate random variable with its PDF denoted by $\mathrm{pdf}_Y(y)$. Then the characteristic function (CF) of the distribution of Y is given by the Fourier transform of its PDF,

$$\mathrm{cf}_Y(t) = \int_{-\infty}^{\infty} e^{ity}\,\mathrm{pdf}_Y(y)dy. \quad (1)$$

Exact analytical expressions of the characteristic functions are known for many standard probability distributions. Table 1 shows the characteristic functions of selected continuous univariate distributions (symmetric and zero-mean) commonly used in modelling measurements in metrological applications, together with their standard deviation, kurtosis and the coverage factor associated with the specified probability P. In general, analytical inversion of CFs is often difficult or impossible. Numerical inversion requires the integration of a real-valued function. Under mild conditions, Gil-Pelaez has derived the inversion formulae suitable for the numerical evaluation of the PDF and/or the CDF, which only require the integration of a real-valued function, see [8],

$$\mathrm{pdf}_Y(y) = \frac{1}{\pi}\int_0^\infty \Re\left(e^{-ity}\,\mathrm{cf}_Y(t)\right)dt, \quad (2)$$

$$\mathrm{cdf}_Y(y) = \frac{1}{2} - \frac{1}{\pi}\int_0^\infty \Im\left(\frac{e^{-ity}\,\mathrm{cf}_Y(y)}{t}\right)dt. \quad (3)$$

Here, by $\Re\left(f(t)\right)$ and $\Im\left(f(t)\right)$ we denote the real and imaginary part of the complex function $f(t)$, respectively. Typically, these integrals require integration of the (highly) oscillatory functions. For the numerical evaluation of these integrals we can use the trapezoidal rule of integration, which works surprisingly well for most typical cases, for more details see e.g. [9]. In particular,

$$\mathrm{pdf}_Y(y) \approx \frac{\delta_t}{\pi}\sum_{j=0}^{N} w_j \Re\left(e^{-it_j y}\,\mathrm{cf}_Y(t_j)\right), \quad (4)$$

$$\mathrm{cdf}_Y(y) \approx \frac{1}{2} - \frac{\delta_t}{\pi}\sum_{j=0}^{N} w_j \Im\left(\frac{e^{-it_j y}\,\mathrm{cf}_Y(t_j)}{t_j}\right), \quad (5)$$

where N is a sufficiently large number of (equidistant) sub-intervals of the interval (0, T). Here, w_j are the appropriate quadrature weights ($w_0 = w_N = \frac{1}{2}$ and w_j = 1 for j = 1, ... , N-1), and t_j denote the appropriate (equidistant) nodes from the interval (0, T), for sufficiently large T. Here, we set $\delta_t = \frac{2\pi}{B-A}$, where $(A,\ B)$ specifies the support of the distribution of the random variable Y, i.e. the range of typical values y of the distribution of Y, which gives $= \frac{N2\pi}{B-A}$. In general, other, more sophisticated methods are required in more complex situations, as e.g. the double exponential formula for the Fourier-type integrals [12].

The numerical inversion of the appropriate CF is applicable in parametric, non-parametric, as well as semi-parametric settings. Working with CFs offers an alternative and often simpler way than working directly with PDFs and CDFs. In particular, CF of a random variable defined as a linear combination of independent random variables, e.g. $Y = c_1X_1 + \ldots + c_nX_n$, where X_j have known $\mathrm{cf}_{X_j}(t)$ and the coefficients c_j, is given by

$$\mathrm{cf}_Y(t) = \mathrm{cf}_{X_1}(c_1t) \times \ldots \times \mathrm{cf}_{X_n}(c_nt). \tag{6}$$

Similarly, CF of a weighted mixture distribution, say $F_w = \sum_{i=1}^{n} w_iF_i$, with weights such that $\sum_{i=1}^{n} w_i = 1$, is

$$\mathrm{cf}_{F_w}(t) = \sum_{i=1}^{n} w_i\,\mathrm{cf}_{F_i}(t). \tag{7}$$

Finally, CF of the empirical characteristic function, say $\hat{F}_n$, based on the observed data, say $x_1, \ldots, x_n$, is a mixture of the CFs of the Dirac distributions centred at x_j,

$$\mathrm{cf}_{\hat{F}_n}(t) = \frac{1}{n}\sum_{j=1}^{n} e^{(itx_j)}. \tag{8}$$

The implementation of the algorithms for the numerical evaluation of the selected characteristic

Table 2

List of algorithms for computing characteristic functions. A simple naming structure is chosen to specify the characteristic function associated with the specific type of probability distribution

CharFunTool Characteristic Functions		
Continuous distributions:	cf_TSPSymmetric	*Discrete distributions:*
	cf_WignerSemicircle	
cf_ArcsineSymmetric		cfN_Binomial
cf_Beta	*Empirical probability distributions:*	cfN_Delaporte
cf_BetaNC		cfN_GeneralizedPoisson
cf_BetaSymmetric	cfE_DiracMixture	cfN_Geometric
cf_BirnbaumSaunders	cfE_Empirical	cfN_Logarithmic
cf_Chi	cfE_EmpiricalBootstrapped	cfN_NegativeBinomial
cf_ChiNC	cfE_EmpiricalOgive	cfN_Poisson
cf_ChiSquare		cfN_PolyaEggenberger
cf_Exponential	*Log-transformed random variables:*	cfN_Quinkert
cf_FisherSnedecor		cfN_Waring
cf_FisherSnedecorNC	cf_LogRV_Beta	
cf_FoldedNormal	cf_LogRV_BetaNC	
cf_Gamma	cf_LogRV_Exponential	*Other non-negative distributions:*
cf_GeneralizedExponential	cf_LogRV_Chi	
cf_GeneralizedLindley	cf_LogRV_ChiNC	cfX_GeneralizedPareto
cf_Gumbel	cf_LogRV_ChiSquare	cfX_PearsonVI
cf_HalfNormal	cf_LogRV_ChiSquareNC	cfX_Weibull
cf_HalfNormalNC	cf_LogRV_FisherSnedecor	cfX_LogLogistic
cf_InverseGamma	cf_LogRV_FisherSnedecorNC	cfX_LogNormal
cf_InverseGaussian	cf_LogRV_Gamma	cfX_Pareto
cf_Laplace	cf_LogRV_GammaNC	cfX_PearsonV
cf_Logistic	cf_LogRV_HalfNormal	
cf_MaxwellBoltzmann	cf_LogRV_HalfNormalNC	
cf_MaxwellBoltzmannNC	cf_LogRV_InverseGamma	*Multivariate test statistics:*
cf_Nakagami	cf_LogRV_MaxwellBoltzmann	
cf_NakagamiNC	cf_LogRV_MaxwellBoltzmannNC	cfTest_Bartlett
cf_Normal	cf_LogRV_MeansRatio	cfTest_CompoundSymmetry
cf_Rayleigh	cf_LogRV_MeansRatioW	cfTest_EqualityCovariances
cf_RayleighNC	cf_LogRV_Nakagami	cfTest_EqualityMeans
cf_Rectangular	cf_LogRV_NakagamiNC	cfTest_EqualityPopulations
cf_RectangularSymmetric	cf_LogRV_Rayleigh	cfTest_Independence
cf_Rice	cf_LogRV_RayleighNC	cfTest_Sphericity
cf_SkewNormal	cf_LogRV_Rectangular	
cf_Stable	cf_LogRV_Rice	
cf_Student	cf_LogRV_Weibull	
cf_TrapezoidalSymmetric	cf_LogRV_WilksLambda	
cf_TriangularSymmetric	cf_LogRV_WilksLambdaNC	

function is realised by the developed MATLAB package CharFunTool together with the tools for their combinations and numerical inversion. Table 2 shows the current list of algorithms for computing the characteristic functions.

The included algorithms for calculation of the characteristic functions of the univariate continuous distributions have a uniform structure of the input arguments:

$$\text{cf\_Distribution}(t,\ \text{par1},\ \ldots\ ,\ \text{park},\ \text{coef}),\quad (9)$$

- t represents a vector of values where the characteristic function will be evaluated,
- the second group of input arguments are the distribution parameters, par1, ..., park (the number of the input parameters depend on particular distribution), the input parameters should be scalars or vectors of equal sizes,
- the third input argument coef is a vector of coefficients of the same size as the parameter vectors.

For example, consider linear combination of independent random variables, say $Y = 2X_1 + 3X_2 - X_3$, where X_i ~ Gamma(α_i, β_i) are independent (however not identically) gamma distributed RVs with parameters $\alpha_1 = \alpha_2 = \alpha_3 = 2$ and $\beta_1 = 1; \beta_2 = 2; \beta_3 = 3$. Then, in CharFunTool, the characteristic function of Y, say cf(t), is given as an anonymous function of the vector argument t, as

$$\text{cf} = @(t)\ \text{cf\_Gamma}(t, [2, 2, 2], [1, 2, 3], [2, 3, -1]).\quad (10)$$

The combined characteristic function can be further numerically inverted to obtain the PDF, the CDF or the quantile function QF. The input arguments of the inversion algorithms also have a uniform argument structure:

$$\text{result} = \text{cf2DistGP}(\text{cf},\ x,\ p,\ \text{options}),\quad (11)$$

- the first argument cf is the anonymous characteristic function of the argument t,
- the second argument x is a vector of values, for which the PDF/CDF is to be evaluated,
- the third argument p is a vector of probabilities where the quantiles of the distribution are to be evaluated,
- the fourth argument options are an optional structure used to control the inversion algorithm.

Other currently available inversion algorithms: cf2DistGPT – algorithm based on the Gil-Pelaez inversion formula and the trapezoidal rule used for integration, cf2DistGPR – algorithm based on the Gil-Pelaez inversion formula and the Riemann sum used for integration, cf2DistGPA – algorithm based on the Gil-Pelaez inversion formula and the adaptive Gauss-Kronod quadrature with acceleration, cf2DistFFT – algorithm based on using the fast Fourier transform (FFT) algorithm, and cf2DistBV – algorithm based on using the Bakhvalov-Vasileva approximation.

3. Calibration of a coaxial step attenuator

To illustrate the CFA and its comparison with MCM and KUM, we consider here as an example the linear measurement model for the calibration of a coaxial step attenuator as considered in [15]. The linear measurement model of the attenuation L_X of the attenuator to be calibrated is given by

$$L_X = \text{const} + L_S + \delta L_S + \delta L_D + \\ + \delta L_M + \delta L_K + \delta L_{ib} - \delta L_{ia} + \delta L_{0b} - \delta L_{0a},\quad (12)$$

where const = 30.043, and the other input quantities are represented as independent random variables with the following probability distributions (here with unspecified measurement units):

L_S~$0.0090 \times N(0.1)$, with the standard uncertainty $u = 0.0090$, and the kurtosis parameter $\eta = 0$,

δL_S~ $(0.0025\sqrt{3}) \times R(-1.1)$, with $u = 0.0025$, and $\eta = -1.2$,

δL_D~$(0.0011\sqrt{2}) \times U(-1.1)$, with $u = 0.0011$, and $\eta = -1.5$,

δL_M~$(0.0200\sqrt{2}) \times U(-1.1)$, with $u = 0.0200$, and $\eta = -1.5$,

δL_K~$(0.0017\sqrt{2}) \times U(-1.1)$, with $u = 0.0017$, and $\eta = -1.5$,

δL_{ib}~$(0.0003\sqrt{3}) \times R(-1.1)$, with $u = 0.0003$, and $\eta = -1.2$,

δL_{ia}~$(0.0003\sqrt{3}) \times R(-1.1)$, with $u = 0.0003$, and $\eta = -1.2$,

δL_{0b}~$0.0020 \times N(0.1)$, $u = 0.0020$, and $\eta = 0$,

δL_{0b}~$0.0020 \times N(0.1)$, $u = 0.0020$, and $\eta = 0$,

where by $N(0.1)$ we denote the standard normal distribution with mean 0 and standard deviation 1, by R(-1.1) the symmetric rectangular distribution on the interval (-1.1), and by U(-1.1) the symmetric U-shaped (Arcsine) distribution on the interval (-1.1).

Using the characteristic functions approach (CFA) with the CharFunTool package the numerically exact value of the expanded uncertainty $U(y)$, i.e. the upper 97.5% quantile of the (zero-mean) distribution of the output quantity $Y = L_X$ – const, was determined as $U(y)$ = 0.03900448275179 in 3.9×10^{-4} seconds.

On the other hand, by using the Monte Carlo method (MCM) we have estimated the expanded un-certainty $U(y)$, i.e. the upper 97.5% quantile of the (zero-mean) distribution of the output quantity $Y = L_X$ – const, based on using $M = 10^6$ randomly generated realisations of Y, as $U(y)$ = 0.0389525 in 0.75 seconds. Moreover, based on $M = 10^8$ randomly generated realisations of Y we obtain $U(y)$ = 0.039003626106614 in 153.2 seconds.

Finally, using the kurtosis uncertainty method (KUM) proposed in [14], we obtain the standard uncertainty of the output quantity Y as $u(y) = 0.0224$ with the calculated kurtosis

$$\eta(y) = \frac{\sum_{j=1}^{m} \eta_j c_j^4 u^4(x_j)}{u^4(y)} = -0.9621.$$

For the required coverage probability $P = 0.95$ the estimated coverage factor is $k_{0.95}(\eta) = 0.1085\eta^3 + 0.1\eta + 1.96 = 1.7672$, and thus, theestimated expanded uncertainty is $U(y) = k_{0.95}(\eta) \times u(y) = 0.0395$.

This clearly illustrates the advantages and computational efficiency of the proposed CF approach over the other alternative methods, especially in the situation when the measurement model is linear and high precision of the computed (estimated) quantiles is required.

Реалізація підходу з використанням характеристичних функцій для оцінювання невизначеності вимірювань

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Анотація

У метрологічній практиці оцінювання невизначеності вимірювань зазвичай засновано на стандартному підході, як описано в “Настанові з подання невизначеності вимірювань” (GUM), з використанням закону поширення невизначеності. Цей підхід є наближеним, оскільки в його основу покладено центральну граничну теорему теорії ймовірності з апаратом числа ступенів свободи, що визначають недостовірність оцінок розширеної невизначеності через ігнорування впливу законів розподілу вхідних величин на закон розподілу вимірюваної величини. Другим відомим підходом до оцінювання невизначеності вимірювань є закон поширення ймовірності, заснований на використанні методу Монте-Карло (ММК). Його недоліком є неможливість отримання існуючими програмними засобами, що реалізують ММК, повного бюджету невизначеності вимірювань. Іншим відомим методом оцінювання невизначеності вимірювань є метод ексцесів (KUM), заснований на обчисленні ексцесу вимірюваної величини через ексцеси вхідних величин. Як альтернатива GUM, MCM та KUM в статті описується підхід характеристичних функцій (CFA), заснований на використанні точного розподілу ймовірностей вимірюваної величини у моделях лінійних вимірювань шляхом інвертування пов’язаної з нею характеристичної функції, визначеної як Фур’є перетворення функції густини ймовірності. Для його реалізації застосовується панель інструментів MATLAB CharFunTool. Використання цього підходу ілюструється на простому прикладі оцінювання невизначеності вимірювань під час калібрування коаксіального ступінчастого атенюатора. Результати, отримані за допомогою пропонованого підходу, порівнюються з результатами, отриманими за допомогою GUM, MCM та методом ексцесів (KUM). Демонструється обчислювальна ефективність запропонованого методу в порівнянні з відомими.

Ключові слова: невизначеність вимірювань; методика GUM; метод Монте-Карло; метод ексцесів; підхід, заснований на характеристичних функціях; числова інверсія.

Реализация подхода с использованием характеристических функций для оценивания неопределенности измерения

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Аннотация

Распределения вероятностей, подходящие для моделирования измерений и оценивания их неопределенностей, обычно основаны на стандартном приближенном подходе, как описано в GUM, то есть на структуре неопределенности GUM (GUF – GUM Uncertainty Framework), с использованием закона распространения неопределенности (также известного как дельта-метод) или более точном методе, основанном на законе распространения вероятности, рассчитанном с использованием метода Монте-Карло (MCM – Monte Carlo Method).

В качестве альтернативы GUF и MCM представлен подход характеристических функций (CFA – Characteristic Funtions Approach), который подходит для определения неопределенности измерения на основе использования точного распределения вероятностей измеряемой величины в моделях линейных измерений путем инвертирования связанной с ней характеристической функции (CF), определенной как Фурье преобразования функции плотности вероятности (PDF). Для реализации подхода характеристической функции используется панель инструментов MATLAB CharFunTool. Предлагаемый подход сравнивается с GUM, MCM и методом неопределенности эксцессов (KUM – Kurtosis Uncertainty Method).

Ключевые слова: неопределенность измерений; методика GUM; метод Монте-Карло; метод эксцессов; подход, основанный на характеристической функции; числовая инверсия.

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