




Good Practice Guide on the calculation of uncertainties of integral quantities determined from correlated spectral input data

Authors	Armin Sperling, PTB; Fabien Eloi, LNE; Jimmy Dubard, LNE; Şenel Yaran, TUBITAK; Yasaman Rezazadeh, Aalto; Zühal Alpaslan Kösemen, TUBITAK
Partners	TUBITAK, PTB, LNE, TechnoTeam, JETI, Aalto
EMPIR Grant Agreement Number	EMPIR 19NRM02 RevStdLED
Due date of the deliverable	31 August 2023
Actual submission date of the deliverable	10 December 2023
Acknowledgement	<p>This project has received funding from the EMPIR programme co-financed by the Participating States and from the European Union's Horizon 2020 research and innovation programme.</p> <p>EMPIR  EURAMET</p> <p>The EMPIR initiative is co-funded by the European Union's Horizon 2020 research and innovation programme and the EMPIR Participating States</p>



19NRM02 RevStdLED



Content

Introduction	3
Using Classical GUM for Uncertainty Calculation	5
Example for Classical GUM	7
Using a Monte Carol Method for Uncertainty Calculations	9
Example for Basic Uncertainty Calculation for Luminous Intensity with Monte Carlo Method	9
Correlation between PDFs using Monte Carlo	13
Basic considerations	13
Multivariate output quantities	16
Example of PDF Monte Carlo: Detector spectral irradiance responsivity calibration	17
Example of Spectral Correlation in Colour Measurement	20
Unknown correlations in the uncertainty analysis of spectral integrals	22
Example of calculation of unknown correlation for spectral mismatch correction factor	23
Acknowledgements	26
References	26
Annex	28
empir19nrm02: "Phyton toolbox for photometric and colorimetric measurement uncertainty calculations"	28



Introduction

This Good Practice Guide (GPG) refers to integral quantities, such as the total flux of a light source or the sensor responsivity, the spectral mismatch or also colour coordinates and the like, which are calculated by integrating individual spectral measured quantity, such as spectral irradiance of a light source, over a range of wavelengths. The radiometric or photometric spectral values may be correlated between each other at different wavelengths. The correlation affects the combined uncertainty of the integral quantities when the spectral values are integrated. Correlation is a statistical measure of the relationship between two variables. In the context of spectral data, correlation means that the individual uncertainties of the spectral values at different wavelengths are not independent from one another but influenced by another common effect. This can have various reasons, e.g. the optical properties of the measuring system change depending on the wavelength or the measured source changes during the measurement. If the spectral values are correlated, the combined uncertainty must be calculated more carefully.

There are two main approaches to calculating the combined uncertainty of an integral quantity from correlated spectral data. In general, a sufficiently complete model of the measurement task must be created for both approaches, which includes all measured variables, factors and components that contribute to the measurement result. This evaluation model is a mathematical expression of the physical model that describes the measurement process, including the necessary correction factors. In addition, the estimated or calculated uncertainty of each individual input component or input variable or correction factor is required. Moreover, in the case of spectral measurements, we usually also have to form integrals or sums of spectral contributions. An important part of calculating the combined uncertainty is determining the correct weighting of the uncertainty contributions of the individual input variables.

1. Analytical approach: To determine the sensitivity of the input quantities, this approach involves analytically differentiating the integral expression with respect to each of the spectral variables and then propagating the uncertainties of the spectral variables through the (partial) derivatives. This approach can be complex and time-consuming, especially for integrals with multiple variables. Moreover, the correlation of the spectral values at different wavelengths are not included in this approach [1]. But spectral uncertainties can arise from various sources such as wavelength scales, slit width, stray light, etc. and include both recurrent and random fluctuations. These fluctuations can be recurrent, occurring consistently during measurements, or random, occurring occasionally and unpredictably [2]. Understanding and accounting for these fluctuations is critical to obtaining reliable and reproducible results. For instance, in spectral irradiance or spectral responsivity calibration are done at specific wavelengths and need to interpolation to provide data at full wavelength range. New data are fully correlated by input so correlation between wavelengths must count into propagation of uncertainty [3,4] Therefore, the correlation of spectral values at different wavelengths must be handled separately.



19NRM02 RevStdLED



2. Monte Carlo approach: Instead of analytically determining the gradients of the influences of the input variables, the Monte Carlo approach directly exploits the scatter of the modelled individual results due to the uncertainty of the input variables. For this purpose, this approach involves a large number of random draws of the measured values that provide the spectral data, each consistent with the known uncertainties of the spectral data. The integration or summation is then calculated for each random sample, and the uncertainty of the integral quantity is estimated from the distribution of the calculated values. The Monte Carlo approach is more straightforward to implement than the analytical approach, but it can be computationally expensive [5].

In this document, it is summarized how to deal with the uncertainty of integral quantities from the basics to more complex implementations with examples. The uncertainty calculations of the integral quantities are complex and time consuming. However, once the model of evaluation has been properly written down, the determination of uncertainty is mainly a software task, the work procedures are strongly connected to software code, an example of which is freely available from the 19NRM02 RevStdLED project in a repository on GitHub.com [6]. The source code is also more permanently archived at zenodo.org [7] for referencing. As a matter of fact, there are a huge variety of software products available on the market (like Mathcad©, Mathematica©, Origin©, etc.) which can be used to calculate the combined uncertainty of measurements including correlations. However, to allow even small test laboratories to implement software code and to adapt it for their own purpose to enable the dissemination of GUM conform uncertainty estimations, it was decided to use the open-source language Python as the basis for the guidelines of this project.

Using Classical GUM for Uncertainty Calculation

The Guide to the Expression of Uncertainty in Measurement (GUM) provides a framework for the calculation of measurement uncertainty [1]. The GUM approach can be used to deal with correlation in spectral data by following these steps:

The first step is to write down the model of evaluation and to identify all of the sources of uncertainty that could affect the spectral data. This includes both random and systematic uncertainties. Once the sources of uncertainty have been identified, the uncertainty of each component must be estimated. This can be done using a variety of methods, such as statistical analysis or expert judgment.

According to GUM, the combined uncertainty $u(y)$ of the output quantity value y is calculated as linear approach of the model function using the standard uncertainty $u(x_i)$ and $u(x_j)$ associated with the N input quantity values x_i and x_j with $1 \leq i, j \leq N$, and the related sensitivity coefficients c_i, c_j and the correlation coefficients $r(x_i, x_j)$.

$$u^2(y) = \sum_{i=1}^N [c_i \cdot u(x_i)]^2 + 2 \sum_{i=1}^{N-1} \sum_{j=i+1}^N c_i c_j u(x_i) u(x_j) r(x_i, x_j) \quad \text{with} \quad \begin{cases} -1 \leq r(x_i, x_j) \leq 1 \\ \text{for } i \neq j \end{cases} \quad (1)$$

Using classical GUM, the sensitivity coefficients are determined by partially differentiating the model of evaluation. If the values $x_{i,k}, x_{j,k}$ of two input quantities (index i, j) are measured simultaneously several times with $1 \leq k \leq n$ then their empirical standard deviation of the means $s(\bar{x}_i), s(\bar{x}_j)$ and the covariance $s(\bar{x}_i, \bar{x}_j)$ with

$$s(\bar{x}_i, \bar{x}_j) = \frac{\sum_{k=1}^n (x_{i,k} - \bar{x}_i) \cdot (x_{j,k} - \bar{x}_j)}{n(n-1)} \quad \text{and} \quad s(\bar{x}_i) = \sqrt{\frac{1}{n(n-1)} \sum_{k=1}^n (x_{i,k} - \bar{x}_i)^2} \quad (2)$$

are used to determine the correlation coefficient between input quantities.

In this way, we obtain the dimensionless correlation coefficient.

$$r(x_i, x_j) = \frac{s(\bar{x}_i, \bar{x}_j)}{s(\bar{x}_i) \cdot s(\bar{x}_j)} = \frac{\sum_{k=1}^n (x_{i,k} - \bar{x}_i) \cdot (x_{j,k} - \bar{x}_j)}{\sqrt{\sum_{k=1}^n (x_{i,k} - \bar{x}_i)^2 \cdot \sum_{k=1}^n (x_{j,k} - \bar{x}_j)^2}} \quad (3)$$

where

$$-1 \leq r(x_i, x_j) \leq 1$$

Calculating the correlation coefficient for all possible variation i, j , the $N \times N$ correlation matrix \mathbf{R}_x of the measurement can be determined.



19NRM02 RevStdLED

$$\mathbf{R}_x = \begin{bmatrix} r(x_1, x_1) & \cdots & r(x_1, x_N) \\ \vdots & \ddots & \vdots \\ r(x_N, x_1) & \cdots & r(x_N, x_N) \end{bmatrix} \quad (4)$$

where $r(x_i, x_i) = 1$ and $r(x_i, x_j) = 0$ when elements x_i and x_j are uncorrelated.

The correlation matrix is a “table” that shows the correlation between each pair of input quantities. The correlation coefficient can be used to quantify the strength of the relationship between two input quantities. Eq. (1) could also be written down as a function of the covariance, with the difference the covariance is expressed with a measurement unit, while the correlation coefficient is dimensionless. According to Eq. (3), the elements (i, j) of the $N \times N$ covariance matrix \mathbf{U}_x (also named uncertainty matrix) are given by:

$$u(x_i, x_j) = r(x_i, x_j)u(x_i)u(x_j) \quad (5)$$

In practice, correlation between measured data can already occur during the measurement at a single wavelength, e.g. if a slight ambient temperature drift occurs during the measurement series, which not only affects the responsivity of the detector of the spectroradiometer but also that of the monitor detector. Therefore, to determine the combined uncertainty of the measurement at a single wavelength using the model of evaluation for the output quantity at a single wavelength, multiple readings must be carried out to be able to determine the covariance of the measured input signals. In principle, this has to be done at every wavelength to be measured. This is significantly simplified by the use of array spectroradiometers, which record all spectral components in a single measurement process.

Using the model of evaluation for the determination of the spectrally integrated quantity, the final combined uncertainty of the integral quantity may also be affected by correlations, e.g. correlations between neighbouring wavelengths/pixels. Here, the same procedure as explained previously may apply. In case of array-spectroradiometers, the multiple readings of the individual pixels taken before can be used to determine the covariance or correlation matrix, respectively.

However, an important note should be given here:

Even if two input variables are correlated with each other (e.g. via the temperature), the covariances will be zero and the measurement results will appear uncorrelated if, for example, the temperature is kept constant during the repeat measurements. However, if the measuring instrument was calibrated on a different day under slightly different conditions, for example, the correlation would be fully effective. Therefore, it is important to either vary the conditions during the repeat measurements to capture the relative effects that might change between the calibration of the system and the actual measurement so that these can be included in the uncertainty budget, or at least to accurately specify the measurement conditions during calibration for which the calibration results are exclusively valid.



19NRM02 RevStdLED



Example for Classical GUM

The output value of a system can be calculated using a model of evaluation. This model function is a mathematical expression that relates the output value to the input values. In the case of a system in which two measured values A , B and a constant value C are multiplied, the model function can be written as follows:

$$Y = F(X_1, X_2, X_3) = A \cdot B \cdot C \quad (6)$$

According to the model the output quantity is derived from multiplication of three input quantities (A, B, C) with input values (a, b, c) where two of them are measured simultaneously providing a statistical variance while the third is constant having a Type B uncertainty based on a rectangular distribution given in Table 1.

Table 1. Example of input values

	a	b	c
1	100.35	0.83	7
2	100.34	1.00	7
3	100.82	1.07	7
4	100.68	1.24	7
5	100.98	1.29	7
6	100.81	1.31	7
7	101.14	1.59	7
8	101.48	1.60	7
9	101.27	1.76	7
10	101.39	1.74	7
$\bar{x} \equiv$	100.926	1.343	7
$\overline{u(\bar{x})} =$	0.127	0.102	$0.3/\sqrt{3}=0.17$
$r(\bar{x}_i, \bar{x}_j) =$	0.926		0

Value of the output is

$$y = \bar{a} \cdot \bar{b} \cdot \bar{c} = 948.81$$

Uncertainty propagation of the model function according to Eq. (1):

$$u(y) = \sqrt{\left((c_a \cdot u(a))^2 + (c_b \cdot u(b))^2 + (c_c \cdot u(c))^2 \right) + 2(c_a c_b u(a) u(b) r(a, b))}$$



19NRM02 RevStdLED



Using the linear approach to determine the sensitivity coefficients in Eq. (1), (see also CIE 198:2011, Eq.13):

$$c_i = \frac{f(x_1, x_2, \dots, x_i + u(x_i), \dots, x_N) - f(x_1, x_2, \dots, x_i - u(x_i), \dots, x_N)}{2 \cdot u(x_i)}$$

it follows

$$(c_a \cdot u(a)) = \frac{1}{2} \cdot ((a + \Delta u(a)) \cdot b \cdot c - (a - \Delta u(a)) \cdot b \cdot c) = 1.193$$

$$(c_b \cdot u(b)) = \frac{1}{2} \cdot ((b + \Delta u(b)) \cdot a \cdot c - (b - \Delta u(b)) \cdot a \cdot c) = 72.061$$

$$(c_c \cdot u(c)) = \frac{1}{2} \cdot ((c + \Delta u(c)) \cdot a \cdot b - (c - \Delta u(c)) \cdot a \cdot b) = 23.042$$

$$u(y) = \sqrt{(1.193^2 + 72.061^2 + 23.042^2 + 2 \cdot (1.193 \cdot 72.06 \cdot 0.926)}$$

$$u(y) = 75.66 \quad \text{without correlation} \quad r(a, b) = 0$$

$$u(y) = 80.10 \quad \text{with correlation:} \quad r(a, b) = 0.926$$

$$u(y) = 96.30 \quad \text{with full correlation} \quad r(a, b) = 1$$

In this case, the partially correlated case lies between the uncorrelated and the fully correlated case. However, this should not be taken for granted, because if, for example, the values b are an order of magnitude greater with unchanged uncertainties, the partially correlated uncertainty is greater than the fully correlated uncertainty.

It is obvious that the classical GUM approach to the spectral measurements can be very time consuming. If the correlation is only very small, it is likely that the uncertainty of the integral quantity is not significantly affected. In this case, it may be possible to ignore the correlation and use the standard GUM approach without a correlation term. If the correlation between the spectral data is strong, then it is important to carefully account for the correlation when calculating the uncertainty of the integral quantity. In this case, the GUM approach may become tedious in the calculation, and it may be necessary to use a more sophisticated method, such as the Monte Carlo approach.



Using a Monte Carlo Method for Uncertainty Calculations

While the linear approach of the classical GUM works well for a lot of measurement tasks with simple models of evaluation, it becomes very complicated and demanding for more complex evaluation models, e.g. of spectrally integrated data, and multivariate quantities, i.e. output results with more than one output quantity (e.g. colour coordinates), or for strongly correlated input quantities and for nonlinear models of evaluation. In all these cases, it is much easier to use a so-called Monte Carlo Method for the uncertainty determination and for assigning the best estimated result of the measurement process.

The Monte Carlo method is not used in metrology to simulate the result of a measurement per se, but to simulate the combined uncertainty of a measurement result based on the knowledge of the uncertainties and the PDFs (Probability Density Function) of the input variables of the measurement.

A probability density function (PDF) is a function that describes the probability of a continuous random variable taking on a certain value. The PDF is a non-negative function that integrates to 1 over the support of the random variable. The PDF is often used to represent the uncertainty of a measurement.

PDFs can be classified into a number of different types. The normal and uniform distributions, explained below, are the most common in metrology.

Normal distribution: The PDF of a normal distribution is bell-shaped, with the most likely value occurring at the mean.

Uniform distribution: The PDF of a continuous uniform distribution is constant over a given interval.

The choice of PDF to be used for a particular application depends on the type of data and the assumptions that can be made about the statistical deviations from the mean during the measurement, which must be mimicked by the random variable used to create the PDF. A particular case to note are uncertainties taken from calibration certificates or other uncertainties combined from multiple sources, in which case the PDF is generally taken as Normal distribution.

As with the classical GUM, the starting point for Monte Carlo Method is the complete model of evaluation which includes all interdependencies of the input parameters and input quantities of the measurement. In addition, the standard deviation / uncertainty and the probability function of every single input quantity has to be known. In principle, the Monte Carlo method allows to determine the combined uncertainty without determining the sensitivity coefficients by derivation of highly complex measurement models. However, it is also possible to determine the sensitivity coefficients if needed.

In the example given below, Monte Carlo Method is explained in detailed.

Example for Basic Uncertainty Calculation for Luminous Intensity with Monte Carlo Method

In photometry and radiometry a typical univariate model function for evaluation depends on multiple input quantities. The estimate of such a multivariate input quantity $\mathbf{X} = (X_1, X_2, \dots, X_N)^T$, a matrix of dimension $N \times 1$, where “T” denotes “transpose”, is interpreted as a multivariate vector x_r which is drawn at random from the PDFs of the N input quantities and provides the model output value y_r with $r = 1, \dots, M$ the number of draws.



This can be most easily explained by an example:

Example for model of a univariate measurement function:

$$I = d^2 \cdot J^1 \cdot s_v^{-1} \cdot k_1^1 \quad (7)$$

The covariance matrix (i.e. the uncertainty matrix), containing the uncertainties of the input quantities is given by:

$$\mathbf{U}_x = \begin{bmatrix} u^2(d) & 0 & 0 & 0 \\ 0 & u^2(J) & 0 & 0 \\ 0 & 0 & u^2(s_v) & 0 \\ 0 & 0 & 0 & u^2(k_1) \end{bmatrix} \quad (8)$$

As the components of the input vector $\mathbf{X} = (d, J, s_v, k_1)^T$ * are expected to be uncorrelated, the off-diagonal elements (e.g. $u(d)u(J)$, $u(d)u(s_v)$, $u(d)u(k_1)$, ...) of the matrix are zero.

Random Generator: $R(\mathbf{x}_r, u(\mathbf{x}_r)) := \text{Random}(\mathbf{x}_r, u(\mathbf{x}_r))$

Explanation: A random value of an input variable with its mean value x_r is drawn, where, as a boundary condition, its value is randomly distributed around its mean and within the limit given by the uncertainty $u(\mathbf{x}_r)$ of the input value. The uncertainties of the input components are taken from the covariance matrix. To correctly reflect the characteristics of the input variable, the distribution function of the draws used must reflect the behaviour of the input variable. If only the mean value (expectation value) and its uncertainty is known, it is expected that the measurement values of the input quantity are normal (i.e. Gaussian) distributed (see 6.4.7.1. in JCGM101:2008)

Simulation by multiple draws:

$$\begin{aligned} y_r &= f(\mathbf{x}_r), \quad r = 1, \dots, M \\ I_1 &= R(d^2, u(d)) \cdot R(J^1, u(J)) \cdot R(s_v^{-1}, u(s_v)) \cdot R(k_1^1, u(k_1)) \\ I_2 &= R(d^2, u(d)) \cdot R(J^1, u(J)) \cdot R(s_v^{-1}, u(s_v)) \cdot R(k_1^1, u(k_1)) \\ I_3 &= R(d^2, u(d)) \cdot R(J^1, u(J)) \cdot R(s_v^{-1}, u(s_v)) \cdot R(k_1^1, u(k_1)) \\ &\dots \\ I_M &= R(d^2, u(d)) \cdot R(J^1, u(J)) \cdot R(s_v^{-1}, u(s_v)) \cdot R(k_1^1, u(k_1)) \end{aligned} \quad (9)$$

After a sufficient number of draws we get the estimate of the output quantity

$$\bar{y} = \frac{1}{M} \sum_{r=1}^M y_r \xrightarrow{\text{Example:}} I = \frac{1}{M} \sum_{r=1}^M I_r \quad (10)$$

and its associated standard uncertainty

$$u^2(\bar{y}) = \frac{1}{M-1} \sum_{r=1}^M (y_r - \bar{y})^2 \xrightarrow{\text{Example:}} u(I) = \sqrt{\frac{1}{M-1} \sum_{r=1}^M (I_r - I)^2} \quad (11)$$

* In this example, no distinction is made between the nomenclature of the expectation value and the nomenclature of the quantity.

19NRM02 RevStdLED

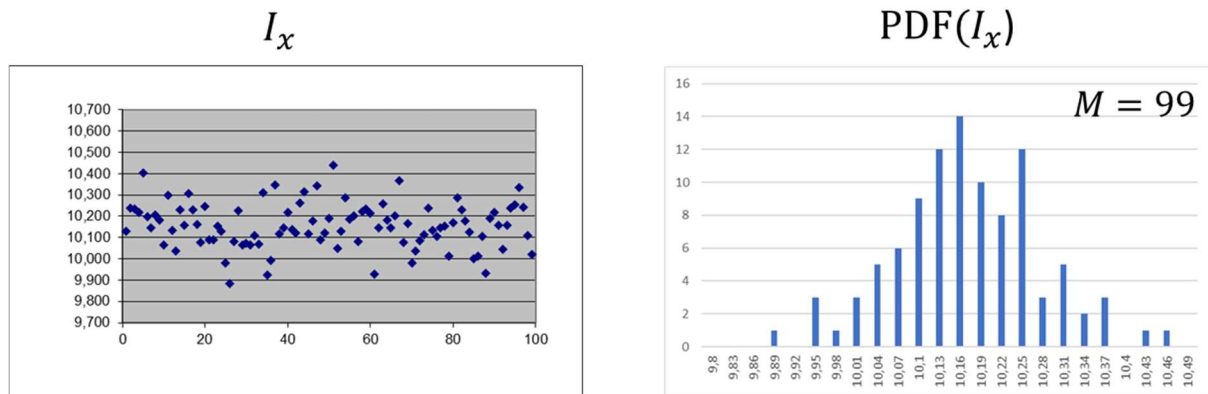


Fig. 2. Discrete representation of the PDF. More examples can be found in CIE 198, CIE 198-sp1 to CIE 198-sp4 [9-12]

If the output quantity Y itself becomes an input quantity for further uncertainty calculations, random draws from its distribution $y(r)$, $r = 1, \dots, M$ with the same probability distribution are to be used. See Annex for further information on implementation of MCS using Python language.



Correlation between PDFs using Monte Carlo

Basic considerations

Probability density functions (PDFs) describe the likelihood of a random variable taking on particular values. The correlation between two PDFs measures how closely they are related. A positive correlation indicates that the variables tend to move in the same direction, while a negative correlation indicates that they tend to move in opposite directions. A correlation of zero indicates that the variables are independent. There are a number of different ways to measure correlation between PDFs. One common measure is the Pearson correlation coefficient as shown already in Eq. (3). In Literature, the following expression is also frequently used:

$$\rho(X_1, X_2) = \frac{cov(X_1, X_2)}{\sigma(X_1) \cdot \sigma(X_2)} \quad (12)$$

where $\rho(X_1, X_2)$ is the correlation coefficient between X_1 and X_2 , $cov(X_1, X_2)$ is the covariance between X_1 and X_2 , and $\sigma(X_1)$ and $\sigma(X_2)$ are the standard deviations of X_1 and X_2 , respectively.

The Pearson correlation coefficient can range from -1 to 1. A coefficient of -1 indicates a perfect negative correlation, meaning that the variables are always moving in opposite directions. A coefficient of 0 indicates no correlation, meaning that the variables are independent. A coefficient of 1 indicates a perfect positive correlation, meaning that the variables are always moving in the same direction.

For example, when measuring luminous intensity, Eq. (7), the luminous responsivity of the detector and the gain of a transimpedance amplifier used to measure the detector output current (see Fig. 1), can be correlated with each other. If, for example, the temperature is not stable during a measurement, the luminous responsivity of the detector and the gain of the transimpedance amplifier can both change depending on the temperature. As a result, the marginal distributions for the calculation of the common output variable, i.e. the originally univariate PDFs of luminous responsivity and gain, will be distorted by the temperature effect. In other words, the shape of the PDFs will change.

In simplified Monte Carlo simulations (MCS), independent PDFs are often used for modelling, even for correlated variables such as the sensitivity and gain of a detector in the example above. The possible correlation between these two variables mentioned above is therefore not taken into account. However, if such a correlation between the quantities is strong, we need a method that takes into account the correlated distortion of the marginal PDFs to allow us to generate random numbers for both quantities



19NRM02 RevStdLED



that reflect the correlation between them*. For this we need the covariance matrix or the correlation matrix for correlated variables of the model of the evaluation.

If the input quantities of the model of evaluation are viewed as components X_i of a multivariate vector quantity, $\mathbf{X} = (X_1, X_2, \dots, X_N)^T$, given as a matrix of dimension $N \times 1$, the correlation matrix is a matrix that describes the correlations between the components of the vector of input variables. It is formed as a matrix of all pairwise correlation coefficients (Eq. 8) of the elements of the vector quantity:

$$\mathbf{C} = \text{Corr}(\mathbf{X}) = \begin{pmatrix} \rho(X_1, X_1) & \cdots & \rho(X_1, X_N) \\ \vdots & \ddots & \vdots \\ \rho(X_N, X_1) & \cdots & \rho(X_N, X_N) \end{pmatrix} \quad (13)$$

Using the method called the Cholesky decomposition, this correlation matrix can be decompose into a lower and upper triangular matrix. The elements of the lower triangular matrix can then be used to generate the correlated random numbers required for a joint PDF.

The lower triangle matrix \mathbf{L} of Cholesky decomposition (or factorizing) is determined using:

$$\mathbf{A} = \mathbf{L} \cdot \mathbf{L}^T = \mathbf{C} \quad (14)$$

The correlation matrix must be symmetric and positive semidefinite to apply the formalism below.

In the case of a 2 x 2 matrix, then the following applies to the decomposition

$$\begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} = \mathbf{A} = \mathbf{L} \cdot \mathbf{L}^T = \begin{bmatrix} l_{11} & 0 \\ l_{21} & l_{22} \end{bmatrix} \begin{bmatrix} l_{11} & l_{12} \\ 0 & l_{22} \end{bmatrix} \quad (15)$$

In general, the matrix elements of the lower triangle matrix \mathbf{L} can be determined according to the general rule:

$$\begin{aligned} l_{kk} &= (a_{kk} - \sum_{j=1}^{k-1} l_{kj}^2)^{1/2} & \text{for } i = k \\ l_{ik} &= \frac{a_{ik} - \sum_{j=1}^{k-1} l_{ij} \cdot l_{kj}}{l_{kk}} & \text{for } i > k \\ l_{ik} &= 0 & \text{for } i < k \end{aligned} \quad (16)$$

In our example of a 2 × 2 matrix the lower triangle matrix \mathbf{L} becomes:

* If the measurement of two quantities within a model of evaluation are represented by the same PDF (e.g. Gaussian distribution), simply using the same random number for both univariate quantities would imply full correlation, meaning that they would always change together. Hence, it needs a more sophisticated approach to generate correlated random numbers.



19NRM02 RevStdLED



$$L = \begin{bmatrix} 1 & 0 \\ a_{21} & \sqrt{1 - a_{21}^2} \end{bmatrix} \quad (17)$$

The application of the lower triangular matrix is illustrated using the example of the model function of luminous intensity from Fig. 1 (slightly simplified), where the gain (R) and for the luminous responsivity (s_v) are expected to be correlated:

$$I = d^2 \cdot V^1 \cdot c^1 \cdot k_1^1 \cdot [R \cdot s_v \cdot]^{-1} \quad (18)$$

In a first step, one has to draw random numbers for all quantities $X = (X_d, X_V, X_C, X_k, X_R, X_{s_v})^T$ according to their uncorrelated PDFs. This is also done for the correlated gain (R) and luminous responsivity (s_v). The total number of draws for each quantity can be written as ($M \times 1$)-matrices X_R and X_{s_v} composed out of M single draws.

$$X_R = (x_{R1}, x_{R2}, \dots, x_{RM})^T \text{ and } X_{s_v} = (x_{s_{v1}}, x_{s_{v2}}, \dots, x_{s_{vM}})^T \quad (19)$$

As we have only two correlated quantities, the correlation matrix for this example will be simply.

$$C = \begin{bmatrix} 1 & \rho \\ \rho & 1 \end{bmatrix} \quad (20)$$

Where ρ given by Eq. 12 or Eq. 3 has to be calculated based on characterising measurements (as shown in the chapter "Example for classical GUM), where gain and luminous responsivity are measured concurrently depending on the ambient temperature. If the functional temperature behaviour of the two variables is known, a theoretical measurement series can be used instead.

To generate correlated sample vectors Z_R and Z_{s_v} from the uncorrelated sample vectors X_R and X_{s_v} for the MCS the lower triangle matrix of the Cholesky decomposed correlation matrix has to be multiplied with uncorrelated sample vectors $X_R = (X_{R1}, X_{R2}, \dots, X_{RM})^T$ and $X_{s_v} = (X_{s_{v1}}, X_{s_{v2}}, \dots, X_{s_{vM}})^T$ from normal distributions (μ_R, σ_R) and (μ_{s_v}, σ_{s_v}) respectively.

$$L(X_R, X_{s_v})^T = (Z_R, Z_{s_v})^T \quad (21)$$

As a result we get the correlated sample vector of random draws for R and s_v :

$$Z_R = X_R \quad (22)$$

$$Z_{s_v} = \rho X_R + \sqrt{1 - \rho^2} X_{s_v} \quad (23)$$



which have to be used for the Monte Carlo simulation instead.

Multivariate output quantities

In photometry and radiometry some important measurement results cannot be modelled as a measurement function in a single scalar output quantity as in Eq. (7). In these cases, the totality of the output quantities, as a so-called multivariate output quantity, is described by a vector output quantity, similar to the multivariate input quantity described above [13]:

$$\mathbf{Y} = \begin{bmatrix} Y_1 \\ \vdots \\ Y_m \end{bmatrix} \equiv (Y_1, \dots, Y_m)^T \quad j = 1, \dots, m \quad (24)$$

This means that the vector quantity consists of m components Y_j , where each Y_j is represented by an independent univariate model equation. In our case (spectral measurements or chromaticity coordinates), the Y_j can be expressed in most cases directly as a formula in \mathbf{X} with \mathbf{f} as multivariate model function*:

$$\mathbf{Y} = \mathbf{f}(\mathbf{X}) \quad (25)$$

and

$$Y_1 = f_1(\mathbf{X}), \dots, Y_m = f_m(\mathbf{X}) \quad (26)$$

with $j = 1, \dots, m$ model functions and $i = 1, \dots, N$ input quantities, i.e. $\mathbf{X} = (X_1, \dots, X_N)^T$

Example:

In case of spectral irradiance responsivity the model function f_j would correspond to Eq. 19, where Y_j is replaced by $s(\lambda_i)$, and the multivariate input vector \mathbf{X} stands for the input variables $(U_{DUT}, U_{ref}, R_{ref}, R_{DUT}, Mon_{ref}, Mon_{DUT}, S_{\phi,ref}(\lambda_i), A_{ref}, c_{wl}(\lambda_i), c_{bw}(\lambda_i), c_{dist})^T$. Finally the multivariate output quantity \mathbf{Y} can be directly used as a multivariate input quantity again to determine e.g. the luminous responsivity.

If, in case of Monte Carlo simulation of \mathbf{Y} , \mathbf{y}_r (as estimate of the \mathbf{Y}_r) with $r = 1, \dots, M$ is one of M independent realisations (draws) of \mathbf{Y} , the average

$$\mathbf{A} = \frac{1}{M}(\mathbf{y}_1 + \dots + \mathbf{y}_M) \quad (27)$$

is taken as the estimate \mathbf{y} of \mathbf{Y} to determine the estimation of the covariance matrix (uncertainty):

$$\mathbf{U}_A = \frac{1}{M-1}((\mathbf{y}_1 - \mathbf{A})(\mathbf{y}_1 - \mathbf{A})^T + \dots + (\mathbf{y}_M - \mathbf{A})(\mathbf{y}_M - \mathbf{A})^T) \quad (28)$$

* For implicit multivariate measurement models see Chapter 6.2 of JCGM 102:2011

Since the PDF of Y is no longer a simple Gaussian function, as is typical for univariate output variables, there is no single coverage range, but a multidimensional coverage region. For example, for bivariate Gaussian distributions, i.e. for model equations with two output quantities, an ellipse is the smallest area that may covers 95 % of the measurement points. In the general case with more than 2 dimensions, a hyper-ellipsoidal coverage range is expected where y specifies the location of the hyper-ellipsoidal, $U_y := U_A$ specifies its shape and k_p its size. For bivariate output quantities $k_p = 2.45$ is valid.

Example of PDF Monte Carlo: Detector spectral irradiance responsivity calibration

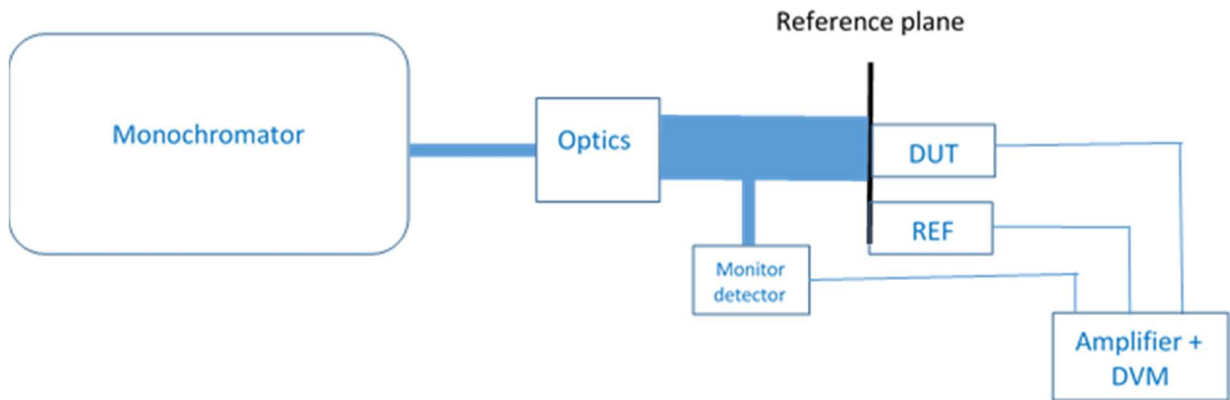


Fig. 3. Responsivity measurement setup

The setup shown in Fig. 3 is used to calibrate the spectrally dependent irradiance responsivity, $s(\lambda)$, of the detector under test (DUT). According to Eq. 24 the responsivity $s(\lambda)$ can be regarded as a multivariate vector quantity of $i = 1, \dots, m$ spectral elements $s(\lambda_i)$, i.e. $s(\lambda) = (s(\lambda_1), \dots, s(\lambda_m))^T$. The model function for the measurement of the spectral irradiance responsivity is given below.

$$s(\lambda_i) = \frac{U_{DUT}}{U_{ref}} \cdot \frac{R_{ref}}{R_{DUT}} \cdot \frac{Mon_{ref}}{Mon_{DUT}} \cdot s_{\phi,ref}(\lambda_i) \cdot A_{ref} \cdot c_{wl}(\lambda_i) \cdot c_{bw}(\lambda_i) \cdot c_{dist} \quad (29)$$

In Monte Carlo simulation, the contribution of the wavelength calibration to the uncertainty is taken into account via a correction factor to mimic a potential wavelength shift, which is relevant for differently shaped relative spectral responsivity functions of the DUT and the reference.

$c_{wl}(\lambda_i)$ is the correction factor to account for the wavelength measurement uncertainty:

$$c_{wl}(\lambda_i) = \frac{c_{wl,DUT}}{c_{wl,ref}} = \frac{1 - \frac{s'(\lambda_i)}{s(\lambda_i)} \cdot \Delta\lambda}{1 - \frac{s'_{ref}(\lambda_i)}{s_{ref}(\lambda_i)} \cdot \Delta\lambda} \quad (30)$$



19NRM02 RevStdLED



The uncertainty contribution of the spectral bandwidth of the radiation used to measure the responsivity of a detector is important when the responsivity changes rapidly within the bandwidth. In other words, if the responsivity is linear or the bandwidth of the source is small, such as for continuous-wave lasers, bandwidth correction may be negligible. Other conditions require the correction of bandwidth effects. $C_{bw}(\lambda_i)$ is the correction factor to account for spectral bandwidth effects for a triangular shaped slit function of the spectroradiometer:

$$C_{bw}(\lambda_i) = \frac{1 - \Delta\lambda^2 \cdot \frac{1}{12} \cdot \frac{s''_{ref}(\lambda_i)}{s_{ref}(\lambda_i)}}{1 - \Delta\lambda^2 \cdot \frac{1}{12} \cdot \frac{s''_{DUT}(\lambda_i)}{s_{DUT}(\lambda_i)}} \quad (31)$$

The random values for M draws generated for these two spectral contributions at a single wavelength will form two column matrices of dimension $M \times 1$, which are used in the MCS together with the column matrices of the other input variables at the same wavelength, based on the measurement model (Eq. 29). The final output of the Monte Carlo simulation for the spectrally dependent responsivity $s(\lambda)$ is a set of m vector elements for all the measured wavelengths λ_i . Each of these elements contain matrix of M individual values of the spectral responsivity $s(\lambda_i)$ corresponding to the number of trials at that specific wavelength. The order of the sorted data should not be changed (general rule for all data generated using Monte Carlo simulation).

$$s(\lambda) = \begin{bmatrix} s(\lambda_1) \\ \vdots \\ s(\lambda_m) \end{bmatrix} \text{ with } i = 1, \dots, m \text{ (number of wavelengths measured)} \quad (32)$$

where

$$s(\lambda_i) = \begin{bmatrix} s(\lambda_i, 1) \\ \vdots \\ s(\lambda_i, M) \end{bmatrix} \text{ with } i = 1, \dots, m \text{ and } r = 1, \dots, M \text{ (number of trials during MCS)} \quad (33)$$

For all wavelength, i.e. for all matrices $s(\lambda_i)$ it is possible to determine the expectation value, which is the average $\bar{s}(\lambda_i)$ of the values, as well as the variance $v^2(\bar{s}(\lambda_i))$.

$$\bar{s}(\lambda_i) = \frac{\sum_{r=1}^M s(\lambda_i, r)}{M} \quad (34)$$

$$v^2(\bar{s}(\lambda_i)) = \frac{\sum_{r=1}^M (s(\lambda_i, r) - \bar{s}(\lambda_i))^2}{(M - 1)} \quad (35)$$

To obtain covariance, we consider two matrices $s(\lambda_i)$ and $s(\lambda_j)$ from the matrix vector $s(\lambda)$ corresponding to wavelengths λ_i and λ_j . For these matrices the covariance $v(s(\lambda_i), s(\lambda_j))$ between pairs i, j of single spectral data can be determined as follows:

$$v(s(\lambda_i), s(\lambda_j)) = \frac{\sum_{k=1}^N (s(\lambda_i, k) - \bar{s}(\lambda_i)) \cdot (s(\lambda_j, k) - \bar{s}(\lambda_j))}{(M - 1)} \quad (36)$$

which results in the correlation coefficient $r(s(\lambda_i), s(\lambda_j))$

$$r(s(\lambda_i), s(\lambda_j)) = \frac{v(s(\lambda_i), s(\lambda_j))}{v(\bar{s}(\lambda_i), v(\bar{s}(\lambda_j)))}$$

where

$$r(s(\lambda_i), s(\lambda_i)) = 1 \quad (37)$$

$$-1 < r(s(\lambda_i), s(\lambda_j)) < +1$$

$$r(s(\lambda_i), s(\lambda_j)) = r(s(\lambda_j), s(\lambda_i))$$

As shown in Eq. 38 for five wavelengths, the correlation matrix is therefore symmetrical to the diagonal, whereby the diagonal elements equal to “1”.

$$\begin{bmatrix} 1 & r(s(\lambda_2), s(\lambda_1)) & r(s(\lambda_3), s(\lambda_1)) & r(s(\lambda_4), s(\lambda_1)) & r(s(\lambda_5), s(\lambda_1)) \\ r(s(\lambda_2), s(\lambda_1)) & 1 & r(s(\lambda_3), s(\lambda_2)) & r(s(\lambda_4), s(\lambda_2)) & r(s(\lambda_5), s(\lambda_2)) \\ r(s(\lambda_3), s(\lambda_1)) & r(s(\lambda_3), s(\lambda_2)) & 1 & r(s(\lambda_4), s(\lambda_3)) & r(s(\lambda_5), s(\lambda_3)) \\ r(s(\lambda_4), s(\lambda_1)) & r(s(\lambda_4), s(\lambda_2)) & r(s(\lambda_4), s(\lambda_3)) & 1 & r(s(\lambda_5), s(\lambda_4)) \\ r(s(\lambda_5), s(\lambda_1)) & r(s(\lambda_5), s(\lambda_2)) & r(s(\lambda_5), s(\lambda_3)) & r(s(\lambda_5), s(\lambda_4)) & 1 \end{bmatrix} \quad (38)$$

For further use, it has to be proven that this matrix is symmetric positive semi-definite $m \times m$ matrix.

The correlation matrix of the relative spectral responsivities of a PTB measurement system is drawn in Fig.4 showing strong positive correlations between responsivities on the same edge of the spectral responsivity function and strong negative correlations between responsivities on different edges.

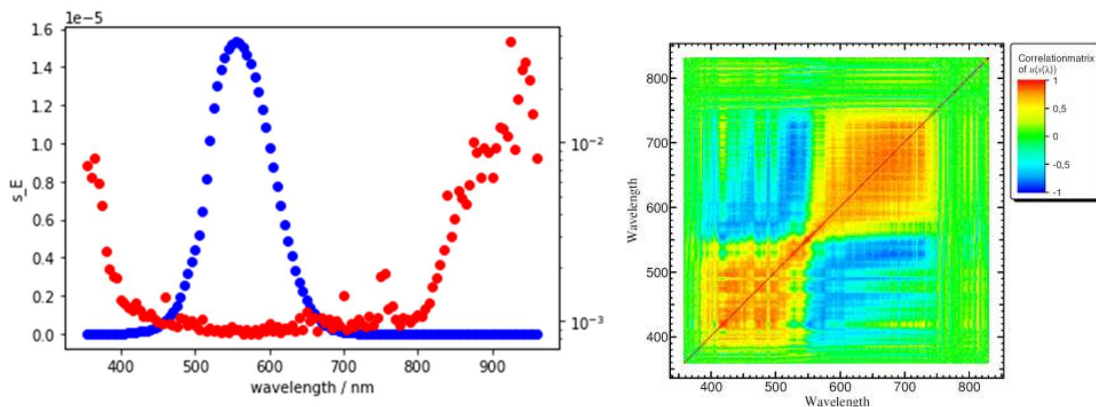


Fig. 4. Left: spectral irradiance responsivity (blue; left axis) and the relative standard uncertainty (red; right axis) of a photometer; Right: the corresponding correlation matrix [14]

More examples of the codes including methods to clean up ill conditioned correlation matrices can be found in the GitHub repository [6]

Example of Spectral Correlation in Colour Measurement

For the determination of the chromaticity coordinates of a source, the required spectrum of the source $S_{DUT}(\lambda)$ can be measured by reflexion on a white diffuser $R_{Diff}(\lambda)$ using a spectroradiometer $S_{Spect}(\lambda)$:

$$S_{DUT}(\lambda) = \frac{S_{Spect}(\lambda)}{R_{Diff}(\lambda)} \quad (39)$$

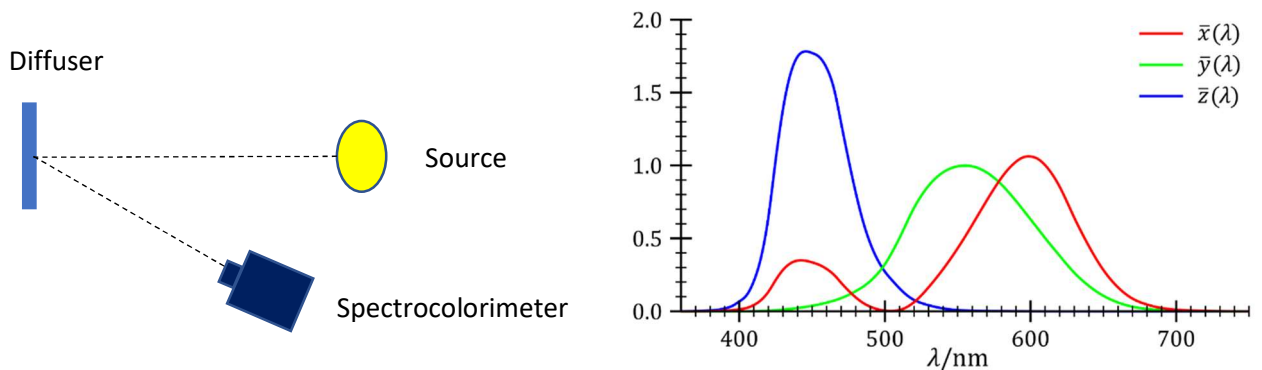


Fig. 5. Left: Measurement setup; Right: CIE 1931 XYZ Color Matching Functions

The chromaticity coordinates x, y of the source as output quantities are determined from $S_{DUT}(\lambda)$ as follows:

$$\begin{aligned} X &= \int S_{DUT}(\lambda) \bar{x}(\lambda) d\lambda \\ Y &= \int S_{DUT}(\lambda) \bar{y}(\lambda) d\lambda \\ Z &= \int S_{DUT}(\lambda) \bar{z}(\lambda) d\lambda \\ x &= \frac{X}{X + Y + Z} \\ y &= \frac{Y}{X + Y + Z} \end{aligned} \quad (40)$$

According to Eq. 40, both components x and y of the chromaticity coordinate are physically correlated. Hence, the chromaticity coordinates are treated as a bivariate output matrix vector $(x, y)^T$ where the respective uncertainty matrix requires to take correlations into account.

Fig. 6 and 7 show the results of Monte Carlo simulations where different contributions are highlighted, depending on whether only the physically correlation, additional correlations due to the spectral measurement or full correlation of all measured data are taken into account.

Some contributions come from the reference reflectance plate and the spectrometer. The correlation between the chromaticity coordinates of a source and the uncertainty contribution of the reflectance values is shown in Fig. 6.

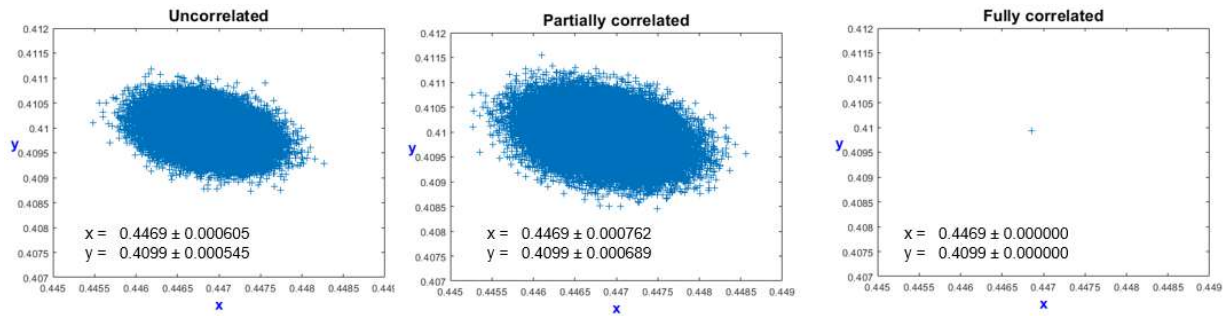


Fig. 6. left: Correlation due to overlapping colour-matching functions and with no additional correlation within the measurement process of the spectral data; centre: Additional partial correlation due to the measurement procedure of the spectral data; right: Additional full correlation of all the spectral data. *Note: The uncertainty of the reflection calibrations leads to an amplitude shift, which is cancelled out in the ratio of Eq. 40 if the correlation is complete.*

Fig. 7 shows the correlation between the colour coordinates of a source and the uncertainty contribution of the wavelength scale calibration.

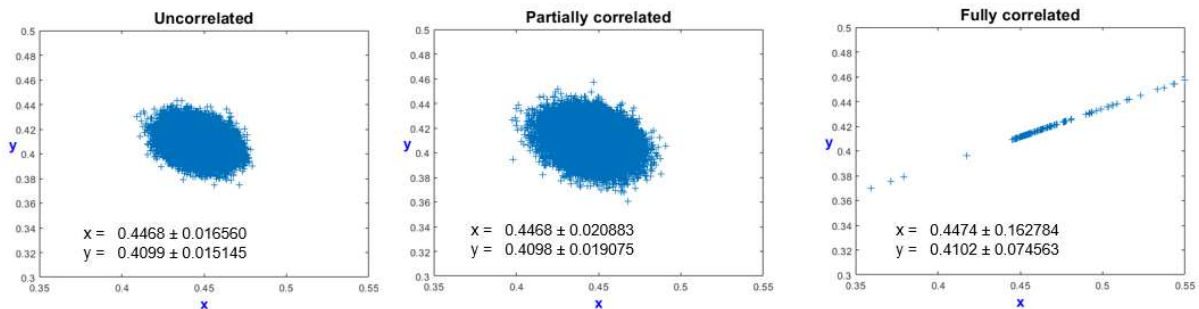


Fig. 7. left: Correlation due to overlapping colour-matching functions and with no additional correlation within the measurement process of the spectral data; centre: with additional partially correlated measurement procedure of the spectral data; right: with additional full correlation of all the spectral data. *Note: The uncertainty of the wavelength scale calibration leads to a shift of the spectral points which does not cancel out in x and y .*

The uncertainties provided in Fig. 6 and 7 are standard uncertainties. The respective expanded uncertainties require a coverage factor of $k_p = 2.45$.



Unknown correlations in the uncertainty analysis of spectral integrals

Quantities like colour coordinates, colour temperature and spectral mismatch correction factor are defined in terms of ratios of spectral integrals of irradiance. Such quantities are not affected by multipliers of spectral irradiance which are the same at all wavelengths (see Figure 6), and the related uncertainty components can be left out of the following analysis. In measuring spectral irradiance, the correlation between measured values at different wavelengths plays an important role in uncertainty evaluations. These correlations manifest themselves in three distinct types of uncertainty components: fully uncorrelated components, like noise, partial correlation with known spectral structure, like lamp filament temperature, and partial correlation with unknown spectral structure that is the most challenging case because of unknown features. It is straightforward to analyse the effects of the two former correlation types. In order to overcome the challenge of accounting for unknown correlations in uncertainty analysis, a method that offers greater reliability compared to previous approaches is used for the spectral integrals. Background to the method is described in Refs. [15-20].

In analysing the effect of partial correlations, in colour coordinates, colour temperature, spectral mismatch correction factor and other similar quantities, nominal spectral irradiance $E(\lambda)$ is modified by:

$$E_e(\lambda) = [1 + \delta(\lambda)u_c(\lambda)]E(\lambda) \quad (41)$$

where λ is the wavelength within the limits of integration of λ_1 and λ_2 , $u_c(\lambda)$ is the relative combined standard uncertainty of spectral irradiance, consisting of various uncertainty components with unknown spectral correlations. $\delta(\lambda)$ is a randomly varying error function calculated according to:

$$\delta(\lambda) = \sin(\theta) + \frac{\cos(\theta)}{\sqrt{\sum_{i=1}^N \frac{1}{i^2}}} \sum_{i=1}^N \frac{f_i(\lambda)}{i} \quad (42)$$

where θ is a random uniformly distributed variable within $[-\pi, \pi]$ and N is the number of non-constant basis functions f_i . The basis functions are defined using Legendre polynomials P_i as

$$f_i(\lambda) = g_{2i-1}(\lambda) \cos(\phi_i) + g_{2i}(\lambda) \sin(\phi_i) \quad (43)$$

where ϕ_i is a random variable uniformly distributed within the interval $[-\pi, \pi]$ and

$$g_i(\lambda) = P_i\left(\frac{2\lambda - \lambda_1 - \lambda_2}{\lambda_2 - \lambda_1}\right) / \sigma_i \quad (44)$$

with σ_i as the standard deviation of P_i when integrated from λ_1 to λ_2 . Legendre polynomials are defined within the interval $[-1, 1]$.

Example of calculation of unknown correlation for spectral mismatch correction factor

Spectral mismatch correction factor

$$F = \frac{\int E(\lambda)V(\lambda)d\lambda}{\int E(\lambda)s_{rel}(\lambda)d\lambda} \quad (45)$$

is used here as a model quantity of ratios of spectral integrals. In Eq. (45), $V(\lambda)$ is the spectral luminous efficacy of photopic vision, the limits of integration are $\lambda_1 = 360$ nm, $\lambda_2 = 830$ nm, and $s_{rel}(\lambda)$ is the relative spectral responsivity of the photometer, normalized to 1 at $\lambda_0 = 555$ nm. The uncertainty analysis of the spectral mismatch correction factor is carried out for carefully characterized spectral irradiance values and main uncertainty components of a 1000-W FEL lamp [21]. Fig.8 shows the relative spectral responsivity of the selected photometer. The uncertainties related to the photometer are not considered here.

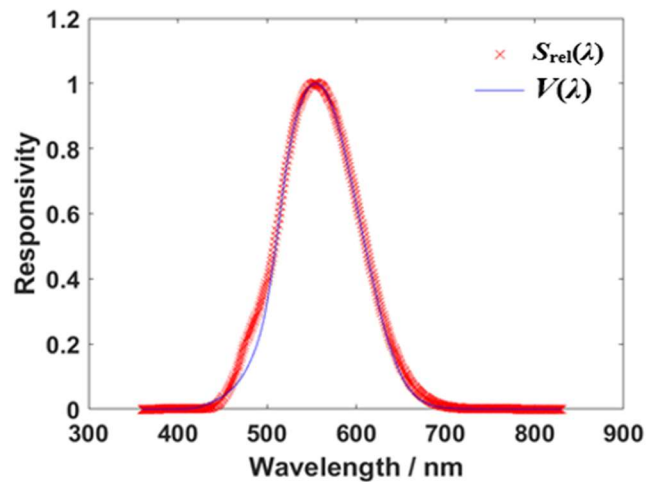


Fig. 8. Relative spectral responsivity $s_{rel}(\lambda)$ of the studied photometer and $V(\lambda)$ curve in the wavelength range 360 nm – 830 nm. The photometer quality index f_1' is 7.3 %.

The uncertainty budget of the spectral irradiance of the studied FEL lamp at 500 nm wavelength is shown in Table 2 [21]. Each of the uncertainty components in Table 2 have specific spectral correlation features. Row (i) describes noise in the calibration which is fully uncorrelated at different measurement wavelengths. The uncertainty of the lamp filament temperature is 0.7 K on row (ii) of Table 1. The variation of the nominal temperature of 3100 K of the lamp filament within the Gaussian probability distribution of $(0.7 K)^2$ variance causes changes of the irradiance spectrum which can be calculated by the Planck radiation law. The third component (iii), related to drift and repeatability of the lamp irradiance, is assumed to have unknown partial correlations between the spectral irradiance values measured at different wavelengths. That component is the main interest here.



19NRM02 RevStdLED

Table 2. Main uncertainty components ($k=1$) of the spectral irradiance of a 1000-W FEL lamp [21], for the uncertainty analysis of F in Eq. (37).

	Component	Relative uncertainty of the spectral irradiance at 500 nm (as an example)
(i)	Noise in the calibration	0.05 %
(ii)	Temperature deviation of the lamp	0.2 %
(iii)	Uncorrected drift & repeatability of the lamp	0.2%

As determined from Eq. (45), the value of spectral mismatch correction factor F is 0.95414 for the photometer of Fig. 8 and a Planckian radiator of temperature 3100 K. Monte Carlo simulations were then carried out corresponding to the uncertainty components of Table 2. The noise in calibration is entirely uncorrelated across different measurement wavelengths of spectral irradiance. To evaluate the effect of this uncertainty component, independent random numbers from a Gaussian distribution at each wavelength were generated for the uncertainty evaluation and the nominal spectral irradiance was deviated accordingly. The standard deviation of F was found to be $0.2 \cdot 10^{-5}$ due to noise in the calibration. The variation in temperature, specifically at 3100 K, of the FEL lamp filament follows a Gaussian distribution with $(0.7 \text{ K})^2$ variance. This temperature uncertainty leads to alterations in the irradiance spectrum, which are computed using the Planck radiation law. The standard deviation of F was found to be $0.07 \cdot 10^{-5}$ due to uncertainty in the lamp filament temperature.

For analysis of the effects of partial correlations, the drift & repeatability component of Table 2 was used for in Eq. (41). Fig. 9 shows the resulting standard deviation of F calculated by Eqs. (41-45) as a function of N . At each value of N , 10000 Monte Carlo cycles were repeated. The standard deviation obtained does not depend on N with large values of N . This convenient feature allows to use the stable standard deviation of $2.3 \cdot 10^{-5}$ of F as the uncertainty due to the drift & repeatability component.

19NRM02 RevStdLED

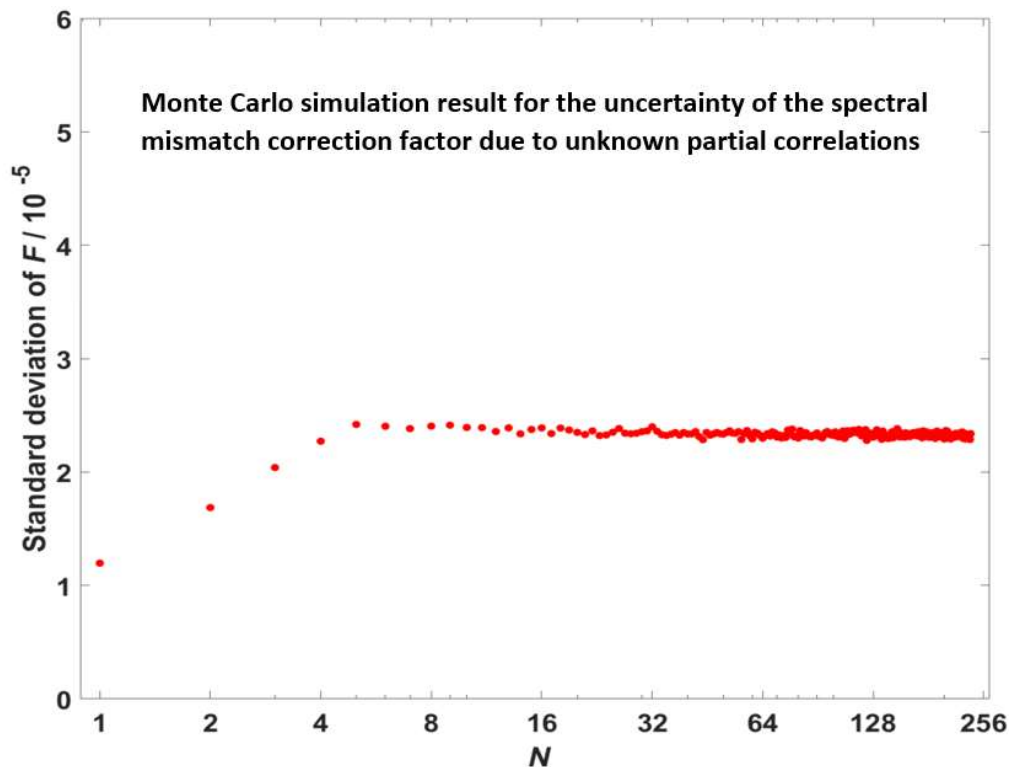


Fig. 9. Standard deviation of F due to unknown partial correlations. Parameter N describes the number of non-constant basis functions used

The uncertainty due to each type of uncertainty components of Table 3 is summarized in Table 3. It is seen that the uncertainty component due to unknown partial correlations is by far the largest. The total standard uncertainty of F is the quadratic sum of components (i) to (iii) leading to $2.3 \cdot 10^{-5}$.

Table 3. Main uncertainty components of the spectral irradiance of a 1000-W FEL lamp [21] and their contribution to the uncertainty of spectral mismatch correction factor F .

	Component	Contribution to standard uncertainty of F
(i)	Noise in the calibration	$0.2 \cdot 10^{-5}$
(ii)	Temperature deviation of the lamp	$0.07 \cdot 10^{-5}$
(iii)	Uncorrected drift & repeatability of the lamp	$2.3 \cdot 10^{-5}$

Uncertainty analysis of quantities defined in terms of ratios of spectral integrals should start from study of the uncertainty budget of the related spectral quantity, such as spectral irradiance. The uncertainty components should then be separated into the following four types: fully correlated, fully uncorrelated, partially correlated with known spectral dependence, and partially correlated with unknown spectral dependence. The remaining steps of the uncertainty analysis are:



19NRM02 RevStdLED



- 1) Remove uncertainty components which are described by a constant multiplier (fully correlated components) because they do not affect the ratio of spectral integrals. (However, these components should remain if the uncertainty of a single spectral integral is needed.)
- 2) Collect uncertainty components which are fully uncorrelated at different wavelengths and carry out a Monte Carlo simulation to evaluate the effect of these components.
- 3) For each of the partially correlated uncertainty components with known spectral dependence, carry out the uncertainty analysis using their known spectral behavior.
- 4) For each of the partially correlated uncertainty components with unknown spectral dependence, carry out the uncertainty analysis using Eqs. (41-44).
- 5) Collect the results from points 1 to 4 above and add them quadratically to determine the total uncertainty of the quantity of interest. [22]

Acknowledgements

This project (19NRM02 RevStdLED) has received funding from the EMPIR programme co-financed by the Participating States and from the European Union's Horizon 2020 research and innovation programme.



References

- [1] JCGM 100:2008 Evaluation of measurement data – Guide to the expression of uncertainty in measurements
- [2] I. Nimeroff, "Propagation of Errors in Spectrophotometric Colorimetry," J. Opt. Soc. Am. 43, 531-533 (1953)
- [3] Gardner JL. Uncertainty Propagation for NIST Visible Spectral Standards. J Res Natl Inst Stand Technol. 2004 Jun 1;109(3):305-18. doi: 10.6028/jres.109.023. PMID: 27366615; PMCID: PMC4854317.
- [4] Woolliams E. Uncertainty analysis for filter radiometry based on the uncertainty associated with integrated quantities. Int J Ther-mophys. 2014;35:1353–1365
- [5] JCGM 101:2008 Evaluation of measurement data — Supplement 1 to the “Guide to the expression of uncertainty in measurement” — Propagation of distributions using a Monte Carlo method
- [6] Github repository of Project 19NRM02 RevStdLED: <https://github.com/empir19nrm02>
- [7] Zenodo repository of Project 19NRM02 RevStdLED: <https://zenodo.org/records/6860393>
- [8] CIE 127:2007 Measurement of LEDs



19NRM02 RevStdLED



- [9] CIE 198-SP1.1:2011 Determination Of Measurement Uncertainties In Photometry Supplement 1: Modules And Examples For The Determination Of Measurement Uncertainties Part 1: Modules for the Construction of Measurement Equations
- [10] CIE 198-SP1.2:2011 Determination Of Measurement Uncertainties In Photometry Supplement 1: Modules And Examples For The Determination Of Measurement Uncertainties Part 2: Examples for Models with Individual Inputs
- [11] CIE 198-SP1.3:2011 Determination Of Measurement Uncertainties In Photometry Supplement 1: Modules And Examples For The Determination Of Measurement Uncertainties Part 3: Examples for the Solving of Systems of Equations
- [12] CIE 198-SP1.4:2011 Determination Of Measurement Uncertainties In Photometry Supplement 1: Modules And Examples For The Determination Of Measurement Uncertainties Part 4: Examples for Models with Distributions
- [13] JCGM 102:2008 Evaluation of measurement data — Supplement 2 to the “Guide to the expression of uncertainty in measurement” —Extension to any numbers of output quantities
- [14] S. Winter, et al Uncertainty Analysis of a photometer calibration at the DSR setup of the PTB, 2016 CIE x029:2006, 139-142 2016
- [15] P. Kärhä *et al*, Method for estimating effects of unknown correlations in spectral irradiance data on uncertainties of spectrally integrated colorimetric quantities, *Metrologia* **54**, 524 – 534 (2017)
- [16] A. Vaskuri et al, Uncertainty analysis of total ozone derived from direct solar irradiance spectra in the presence of unknown spectral deviations, *Atmos. Meas. Tech.*, **11**, 3595–3610 (2018)
- [17] P. Kärhä *et al*, Key comparison CCPR-K1.a as an interlaboratory comparison of correlated color temperature, *J. Physics: Conf. Ser.* **972**, 012012 (2018)
- [18] K. Maham *et al*, Spectral mismatch uncertainty estimation in solar cell calibration using Monte Carlo simulation, *IEEE Journal of Photovoltaics*, doi: 10.1109/JPHOTOV.2023.3311890
- [19] U. Krueger *et al*, Sensitivity evaluation of measurement uncertainty contributions of spectral data for calculated integral quantities (submitted)
- [20] K. Maham *et al*, Spectral analysis of deviations from key comparison reference values (submitted)
- [21] A. Sperling *et al*, 19NRM02 Summary report on traceability of spectral calibrations (<https://www.ptb.de/empir2020/revstdled/information-communication/download/>)
- [22] Jupyter Notebook on investigations carried out for NewRad2023 regarding basis functions: <https://github.com/empir19nrm02/empir19nrm02/blob/main/empir19nrm02/Jupyter/NewRad2023.ipynb>



19NRM02 RevStdLED



Annex

empir19nrm02: “Phyton toolbox for photometric and colorimetric measurement uncertainty calculations”

The free available "empir19nrm02" Python software toolbox for photometric and colorimetric measurement uncertainty calculations (<https://github.com/empir19nrm02/empir19nrm02>) was developed by project partners and offers a wide range of functionalities with its application examples, which were mainly written in the high-level open source language Python®. Users can utilize the tool to perform various tasks, including but not limited to:

1. **Uncertainty calculation with the aid of Monte Carlo Simulations (MCS):** The software examples facilitates the computation of uncertainty by employing different level of Monte Carlo simulations. In addition MCS is used in the included tools to model and analyze the impact of various sources of uncertainty in the data.
2. **Analyzing data with complex correlations:** The tool is able to process data sets with complicated correlations, e.g. the correlations between at different wavelengths. This feature is particularly valuable for users who have to deal with complex relationships within their data sets.
3. **Multi-functional capabilities within a computer-based environment:** "empir19nrm02" is designed to fit seamlessly into a computer-based environment and provides the user with a comprehensive set of tools for diverse analytical tasks. This increases the usefulness of the tool for a wide range of applications.

Furthermore, the "empir19nrm02" Python software tool is adaptable to the specific needs of the user. It is compatible with Python 3.10 versions, making it versatile enough to be utilized across different environments such as Google Colab ©, Anaconda ©, GitHub Desktop ©, and more.

This adaptability allows users to integrate the tool into their preferred working environments, promoting accessibility and ease of use. Whether employed in collaborative online platforms like Google Colab or local development environments like Anaconda, the tool ensures consistent performance and functionality.

Users can easily employ the specified tool on their computers by referring to a brief guide provided in the link below, which outlines the installation process for Python and all essential packages

<https://github.com/empir19nrm02/empir19nrm02/tree/main/Doc>.

During the project, the data used in calculations is provided in the DATA folder (see link below) to allow the users to experiment with the code and enhance their experience with the tool. The aim is to make it easier for users to work with and test the codes in practice and encourage a better understanding of how to use the tool.

<https://github.com/empir19nrm02/empir19nrm02/tree/main/empir19nrm02/data>In the Jupyter® folder (see link below), numerous example applications are provided, ranging from the simplest to the most complex. The User can revise and create their own programs based on these examples to meet their specific needs. This allows users to effectively utilize the given examples as a starting point for their own projects.



19NRM02 RevStdLED



<https://github.com/empir19nrm02/empir19nrm02/tree/main/empir19nrm02/Jupyter>

Below you will find some Jupyter notebooks for the examples covered in this guide, which describe the Python code for a possible realisation of the Monte Carlo simulation. In addition to the software code, the Jupyter notebooks also contain further information and graphical intermediate results to illustrate the individual process steps.

Basic Luminous Intensity with Monte Carlo:

https://github.com/empir19nrm02/empir19nrm02/blob/main/empir19nrm02/Jupyter/MCS_TestApplication.ipynb

Spectral Irradiance Responsivity:

https://github.com/empir19nrm02/empir19nrm02/blob/main/empir19nrm02/Jupyter/MCSim_PTBTTest.ipynb

Multivariate Quantities:

<https://github.com/empir19nrm02/empir19nrm02/blob/main/empir19nrm02/Jupyter/DoETest.ipynb>