

# NIST Uncertainty Machine — User's Manual

Thomas Lafarge      Antonio Possolo

Statistical Engineering Division  
Information Technology Laboratory  
National Institute of Standards and Technology  
Gaithersburg, Maryland, USA

November 26, 2020

## 1 NIST Uncertainty Machine for the Impatient

- Using a Web browser, visit <https://uncertainty.nist.gov/>.
- Choose the number of input quantities from the drop-down menu, and change their names if desired.
- Select a probability distribution for each of the input quantities, and enter values for its parameters (in the absence of cogent reason to do otherwise, assign Gaussian distributions to the input quantities, with means equal to estimates of their values, and standard deviations equal to their standard uncertainties);
- If there are correlations between the input quantities, then activate **Correlations**, enter the values of the non-zero correlations, and select a copula to apply them with (cf. Figure 6 on Page 26).
- Specify the size of the Monte Carlo sample to be drawn from the probability distribution of the output quantity (no larger than 5 000 000).
- Enter one or more valid R expressions (one per line) into the box labeled **Value of output quantity (R expression)** such that the last line evaluates to  $f(x_1, \dots, x_n)$ , the right-hand side of the measurement equation. (Refer to (U-8) on Page 11 for the case when the output quantity is a vector.)
- Click the button labeled **Run the computation**.

## 2 Purpose

The NIST Uncertainty Machine (<https://uncertainty.nist.gov/>) is a Web-based software application to evaluate the measurement uncertainty associated with an output quantity defined by a measurement model of the form  $y = f(x_1, \dots, x_n)$ .

The function  $f$  must be specified fully and explicitly, either as a formula or as an algorithm that, given vectors of values of the inputs, all of the same length, produces a vector of values of the output, also of the same length as the inputs — this is the sense in which we say, throughout this manual, that  $f$  must be “vectorized.”

The input quantities are modeled as random variables whose joint probability distribution also has to be fully specified. In many applications,  $f$  is real-valued (but vectorized as just mentioned). Section 12, beginning on Page 27, shows how the NIST Uncertainty Machine may also be used to produce the elements needed for a Monte Carlo evaluation of uncertainty for a multivariate measurement: that is, when, given a single set of scalar inputs  $x_1, \dots, x_n$ ,  $y$  is a vector (whose length may be different from  $n$ ). The example presented in section 12 (*Voltage Reflection Coefficient*) illustrates this case.

Lafarge and Possolo [2015] describe an early version of the NIST Uncertainty Machine and an important innovation implemented in it: the computation of the uncertainty budget based entirely on the results of the Monte Carlo method. Both Bell [1999] and Hall and White [2018] provide succinct, very accessible introductions to the concepts and basic techniques for the evaluation of measurement uncertainty. Possolo [2015] and Possolo and Iyer [2017] provide more extensive introductions that include many illustrative examples drawn from the practice of measurement science.

The NIST Uncertainty Machine evaluates measurement uncertainty by application of two different methods:

- The method introduced by Gauss [1823] and popularized by Kline and McClintock [1953], particularly among the engineering and physics communities — this method is described succinctly by Taylor and Kuyatt [1994], and more detailedly in the *Guide to the Evaluation of Uncertainty in Measurement* (GUM) [Joint Committee for Guides in Metrology, 2008a];
- The Monte Carlo method described by Morgan and Henrion [1992] in the context of measurement science, which is specified in Supplements 1 (GUM-S1) and 2 (GUM-S2) to the GUM [Joint Committee for Guides in

[Metrology, 2008b, 2011](#)] — [Possolo et al. \[2009\]](#) dispel some common misunderstandings about the application of the techniques described in the GUM-S1.

### 3 Gauss's Formula vs. Monte Carlo Method

The method described in the GUM produces an approximation to the standard measurement uncertainty  $u(y)$  of the output quantity, starting from:

- (a) Estimates  $x_1, \dots, x_n$  of the input quantities, which must be specified by the user;
- (b) Standard measurement uncertainties  $u(x_1), \dots, u(x_n)$  associated with the input quantities, which also must be specified by the user;
- (c) Correlations  $\{r_{ij}\}$  between every pair of different input quantities, which the NIST Uncertainty Machine assumes all to be zero unless the user explicitly specifies other values for them;
- (d) Values of the partial derivatives of  $f$  evaluated at  $x_1, \dots, x_n$ , which the user need not concern herself with, because the NIST Uncertainty Machine does all the necessary calculations.

When the probability distribution of the output quantity is approximately Gaussian, then the interval  $y \pm 2u(y)$  may be interpreted as a coverage interval for the measurand with approximately 95 % coverage probability.

By a felicitous coincidence this also holds for some markedly non-Gaussian probability distributions, including many instances of the Student's  $t$ , lognormal, gamma, and Weibull distributions [[Freedman et al., 2007](#)].

However, and in general, the probabilistic meaning of other intervals, for example  $y \pm u(y)$  or  $y \pm 3u(y)$ , typically will be markedly dependent on the probability distribution assigned to  $y$ . For example, if this distribution is Gaussian, then  $y \pm u(y)$  has coverage probability 68 %, but 76 % when the distribution is Laplace (or double exponential).

The GUM also considers the case where the distribution of the output quantity  $y$  is approximately Student's  $t$  with a number of degrees of freedom that is a function of the numbers of degrees of freedom that the  $\{u(x_j)\}$  are based on, computed using the Welch-Satterthwaite formula [[Satterthwaite, 1946](#), [Welch, 1947](#)].

In general, neither the Gaussian nor the Student's  $t$  distributions need model the dispersion of values of the output quantity accurately, even when all the input quantities are adequately modeled as Gaussian random variables.

The GUM suggests that the Central Limit Theorem (CLT) from Probability Theory [DeGroot and Schervish, 2011] lends support to the Gaussian approximation for the distribution of the output quantity. However, without a detailed examination of the measurement function  $f$ , and of the probability distribution of the input quantities (examinations that the GUM does not explain how to do), it is impossible to guarantee the adequacy of the Gaussian or Student's  $t$  approximations.

NOTE. The CLT states that, under specified conditions, a sum of independent random variables has a probability distribution that is approximately Gaussian [Billingsley, 1979, Theorem 27.2]. The CLT is a *limit* theorem, in the sense that it concerns an infinite sequence of sums, and provides no indication about how close to Gaussian the distribution of a sum with a finite number of summands will be. Other results in probability theory provide such indications, but they involve more than just the means and variances that are required to apply Gauss's formula [Friedrich, 1989].

NOTE. The reason why the CLT may be relevant is the following: if the function  $f$  is sufficiently smooth in a neighborhood of the point (in  $n$ -dimensional Euclidean space)  $(\xi_1, \dots, \xi_n)$ , whose coordinates are the true values of the input quantities, then  $f(x_1, \dots, x_n) \approx f(\xi_1, \dots, \xi_n) + \dot{f}_1(x_1, \dots, x_n)(x_1 - \xi_1) + \dots + \dot{f}_n(x_1, \dots, x_n)(x_n - \xi_n)$ , where the  $\{\dot{f}_i\}$  denote the first-order partial derivatives of  $f$ . The right-hand side is a sum of random variables when the  $\{x_i\}$  are modeled as random variables.

Application of the Monte Carlo method produces an arbitrarily large sample from the probability distribution of the output quantity, and it requires that the joint probability distribution of the random variables modeling the input quantities be specified fully.

This sample alone suffices: (i) to compute the standard uncertainty associated with the output quantity; (ii) to compute and to interpret coverage intervals probabilistically; and (iii) to estimate the proportions of the squared uncertainty  $u^2(y)$  that are attributable to the sources of uncertainty corresponding to the the different input quantities (the so-called *uncertainty budget*), using the technique described by Lafarge and Possolo [2015].

EXAMPLE. Suppose that the measurement model is  $y = ab/c$ , and that  $a$ ,  $b$ , and  $c$  are modeled as independent random variables such that:

- $a$  is Gaussian with mean 32 and standard deviation 0.5;

- $b$  has a uniform (or, rectangular) distribution with mean 0.9 and standard deviation 0.025;
- $c$  has a symmetrical triangular distribution with mean 1 and standard deviation 0.3.

Figure 1 on Page 6 shows the graphical user interface of the NIST Uncertainty Machine filled in to reflect these modeling choices, and the results that are returned and displayed by the browser. To load the specifications for this example into the NIST Uncertainty Machine, click [here](#).

The method described in the GUM produces  $y = 32.2$  and  $u(y) = 12.5$ . According to the conventional interpretation, the interval  $y \pm 2u(y) = (18, 67.1)$  may be a coverage interval with approximately 95 % coverage probability. (The results of the Monte Carlo method can be used to show that the effective coverage of this interval is 95.5 %.)

Since the NIST Uncertainty Machine requires that the probability distribution of the input quantities be specified, in the absence of cogent reason to do otherwise, the user may assign Gaussian (or, normal) distributions to them:

- If the input quantities are uncorrelated, then this amounts to assigning a Gaussian distribution to each one of them, with mean and standard deviation equal to the corresponding estimate and standard uncertainty;
- If the input quantities are correlated, then besides assigning Gaussian distributions to them as in the previous case, then the user will also need to select the option marked Correlation in the interface of the NIST Uncertainty Machine, and then specify the values of the correlations, and select a Gaussian copula (if indeed a multivariate Gaussian distribution is desired) to enforce the correlations [[Possolo, 2010](#)].

In many cases there is cogent reason to assign non-Gaussian distributions to at least some of the input quantities.

For example, if the quantity takes values between known lower and upper limits, then a (shifted and re-scaled) beta distribution with suitably chosen parameters may be an appropriate model: the uniform (or, rectangular) distribution is a special case of the beta distribution.

For another example, suppose that  $f(x_1, \dots, x_n)$  involves a ratio, as in the example above, where  $y = ab/c$ . Then  $c$  should not be assigned a normal distribution because the corresponding probability density is positive at 0, and  $y$  will have infinite variance. If the true value of  $c$  is known to be positive, and  $\hat{c}$  is its estimate, and  $u(c)/\hat{c}$  is less than 5 %, say, then  $c$  may be assigned a lognormal

## INPUT

1. Select Inputs & Choose Distributions

Number of input quantities: 3

Names of input quantities:

a b c

a Gaussian (Mean, StdDev) 32 0.5

b Uniform (Mean, StdDev) 0.9 0.025

c Triangular -- Symmetric (Mean, StdDev) 1 0.3

Correlations

2. Choose Options

Number of realizations of the output quantity: 1000000

Random number generator seed: 5

Symmetrical coverage intervals

3. Write the Definition of Output Quantity

Definition of output quantity (R expression):

a\*b/c

Run the computation

## OUTPUT

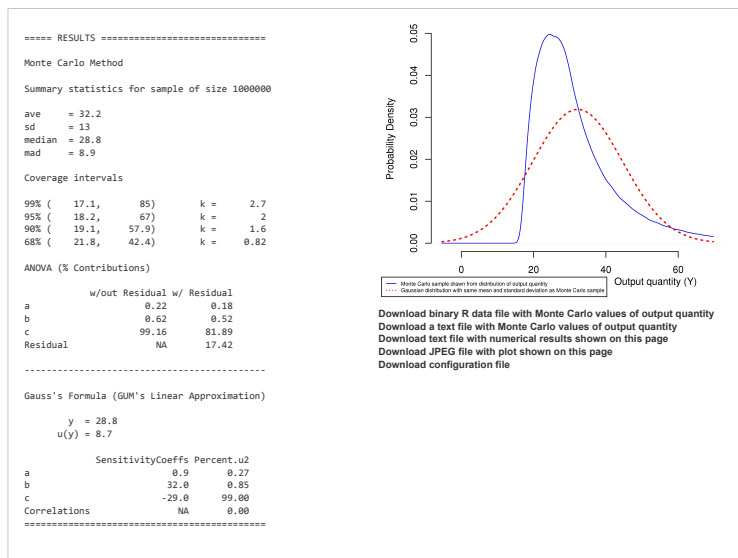


Figure 1: **ABC**. Entries in the Web page correspond to the example discussed in §3. In each numerical result, only the digits that the NIST Uncertainty Machine deems to be significant are printed. Estimate of the probability density of the output quantity (solid blue line), and probability density (dotted red line) of a Gaussian distribution with the same mean and standard deviation as the output quantity. In this case, the Gaussian approximation is very inaccurate.

distribution with mean  $\hat{c}$  and standard deviation  $u(c)$ , and this distribution will be just about indistinguishable from the Gaussian distribution with the same mean and standard deviation.

The NIST Uncertainty Machine offers a rich menu of distributions that may be selected and assigned to the input quantities to characterize the uncertainty associated with them. Possolo and Elster [2014] provide detailed guidance for how to assign probability distributions to input quantities, and illustrate this guidance with examples. The NIST Uncertainty Machine also offers the possibility of importing a file with a sample of values drawn from the distribution one wishes to assign to an input quantity, regardless of what this distribution may be, and without having to specify it.

## 4 Usage

The NIST Uncertainty Machine runs on a NIST Web server, accessible via a Web browser at <https://uncertainty.nist.gov/>. The computational engine of the NIST Uncertainty Machine is written in the R language for statistical computing and graphics [R Core Team, 2015].

NOTE. Some commercial products, and free software, are identified in this manual in order to specify the means whereby the NIST Uncertainty Machine may be employed. Such identification is not intended to imply recommendation or endorsement by the National Institute of Standards and Technology, nor is it intended to imply that the products or software identified are necessarily the only or best available for the purpose.

**Seed.** The box following **Random number generator seed** contains an integer no larger than 100 that serves as the seed for the random number generator. With the same seed, and with the same other inputs, the NIST Uncertainty Machine should always produce exactly the same results. In general, the user does not need to choose a value for the seed: a value is placed in the box automatically when the Web page of the NIST Uncertainty Machine is visited.

**Reset.** Pressing the **Reset** button. will clear all the entries in the input page.

(U-1) If the user wishes to use a previously saved configuration file with inputs for the NIST Uncertainty Machine, then use the rectangle outlined with a dashed line in the input page, **Drop configuration file**

**here or click to upload:** either drag the file onto it, or click inside this rectangle and then look for and select the file where the input parameters will have been saved previously. (U-12) explains how to save a configuration file that may be used subsequently to re-run the same computation.

- (U-2) Choose the number of input quantities from the drop-down menu corresponding to the entry **Number of input quantities**. In response to this, the Web page will update itself and show as many boxes as there are input quantities, and assign default names to them (which may be changed as explained next).
- (U-3) Enter the names of the input quantities into the boxes following **Names of input quantities**. The same names will automatically become the labels of the rows of boxes that appear immediately below and that are used to specify probability distributions for the input quantities.
- (U-4) Assign a probability distribution to each of the input quantities using the drop-down menus in front of them. A few commonly used distributions will be readily available. Clicking on **More choices** will reveal others. Once a choice is made, one or more additional input boxes will appear, where values of parameters must be entered fully to specify the probability distribution that was selected. If the choice is **Sample values** (between 30 and 100000), then a rectangle outlined with a dashed line will appear in the same row, saying **Drop sample file here or click to upload**.

Table 2 on Page 13 lists the distributions implemented currently, and their parametrizations. Note that some distributions can be parametrized in any one of several different ways: in such cases, only one of the parametrizations needs to be specified. For example, specifying a rectangular distribution whose left and right end-points are 0.37 and 0.41 is equivalent to specifying a rectangular distribution whose mean is  $(0.34 + 0.42)/2 = 0.38$  and whose standard deviation is  $(0.42 - 0.34)/\sqrt{12} = 0.023$ .

The NIST Uncertainty Machine does not accept standard deviations that are set to 0 — however, this is detected only at run time (after the user will have pressed the button labeled Run the computation). Declaring the standard deviation to be 0 would be equivalent to specifying the value of a constant, which can be done either by entering this value as a numerical constant in the expression that defines the output



quantity (cf. the example in Section 11 that begins on Page 25), or by selecting Constant as distribution type and entering the value of the constant in the corresponding box.

- (U-5) As already mentioned above, the NIST Uncertainty Machine allows the user to provide a sample drawn from the probability distribution of an input quantity instead of selecting a particular distribution from among those that the NIST Uncertainty Machine offers.

To provide such sample, select Sample values (between 30 and 100000) from the drop-down menu with the list of distributions, and then use the rectangle outlined with a dashed line that will have appeared in the input page, in front of the box corresponding to the input quantity, **Drop sample file here or click to upload**: either drag the file onto it, or click it and then look for and select the file containing the sample values.

The data file is then parsed and all the numbers present in it will be loaded. The numerical values may be arranged in the file in any way that is convenient for the user — one or several per line —, but must be separated from one another by any (not necessarily the same throughout the file) non-numeric character or string of non-numeric characters. The numbers may be written either in decimal or scientific notation, and in this case using **e** or **E** to denote the appropriate power of ten. For example, 1983.76 may also be written either as 1.98376e3 or as 1.98376E3. Once the file has been parsed the number of values loaded will be shown to ensure that it matches the user's expectation. The total number of sample values provided in this way, summed across all input quantities for which samples are provided, cannot exceed 2 400 000 approximately. In case this limit is reached, an error message appears once the computation starts.

The NIST Uncertainty Machine operates essentially in the same way regardless of whether parametric distributions are specified, or samples from otherwise unspecified distributions are provided. The main difference is that, for the latter, the NIST Uncertainty Machine resamples the values in the sample that was provided repeatedly, uniformly at random with replacement (that is, all values in the sample provided are equally likely to be drawn, and all are available for drawing when a draw is made). §13 illustrates this feature, and provides additional information about it.

- (U-6) Enter the size of the Monte Carlo sample to be drawn from the probability distribution of the output quantity, into the box labeled **Number of realizations of the output quantity**: the default value,  $1 \times 10^6$ , is the minimum recommended sample size (currently the NIST Uncertainty Machine is able to generate samples of size from  $1 \times 10^5$  to  $5 \times 10^6$ ).
- (U-7) Enter a valid R expression into the box labeled **Value of output quantity (R expression)** that represents  $f(x_1, \dots, x_n)$ , the right-hand side of the measurement equation that defines the value of the output quantity. This expression should involve only the input quantities, functions and numerical constants that R knows how to evaluate, listed on table 1. (Remember that R is case sensitive.) Refer to the current version of *An Introduction to R*, freely available at <https://cran.r-project.org/manuals.html>, or to one of the tutorials listed in <https://cran.r-project.org/other-docs.html>.

+	-	*	^	%%	%/%
/	abs	sign	sqrt	ceiling	floor
trunc	cummax	cummin	cumprod	cumsum	exp
expm1	log	log10	log2	log1p	cos
cosh	sin	sinh	tan	tanh	acos
acosh	asin	asinh	atan	atanh	cospi
sinpi	tanpi	gamma	lgamma	digamma	trigamma
==	<	>	=	pi	complex
Re	Im	Mod	Arg	{	(
c	function	\$	mapply	matrix	%*%
uniroot	t	solve			

Table 1: **Supported functions.** List of functions and operators currently supported by the NIST Uncertainty Machine.

Alternatively, the definition may comprise several R expressions, but with only one expression per line within this box (pressing Enter on the keyboard, with the cursor in this box, creates a new line), and the last expression must evaluate the output quantity (without assigning this value to any variable), or one component of the output quantity when the output quantity is a vector (*cf.* (U-8)).

EXAMPLE. If the measurement model is  $A = (L_1 - L_0)/(L_0(T_1 - T_0))$ , then the R expression that should be entered into this box is  $(L1 - L0)/(L0*(T1 - T0))$ . Alternatively, the box may comprise these three lines:

```

N = L1-L0
D = L0*(T1-T0)
N / D

```

The NIST Uncertainty Machine requires that the measurement function  $f$  be vectorized: that is, if each of its arguments is a vector of length  $K$ , then the value of  $f$ , specified in the last line of the box, must be a vector of length  $K$  such that the  $k$ th element of this vector is the value of  $f$  at the  $k$ th values of all the input quantities. This may not happen automatically for some intricate measurement equations that involve optimizations, root-finding, or solutions of differential equations, among others. In the example described in §13, vectorization is achieved simply by invoking the R function `mapply`, which applies the same function to sets of corresponding values of its arguments.

NOTE. The NIST Uncertainty Machine may report *Impossible to evaluate the output expression*. This may be caused by the use of an R function that the NIST Uncertainty Machine does not recognize yet. When such message is encountered, please send an eMail message to both [thomas.lafarge@nist.gov](mailto:thomas.lafarge@nist.gov) and [antonio.possolo@nist.gov](mailto:antonio.possolo@nist.gov), showing the inputs that induced such response.

- (U-8) If the output quantity is a vector with  $p$  components, press the “+” button  $p - 1$  times to create a total of  $p$  output fields. Enter an R expression into each one of them similarly to how the specification of the value of the output quantity was described in (U-7).
- (U-9) If symmetrical coverage intervals are desired, then select the option marked **Symmetrical coverage intervals**. These intervals take a little longer to compute than those computed by default (which may be asymmetrical), and are of the form  $\hat{y} \pm ku(y)$  where  $\hat{y}$ , the estimate of the output quantity, is the average of the Monte Carlo sample, and the *coverage factor*  $k$  depends on the specified coverage probability.

NOTE. The default coverage interval with coverage probability  $0 < \gamma < 1$  is  $(y_{(1-\gamma)/2}^*, y_{(1+\gamma)/2}^*)$ , whose endpoints are the  $50(1 - \gamma)$ th and  $50(1 + \gamma)$ th percentiles of the Monte Carlo sample drawn from the probability distribution of the output quantity. These need not be equidistant from the average (or from the median) of the sample. The corresponding coverage factor is computed as  $k = (y_{(1+\gamma)/2}^* - y_{(1-\gamma)/2}^*) / (2u(y))$ , and it is not particularly meaningful when the interval is not symmetrical (that is, when it is not centered on the estimate of the output quantity).

Even for symmetrical intervals (those that are centered on the average of the Monte Carlo sample drawn from the probability distribution of the output quantity), the coverage factor  $k$  is computed only after the coverage interval has been derived from this sample, hence differently from how it is computed in the GUM.

- (U-10) If there are non-null correlations between input quantities that need to be taken into account, then select the option marked **Correlations**, and enter the values of non-zero correlations into the appropriate boxes in the upper triangle of the correlation matrix that the browser will display.

NOTE. Not all combinations of values of the correlations that may be entered produce a valid correlation matrix, which must be symmetrical, have all entries between  $-1$  and  $+1$ , and have only positive eigenvalues. The NIST Uncertainty Machine issues an error message (Illegal correlation matrix) if these conditions are not all met.

- (U-11) If **Correlations** has been selected, then besides having specified correlations in (U-10), also select a copula (currently, either Gaussian or Student's  $t$ ) to manufacture a joint probability distribution for the input quantities. This is needed because there are infinitely many multivariate distributions with the same means, standard deviations, and correlations [Nelsen, 2006]. If the copula chosen is (multivariate) Student's  $t$ , then another box will appear nearby to receive the desired number of degrees of freedom.

NOTE. The resulting joint distribution reproduces the correlation structure that has been specified, and has the distributions specified for the input quantities as margins. Possolo [2010] explains and illustrates the role that copulas play in uncertainty analysis.

- (U-12) Click the button labeled **Run the computation**. In response to this, the browser will open a new tab where numerical and graphical results will be displayed, which are described in §5.

The NIST Uncertainty Machine estimates the number of significant digits in the results, and reports only these. To increase the number of significant digits, another run will have to be done with a larger size for the Monte Carlo specified in Number of realizations of the output quantity, as explained in (U-6).

One of the outputs produced by the NIST Uncertainty Machine is a plot showing two probability densities described in §5 and illustrated in Figure 1 on Page 6.

Below this plot there are five clickable links: if the last one, which reads **Download Configuration File**, is clicked, a plain text file named `config.um` is downloaded to the local machine that specifies the inputs that were used. This file may be renamed at will, and reused in a future run of the NIST Uncertainty Machine, as explained in (U-1).

## 5 Results

The NIST Uncertainty Machine produces output on a Web page, and offers the possibility of downloading its output in the form of four files.

- Numerical output appears to the left, and it is divided into two sections. The top section lists results from the application of the Monte Carlo method. The bottom section lists results from the application of the method described in the GUM.

The results for the Monte Carlo method include a table with summary statistics for the sample that was drawn from the probability distribution of the output quantity: average, standard deviation, median, MAD.

The average is the common estimate of the true value of the output quantity, and the standard deviation is the common evaluation of  $u(y)$ . However, the median may be a reasonable, and in some cases a preferable alternative to the average as estimate of that true value. Similarly, MAD may be a reasonable, and in some cases a preferable alternative to the standard deviation as evaluation of  $u(y)$ . When reporting measurement results, it is the user's responsibility to state how the estimate of the true value of the output quantity was obtained, and how the associated standard uncertainty was evaluated.

NOTE. "MAD" denotes the median absolute deviation from the median, multiplied by a factor (1.4826) that makes the result comparable to the standard deviation when applied to samples from Gaussian distributions.

NOTE. Neither the MAD, nor the MAD divided by the square root of the sample size, are the standard deviation of the sampling distribution of the median. For a sample of large size  $n$  drawn from a continuous

NAME	PARAMETERS	CONSTRAINTS
Bernoulli	Prob. of success	$0 < \text{Prob. of success} < 1$
Binomial	Number of trial, Probability	$\text{nb. of trial} \in \mathbb{N}, 0 < \text{Probability} < 1$
Binomial negative	Mean, Dispersion	$\text{Mean} > 0, \text{Dispersion} > 0$
Beta	Mean, StdDev	$0 < \text{Mean} < 1, 0 < \text{StdDev} < \frac{1}{2}$
	Shape1, Shape2	$\text{Shape1} > 0, \text{Shape2} > 0$
Beta – Shifted & Rescaled	Mean, StdDev, Left, Right	$0 < \text{Mean} < 1, 0 < \text{StdDev} < \frac{1}{2}, \text{Left} < \text{Right}$
	Shape1, Shape2, Left, Right	$\text{Shape1} > 0, \text{Shape2} > 0, \text{Left} < \text{Right}$
Chi-Squared	DF	$\text{DF} > 0$
Constant	Value	—
Exponential	Mean	$\text{Mean} > 0$
Gamma	Mean, StdDev	$\text{Mean} > 0, \text{StdDev} > 0$
	Shape, Scale	$\text{Shape} > 0, \text{Scale} > 0$
Gaussian	Mean, StdDev	$\text{StdDev} > 0$
Gaussian – Truncated	Mean, StdDev, Left, Right	$\text{StdDev} > 0, \text{Left} < \text{Right}$
Lognormal	Mean, StdDev	$\text{Mean} > 0, \text{StdDev} > 0$
Poisson	Rate	$\text{Rate} > 0$
Rectangular	Mean, StdDev	$\text{StdDev} > 0$
	Left, Right	$\text{Left} < \text{Right}$
Student's t	Mean, StdDev, DF	$\text{StdDev} > 0, \text{DF} > 2$
	Center, Scale, DF	$\text{Scale} > 0, \text{DF} > 0$
Triangular – Symmetric	Mean, StdDev	$\text{StdDev} > 0$
	Left, Right	$\text{Left} < \text{Right}$
Triangular – Asymmetric	Left, Right, Mode	$\text{Left} \leq \text{Mode} \leq \text{Right}; \text{Left} \neq \text{Right}$
Uniform	Mean, StdDev	$\text{StdDev} > 0$
	Left, Right	$\text{Left} < \text{Right}$
Weibull	Mean, StdDev	$\text{Mean} > 0, \text{StdDev} > 0$
	Shape, Scale	$\text{Shape} > 0, \text{Scale} > 0$

Table 2: **Distributions.** Several distributions are available with alternative parametrizations: for these, it suffices to select and specify one of them. DF stands for number of degrees of freedom. Left and Right denote the left and right endpoints of the interval to which a distribution assigns probability 1. The mode of a distribution is where its probability density reaches its maximum. The rectangular distribution is the same as the uniform distribution. A quantity  $x$  has a shifted and rescaled beta distribution when  $(x - \text{Left})/(\text{Right} - \text{Left})$  has a conventional beta distribution. For the truncated Gaussian distribution, Mean and StdDev denote the mean and standard deviation without truncation: the actual mean and standard deviation depend also on the truncation points, and it is the actual mean and standard deviation that the GUM and Monte Carlo methods use in their calculations. A Student's  $t$  distribution will have infinite standard deviation unless  $\text{DF} > 2$ , and its mean will be undefined unless  $\text{DF} > 1$ . The values assigned to the parameters must satisfy the constraints listed.

distribution with probability density  $g$ , this standard deviation is approximately equal to  $1/(2g(M)\sqrt{n})$ , where  $M$  denotes the true value of the median.

Also listed are coverage intervals with coverage probabilities 99 %, 95 %, 90 %, and 68 %. The interval with 68 % coverage probability is often called a “1-sigma interval”, and the interval with 95 % coverage probability is often called a “2-sigma interval”: however, these designations are appropriate only when the distribution of the output quantity is approximately Gaussian. Next to each interval is listed the value of the corresponding *coverage factor*  $k$  (cf. GUM 3.3.7, and GUM 6.2). The values of  $k$  are equal to one half the length of the interval divided by the standard uncertainty.

If option mentioned in (U-9) above is selected prior to starting the computations then these intervals will be centered on the mean of the sample of values of the output quantity. Otherwise their endpoints will be computed as explained in (U-9).

The section pertaining to the Monte Carlo method concludes with a table of analysis of variance (ANOVA) that lists, for each input quantity, the proportion of  $u^2(y)$  that the source of uncertainty corresponding to the input quantity is responsible for, computed under the assumption that the output quantity is a *linear* function of the input quantities [Lafarge and Possolo, 2015].

The line labeled “Residual” lists the proportion of  $u^2(y)$  that is left unaccounted for when that assumption of linearity does not hold. Therefore, it provides a single-number summary of the accuracy of the approximation to  $u(y)$  given by Gauss’s formula, which is Equation (13) in the GUM (Page 21).

The ANOVA table has two columns: the column labeled “w/out Residual” lists the proportions recomputed out of a total that excludes the portion deemed “residual”. These should be numerically close to the entries in the similar table that appears at the bottom of the section of results from the application of the method described in the GUM.

The results obtained according to the GUM are listed under Gauss’s Formula (GUM’s Linear Approximation). These include an estimate of the true value of the output quantity and an evaluation of the associated standard uncertainty. The former is computed according to Equation (1) in the GUM, and the latter according to Equation (13), where the

values of the partial derivatives are computed using numerical differentiation as implemented in R function `grad` defined in package `numDeriv` [Gilbert and Varadhan, 2016].

Finally, a table shows the *sensitivity coefficients* as defined in the GUM 5.1.3: the values of the first-order partial derivatives of the measurement function  $f$  evaluated at the estimates of the input quantities.

The same table also shows the percentage contributions that the different input quantities make to the squared standard uncertainty of the output quantity. If the input quantities are uncorrelated, then these contributions add up to 100 % approximately. If they are correlated, then the contributions may add up to more or less than 100 %, depending on the absolute values and signs of the correlations: in this case, the line labeled *Correlations* will indicate the percentage of  $u^2(y)$  that is attributable to those correlations (this percentage is positive if  $u^2(y)$  is larger than it would have been in the absence of correlations).

- The plot included in the output Web page depicts an estimate of the probability density of the output quantity (smooth, continuous version of a histogram, drawn in a solid blue line) computed as described by Silverman [1986] and as implemented in R function `density`. The plot also shows (depicted as a red dashed line) the probability density of the Gaussian distribution with the same mean and standard deviation as the Monte Carlo sample of values of the output quantity.
- Below this plot there are five clickable links that, once clicked, download a file to the local machine.

– **Download binary R data file with Monte Carlo values**

**of output quantity:** a binary file with suffix `Rd` is downloaded that contains (in variable `y`) the Monte Carlo sample of values drawn from the probability distribution of the output quantity — it can be loaded into R using the function `load`.

NOTE. When the output quantity is a vector with  $p \geq 2$  components, as contemplated in (U-8), the NIST Uncertainty Machine will first display download links relevant to all the outputs, followed by  $p$  sections, labeled *Output 1*, *Output 2*, ..., each structured as described above. The links just mentioned, will download the values sampled for all  $p$  outputs. When this file with results is loaded into R, a list named `yList` is made available, with  $p$  elements named `y1`, `y2`, ....



- **Download a text file with Monte Carlo values of output quantity:** a plain text file is downloaded that contains the Monte Carlo sample of values drawn from the probability distribution of the output quantity; since preparing this file involves converting the binary file mentioned above into a plain text version, some noticeable time may elapse before the download actually begins.

NOTE. When the output quantity is a vector with  $p \geq 2$  components, as contemplated in (U-8), the NIST Uncertainty Machine will first display download links relevant to all the outputs, followed by  $p$  sections, labeled Output 1, Output 2, ..., each structured as described above. The links just mentioned will download the values sampled for all  $p$  outputs, arranged into a plain text file with as many rows as the sample size of the Monte Carlo sample, and with  $p$  values per line, separated from each other by blank spaces.

- **Download text file with numerical results shown on this page:** a plain text file with the same results and layout of the numerical results shown on the output Web page.
- **Download JPEG file with plot shown on this page:** a JPEG file with the same plot that is displayed on the Web page, showing two probability densities.
- **Download Configuration File:** a plain text file with extension .um that specifies the inputs that were used and that may be reused as explained in (U-1).

## 6 Transparency for Validation & Verification

Given a configuration file produced by the NIST Uncertainty Machine, which has been saved to the user's local machine as explained in (U-12) on Page 12, and passing the file name as an argument to FullScriptNUM.R, should produce the same results as when the same configuration file is loaded into the NIST Uncertainty Machine and run there, provided R has been installed in the local machine.

Suppose the configuration file is called NUMConfigExample.um. (The default extension for configuration files produced by the NIST Uncertainty Machine is .um, but the file name may be any alphanumeric string that is a legal file name under the applicable operating system — embedded blank spaces are discouraged — and does not even have to have an extension.

The following command, executed in a terminal window (under Linux or MacOS), or at the Windows command prompt, will replicate the results that the specified configuration file would produce if loaded into the NIST Uncertainty Machine and run there. (In Windows other than version 10, click Start, type cmd in the box Search programs and files, and press Enter on the keyboard. In Windows 10 choose Command Prompt from the menu that appears after pressing WIN+X or right-clicking on the Start button.) Note that \$ denotes the terminal prompt, hence is not part of the command:

```
$ Rscript FullScriptNUM.R NUMConfigExample.um
```

The script, which is available on the About page of <https://uncertainty.nist.gov/>, will generate 3 files in the current directory or folder, with the same prefix as the configuration file. In the case of the example above, the output files would be:

- NUMConfigExample-results.txt: a plain text file with the same results and layout of the numerical results shown on the NIST Uncertainty Machine's output Web page;
- NUMConfigExample-density.jpg: a JPEG file with the same plot that is displayed on the NIST Uncertainty Machine's output Web page, showing the graphs of two probability densities;
- NUMConfigExample-values.Rd: a binary R data file with the replicates of the input quantities, and with the corresponding values of the output quantity, corresponding to the Monte Carlo method of the GUM-S1. In R, the command `load("NUMConfigExample-values.Rd")` will create as many vectors as there are input quantities, with their names as specified in the configuration file, and a vector named `y` with the values of the output quantity.

The script will install any necessary R packages that may not have been previously installed in the local version of the R system. The script first writes its version number onto the terminal window, which should be matched to the version of the NIST Uncertainty Machine displayed at the top of the page of the web application, for example: NIST Validation & Verification Script Version 1.4

## 7 Example — Thermal Expansion Coefficient

To measure the coefficient of linear thermal expansion of a cylindrical copper bar, the length  $L_0 = 1.4999$  m of the bar was measured with the bar at temperature  $T_0 = 288.15$  K, and then again at temperature  $T_1 = 373.10$  K, yielding  $L_1 = 1.5021$  m. The measurement model is  $A = (L_1 - L_0)/(L_0(T_1 - T_0))$ .

For the purpose of this illustration we will assume that the input quantities are like (scaled and shifted) Student's  $t$  random variables with 3 degrees of freedom, with means equal to the measured values given, and standard deviations  $u(L_0) = 0.0001$  m,  $u(L_1) = 0.0002$  m,  $u(T_0) = 0.02$  K, and  $u(T_1) = 0.05$  K.

This modeling assumption is appropriate when the estimates of the input quantities are averages of 4 determinations made under conditions of repeatability, which may be regarded as samples from Gaussian distributions, and the associated uncertainties result from Type A evaluations, and are what the GUM calls “experimental standard deviation of the mean”, computed according to Equation (5) in the GUM.

To load the specifications for this example into the NIST Uncertainty Machine, click [here](#). The GUM's approach yields  $\alpha = 1.727 \times 10^{-5} \text{ K}^{-1}$  and  $u(\alpha) = 2 \times 10^{-6} \text{ K}^{-1}$ , and the Monte Carlo method reproduces these results. Figure 2 on Page 20 reflects these facts, and lists the results.

## 8 Example — End-Gauge Calibration

In Example H.1 of the GUM (which is reconsidered by [Guthrie et al. \[2009\]](#)), the measurement model is  $l = l_s + d - l_s[(\delta\alpha)\theta + \alpha_s(\delta\theta)]$ , where  $\delta\alpha$  and  $\delta\theta$  each denotes a single input quantity, not a product of two input quantities.

The estimates and standard measurement uncertainties of the input quantities are listed in Table 3. For the Monte Carlo method, we model the input quantities as independent Gaussian random variables with means and standard deviations equal to these estimates and standard measurement uncertainties. To load the specifications for this example into the NIST Uncertainty Machine, click [here](#).

The GUM's approach yields  $l = 50\,000\,838$  nm and  $u(l) = 32$  nm, while the Monte Carlo method reproduces the value for  $l$  but evaluates  $u(l) = 34$  nm. Refer to Figure 3 on Page 21.

The GUM (Page 84) gives (50 000 745 nm, 50 000 931 nm) as an approximate 99 % coverage interval for  $l$ , and the results of the Monte Carlo method confirm this coverage probability. If the user chooses a coverage interval that is proba-

INPUT

1. Select Inputs & Choose Distributions

Number of input quantities: 4

Names of input quantities:  
L0 T0 L1 T1

L0 Student t (Mean, StdDev, No. of degrees of freedom)

1.4999

0.0001

3

T0 Student t (Mean, StdDev, No. of degrees of freedom)

288.15

0.02

3

L1 Student t (Mean, StdDev, No. of degrees of freedom)

1.5021

0.0002

3

T1 Student t (Mean, StdDev, No. of degrees of freedom)

373.10

0.05

3

Correlations

2. Choose Options

Number of realizations of the output quantity: 1000000

Random number generator seed: 5

Symmetrical coverage intervals

3. Write the Definition of Output Quantity

Definition of output quantity (R expression):  
(L1-L0) / (L0\*(T1-T0))

Run the computation

OUTPUT

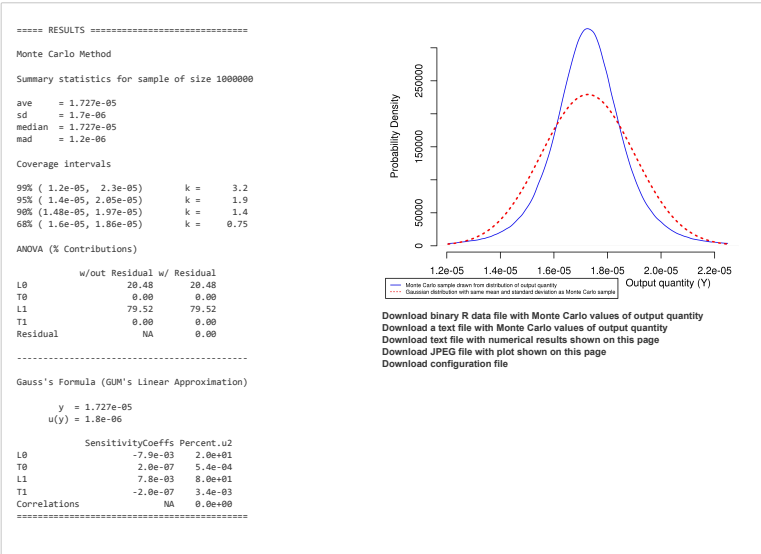


Figure 2: Thermal Expansion Coefficient. Input and output Web pages for the example discussed in §7.

QUANTITY	$x$	$u(x)$
$l_S$	50 000 623 nm	25 nm
$d$	215 nm	9.7 nm
$\delta\alpha$	$0\text{ }^{\circ}\text{C}^{-1}$	$0.58 \times 10^{-6}\text{ }^{\circ}\text{C}^{-1}$
$\theta$	$-0.1\text{ }^{\circ}\text{C}$	$0.41\text{ }^{\circ}\text{C}$
$\alpha_S$	$11.5 \times 10^{-6}\text{ }^{\circ}\text{C}^{-1}$	$1.2 \times 10^{-6}\text{ }^{\circ}\text{C}^{-1}$
$\delta\theta$	$0\text{ }^{\circ}\text{C}$	$0.029\text{ }^{\circ}\text{C}$

Table 3: **End-Gauge Calibration.** Estimates and standard measurement uncertainties for the input quantities in the measurement model of Example H.1 in the GUM.

bilistically symmetric (meaning that it leaves 0.5 % of the Monte Carlo sample uncovered on both sides), then the Monte Carlo method produces (50 000 749 nm, 50 000 927 nm) as 99 % coverage interval, which happens not be quite centered at the estimate of  $y$ .

## 9 Example — Dynamic Viscosity

The dynamic viscosity  $\mu_M$  of a solution of sodium hydroxide in water at  $20\text{ }^{\circ}\text{C}$ , is measured using a boron silica glass ball of mass density  $\rho_B = 2217\text{ kg/m}^3$ , with measurement equation  $\mu_M = \mu_C[(\rho_B - \rho_M)/(\rho_B - \rho_C)](t_M/t_C)$ , where  $\mu_C = 4.63\text{ mPa}\cdot\text{s}$ ,  $\rho_C = 810\text{ kg/m}^3$ , and  $t_C = 36.6\text{ s}$  denote the viscosity, mass density, and ball travel time for the calibration liquid, and  $\rho_M = 1180\text{ kg/m}^3$  and  $t_M = 61\text{ s}$  denote the mass density and ball travel time for the sodium hydroxide solution.

To load the specifications for this example into the NIST Uncertainty Machine, click [here](#).

If the input quantities are modeled as independent Gaussian random variables with means equal to their assigned values, and standard deviations equal to their associated standard uncertainties  $u(\mu_C) = 0.01\mu_C$ ,  $u(\rho_B) = u(\rho_C) = u(\rho_M) = 0.5\text{ kg/m}^3$ ,  $u(t_C) = 0.15t_C$ , and  $u(t_M) = 0.10t_M$ , then the Monte Carlo method of the GUM-S1 as implemented in the NIST Uncertainty Machine produces:  $\hat{\mu}_M = 5.8\text{ mPa}\cdot\text{s}$ ,  $u(\mu_M) = 1.12\text{ mPa}\cdot\text{s}$ , and  $[4.05\text{ mPa}\cdot\text{s}, 8.4\text{ mPa}\cdot\text{s}]$  as an approximate 95 % coverage interval for  $\mu_M$ . This interval is asymmetric relative to the estimate  $\hat{\mu}_M$ .

If, instead, the estimates of the input quantities were substituted into the measurement equation, the resulting estimate of  $\mu_M$  would have been  $5.69\text{ mPa}\cdot\text{s}$ .

## INPUT

1. Select Inputs & Choose Distributions

Number of input quantities:

Names of input quantities:

IS

IS

d

dalphi

theta

alphaS

dtheta

Correlations

2. Choose Options

Number of realizations of the output quantity:

Random number generator seed:

Symmetrical coverage intervals

3. Write the Definition of Output Quantity

Definition of output quantity (R expression):

Run the computation

## OUTPUT

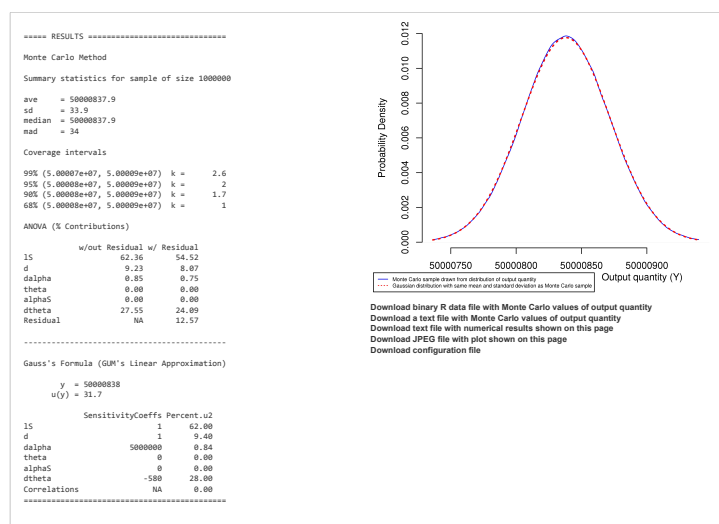


Figure 3: **End-Gauge Calibration.** Input and output Web pages for the example discussed in §8. Note that the value of  $\alpha_S$ ,  $11.5 \times 10^{-6} \text{ }^\circ\text{C}^{-1}$ , was entered as 11.5e-6.

And if Gauss's formula is used to evaluate  $u(\mu_M)$ , the result is 1.11 mPa s.

Interestingly, the evaluation of  $u(\mu_M)$  is close to the evaluation produced by the Monte Carlo method, but the estimates of the measurand produced by one and by the other differ: the reason is the skewness (or, asymmetry) of the distribution of the measurand, apparent in Figure 4 on Page 23.

This figure also shows that the coverage interval given above differs from the interval corresponding to the prescription in clause 6.2.1 of the GUM (estimate of the output quantity plus or minus twice the standard measurement uncertainty evaluated using the approximate propagation of error formula). Figure 5 on Page 24 shows the corresponding input and output Web pages of the NIST Uncertainty Machine.

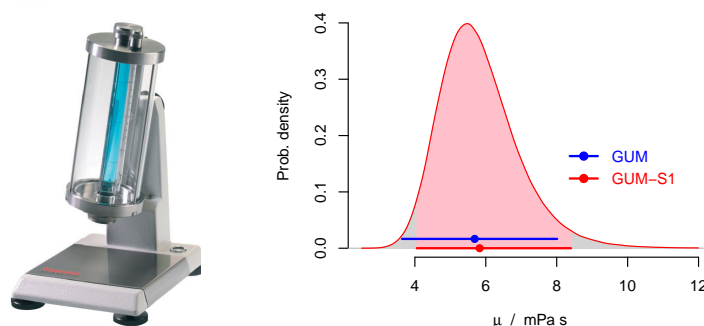


Figure 4: HAAKE™ falling ball viscometer from Thermo Fisher Scientific, Inc., (left panel), and probability density (right panel) corresponding to a Monte Carlo sample of size  $1 \times 10^6$ , also showing 95 % coverage intervals for the value of the dynamic viscosity of the liquid, one corresponding to the prescription in clause 6.2.1 of the GUM, the other whose endpoints are the 2.5th and 97.5th percentiles of the Monte Carlo sample.

## 10 Example — Resistance

In Example H.2 of the GUM, the measurement model for the resistance of an element of an electrical circuit is  $R = (V/I) \cos(\phi)$ . The estimates and standard uncertainties of the input quantities, and the correlations between them, are listed in Table 4 on Page 23.

For the Monte Carlo method, we model the input quantities as correlated Gaussian random variables with means and standard deviations equal to the esti-

INPUT

1. Select Inputs & Choose Distributions

Number of input quantities: 6

Names of input quantities:

muC

rhoB

rhoM

rhoC

tM

tC

muC

Gaussian (Mean, StdDev)

4.63

0.0463

rhoB

Gaussian (Mean, StdDev)

2217

0.5

rhoM

Gaussian (Mean, StdDev)

1180

0.5

rhoC

Gaussian (Mean, StdDev)

810

0.5

tM

Gaussian (Mean, StdDev)

61

6.1

tC

Gaussian (Mean, StdDev)

36.6

5.49

Correlations

2. Choose Options

Number of realizations of the output quantity: 1000000

Random number generator seed: 5

Symmetrical coverage intervals

3. Write the Definition of Output Quantity

Definition of output quantity (R expression):

muC \* ((rhoB-rhoM)/(rhoB-rhoC)) \* (tM/tC)

-

+

Run the computation

OUTPUT

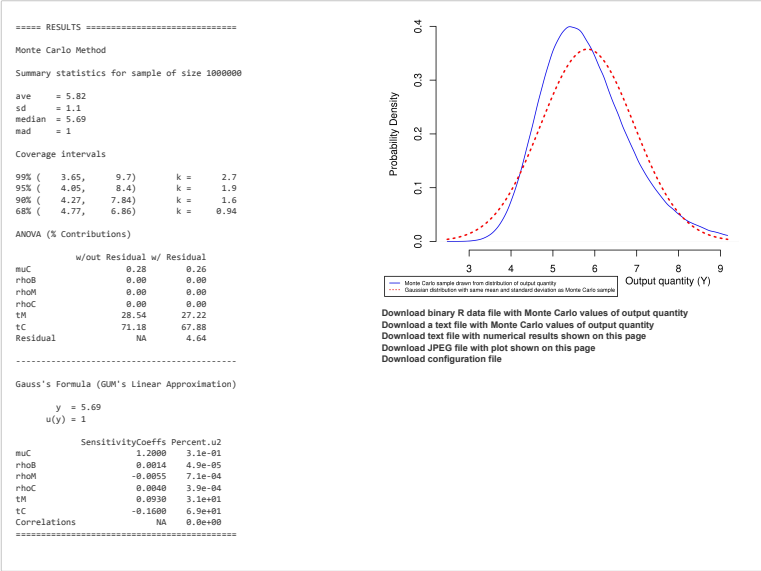


Figure 5: Viscosity. Input and output Web pages for the example discussed in §9.



mates and standard uncertainties listed in Table 4, and with correlations identical to those given in the same table. We also adopt a Gaussian copula to manufacture a joint probability distribution consistent with the assumptions already stated.

To load the specifications for this example into the NIST Uncertainty Machine, click [here](#).

QUANTITY	$x$	$u(x)$
$V$	4.9990 V	0.0032 V
$I$	$19.6610 \times 10^{-3}$ A	$0.0095 \times 10^{-3}$ A
$\phi$	1.044 46 rad	0.000 75 rad
$r(V, I) = -0.36$	$r(V, \phi) = 0.86$	$r(I, \phi) = -0.65$

Table 4: **Resistance.** Estimates and standard measurement uncertainties for the input quantities in the measurement model of Example H.2 in the GUM, and correlations between them, all as listed in Table H.2 of the GUM.

The GUM’s approach and the Monte Carlo method produce the same values of the output quantity  $R = 127.732 \Omega$  and of the standard uncertainty  $u(R) = 0.07 \Omega$ . The Monte Carlo method yields  $(127.595 \Omega, 127.869 \Omega)$  as approximate 95 % coverage interval for the resistance without invoking any additional assumptions about  $R$ . Figure 6 on Page 26 reflects these facts, and lists the results.

## 11 Example — Stefan-Boltzmann Constant

The functional relation used to define the Stefan-Boltzmann constant  $\sigma$  involves the Planck constant  $h$ , the molar gas constant  $R$ , Rydberg’s constant  $R_\infty$ , the relative atomic mass of the electron  $A_r(e)$ , the molar mass constant  $M_u$ , the speed of light in vacuum  $c$ , and the fine-structure constant  $\alpha$ :

$$\sigma = \frac{32\pi^5 h R^4 R_\infty^4}{15 A_r(e)^4 M_u^4 c^6 \alpha^8}. \quad (1)$$

Note that the Greek letter that is conventionally used to denote the Stefan-Boltzmann constant is the same that is also commonly used to denote the standard deviation of a probability distribution. In this example, all instances of “ $\sigma$ ” refer to the Stefan-Boltzmann constant.

Table 5 lists the 2010 CODATA [Mohr et al., 2012] recommended values of the quantities that determine the value of the Stefan-Boltzmann constant, and the

## INPUT

1. Select Inputs & Choose Distributions

Number of input quantities: 3

Names of input quantities:

V I phi

V Gaussian (Mean, StdDev) 4.9990 0.0032

I Gaussian (Mean, StdDev) 19.6610e-3 0.0095e-3

phi Gaussian (Mean, StdDev) 1.04446 0.00075

Correlations

	V	I	phi
V	1	-0.36	0.86
I		1	-0.65
phi			1

Gaussian Copula

2. Choose Options

Number of realizations of the output quantity: 1000000

Random number generator seed: 5

Symmetrical coverage intervals

3. Write the Definition of Output Quantity

Definition of output quantity (R expression):

$(V/I) * \cos(\phi)$

Run the computation

## OUTPUT

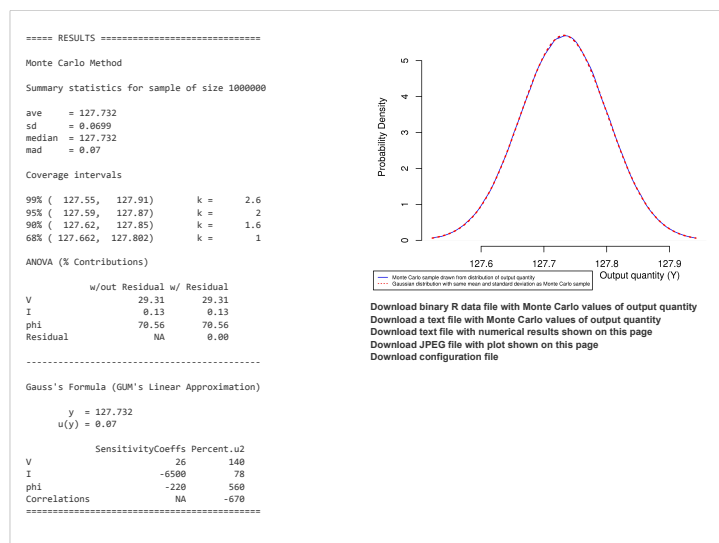


Figure 6: **Resistance**. Input and output Web pages for the example discussed in §10. Note that, in this case, the NIST Uncertainty Machine reconfigured its graphical user interface automatically to accommodate the correlations that had to be specified.

measurement uncertainties associated with them. To load the specifications for this example into the NIST Uncertainty Machine, click [here](#).

	VALUE	STD. MEAS. UNC.	UNIT
$h$	$6.62606957 \times 10^{-34}$	$0.00000029 \times 10^{-34}$	J s
$R$	8.3144621	0.0000075	J mol <sup>-1</sup> K <sup>-1</sup>
$R_\infty$	10973731.568539	0.000055	m <sup>-1</sup>
$A_r(e)$	$5.4857990946 \times 10^{-4}$	$0.000000022 \times 10^{-4}$	u
$M_u$	$1 \times 10^{-3}$	0	kg/mol
$c$	299792458	0	m/s
$\alpha$	$7.2973525698 \times 10^{-3}$	$0.000000024 \times 10^{-3}$	1

Table 5: **Stefan-Boltzmann.** 2010 CODATA recommended values and standard measurement uncertainties for the quantities used to define the value of the Stefan-Boltzmann constant. Once the international system of units (SI) will have been redefined (expected in 2018), the value of  $h$  will be fixed and the associated standard uncertainty will become 0 J s [Newell et al., 2018].

According to the GUM, the estimate of the measurand equals the value of the measurement function evaluated at the estimates of the input quantities, as  $\sigma = 5.67037 \times 10^{-8} \text{ W m}^{-2} \text{ K}^{-4}$ . Both the GUM's approximation and the Monte Carlo method produce the same evaluation of  $u(\sigma) = 2 \times 10^{-13} \text{ W m}^{-2} \text{ K}^{-4}$ .

These evaluations disregard the correlations between the input quantities that result from the adjustment process used by CODATA. However, once these correlations are taken into account via Equation (13) in the GUM, the same value still obtains for  $u(\sigma)$  to within the single significant digit reported above.

Without making additional assumptions, it is impossible to interpret an expression like  $\sigma \pm u(\sigma)$  probabilistically. The assumptions made to apply the Monte Carlo method of the GUM-S1 deliver not only an evaluation of uncertainty, but also enable its probabilistic interpretation.

If the measurement uncertainties associated with  $h$ ,  $R$ ,  $R_\infty$ ,  $A_r(e)$ , and  $\alpha$  are expressed by modeling these quantities as independent Gaussian random variables with means and standard deviations set equal to the values and standard measurement uncertainties listed in Table 5, then the distribution that the Monte Carlo method of the GUM-S1 assigns to the measurand happens to be approximately Gaussian as gauged by the Anderson-Darling test of Gaussian shape [Anderson and Darling, 1952].

Figure 7 on Page 28 reflects these facts and shows the results, which imply that the interval from  $5.670332 \times 10^{-8} \text{ W m}^{-2} \text{ K}^{-4}$  to  $5.6704126 \times 10^{-8} \text{ W m}^{-2} \text{ K}^{-4}$

is a coverage interval for  $\sigma$  with approximate 95 % coverage probability.

Two of the inputs,  $M_u$  and  $c$ , have zero standard uncertainty. Since the NIST Uncertainty Machine requires standard deviations to be strictly positive, the user may either assign very small values to them, or they may be removed from the list of input quantities and their values entered as constants in the expression that defines the output quantity, as shown in the upper panel of Figure 7 on Page 28.

## 12 Example — Voltage Reflection Coefficient

Tsui et al. [2012] consider the voltage reflection coefficient  $\Gamma = S_{22} - S_{12}S_{23}/S_{13}$  of a microwave power splitter, defined as a function of elements of the corresponding 3-port scattering matrix (*S-parameters*). Table 6 reproduces the measurement results for the S-parameters listed in Tsui et al. [2012, Table 5]. Since the S-parameters (input quantities) are complex-valued, so is  $\Gamma$  (output quantity). Therefore, in this example the measurement model is a measurement equation with a vector-valued output quantity,  $(\Re(\Gamma), \Im(\Gamma))$ , whose components are the real and imaginary parts of  $\Gamma$ .

	Mod( $S$ )	$u(\text{Mod}(S))$	Arg( $S$ )	$u(\text{Arg}(S))$
$S_{22}$	0.24776	0.00337	4.88683	0.01392
$S_{12}$	0.49935	0.00340	4.78595	0.00835
$S_{23}$	0.24971	0.00170	4.85989	0.00842
$S_{13}$	0.49952	0.00340	4.79054	0.00835

Table 6: S-parameters expressed in polar form, and associated standard uncertainties, with Arg( $S$ ) and  $u(\text{Arg}(S))$  expressed in radian.

The NIST Uncertainty Machine can handle vectorial output quantities. Additional output fields are added by clicking the “+” button as explained in (U-8) on Page 11. The NIST Uncertainty Machine produces the raw materials that are necessary to characterize the uncertainty of a multivariate output by application of the Monte Carlo method, but it does not provide a full characterization of the uncertainty surrounding the multivariate output.

If  $\mathbf{y} = \mathbf{f}(x_1, \dots, x_n)$  is the measurement model for a  $p$ -dimensional output quantity  $\mathbf{y} = (y_1, \dots, y_p)$ , then the model may be re-written as a system of  $p$  simul-

INPUT

1. Select Inputs & Choose Distributions

Number of input quantities: 5

Names of input quantities:

h

R

Rinf

e

alpha

h

Gaussian (Mean, StdDev)

6.62606957e-34

0.00000029e-34

R

Gaussian (Mean, StdDev)

8.3144621

0.0000075

Rinf

Gaussian (Mean, StdDev)

10973731.56853

0.000055

e

Gaussian (Mean, StdDev)

5.4857990946e-

0.0000000022e-

alpha

Gaussian (Mean, StdDev)

7.2973525698e-

0.0000000024e-

Correlations

2. Choose Options

Number of realizations of the output quantity: 1000000

Random number generator seed: 5

Symmetrical coverage intervals

3. Write the Definition of Output Quantity

Definition of output quantity (R expression):

N = 32 \* (p1^5) \* h \* (R^4) \* (Rinf^4)

D = 15 \* (e^4) \* ((1e-3)^4) \* (299792458^6) \* (alpha^8)

N / D

Run the computation

OUTPUT

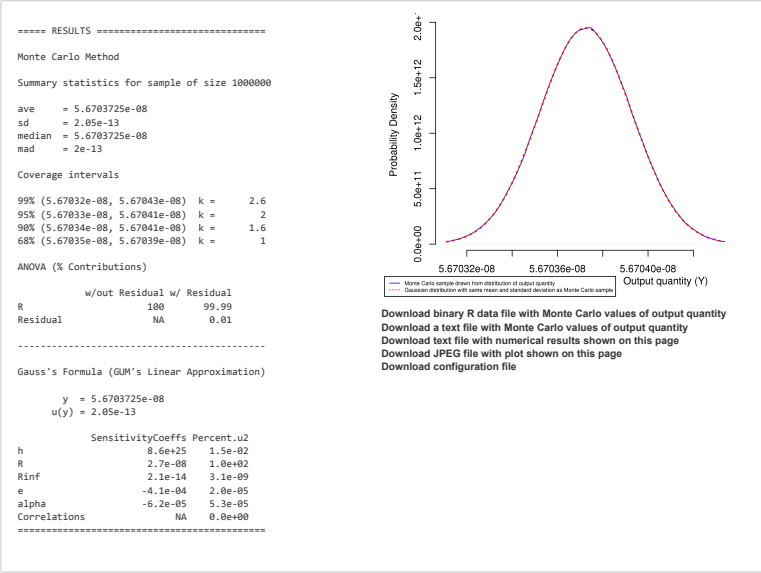


Figure 7: Stefan-Boltzmann Constant. Input and output Web pages for the example discussed in §11.

taneous measurement equations  $y_1 = f_1(x_1, \dots, x_n), \dots, y_p = f_p(x_1, \dots, x_n)$ , where  $f = (f_1, \dots, f_p)$ . The recommended procedure then is this:

- (i) Run the NIST Uncertainty Machine with each output in its own field, and save the file containing the samples drawn from the probability distributions of the  $p$  components  $y_1, \dots, y_p$  of the vectorial output quantity;
- (ii) Read this file into some suitable statistical analysis computing environment, for example R, and complete the uncertainty analysis for the output quantity in this environment.

The S-parameters are assumed to be independent, complex-valued random variables. The modulus and argument of each S-parameter are modeled as independent Gaussian random variables with mean and standard deviation equal to the value and standard uncertainty listed in Exhibit 6. (Note that the results would be different if the same modeling assumptions were made for the real and imaginary parts of the S-parameters instead.)

The real and imaginary parts of  $\Gamma$  are functions of the same eight input quantities, which are the moduli and arguments of the four S-parameters, hence in this case  $p = 2$  and the components of the bivariate output quantity are:  $\Re(\Gamma) = f_1(M_{22}, A_{22}, M_{12}, A_{12}, M_{23}, A_{23}, M_{13}, A_{13})$ , and  $\Im(\Gamma) = f_2(M_{22}, A_{22}, M_{12}, A_{12}, M_{23}, A_{23}, M_{13}, A_{13})$ . Figure 8 on Page 30 shows the corresponding input Web page of the NIST Uncertainty Machine, including the definition of the functions  $f_1$  and  $f_2$ .

To load the specifications for this example into the NIST Uncertainty Machine, click [here](#).

It is also possible to incorporate correlations between the S-parameters, as well as correlations between the modulus and argument of any of the S-parameters, by specifying a suitable correlation matrix and applying it via one of the copulas [Possolo, 2010] that is available in the NIST Uncertainty Machine. Neither was done in this case.

Once the Monte Carlo samples of the two components of the output quantity,  $\Re(\Gamma)$  and  $\Im(\Gamma)$ , will have been downloaded and saved, they may be imported into any statistical computing application to characterize the uncertainty associated with  $\Gamma$ , for example as depicted in Figure 9 on Page 32, and as illustrated in Listing 1. The estimate of  $\Re(\Gamma)$  is 0.0074 and  $u(\Re(\Gamma)) = 0.0050$ . The estimate of  $\Im(\Gamma)$  is 0.0031 and  $u(\Im(\Gamma)) = 0.0045$ . The correlation between  $\Re(\Gamma)$  and  $\Im(\Gamma)$  is 0.0311.

**1. Select Inputs & Choose Distributions**

Number of input quantities:

Names of input quantities:

S22.Mod	S22.Arg	S12.Mod	S12.Arg	S23.Mod	S23.Arg	S13.Mod	S13.Arg
S22.Mod	Gaussian (Mean, StdDev)	0.24776	0.00337				
S22.Arg	Gaussian (Mean, StdDev)	4.86883	0.01392				
S12.Mod	Gaussian (Mean, StdDev)	0.49935	0.00340				
S12.Arg	Gaussian (Mean, StdDev)	4.78595	0.00835				
S23.Mod	Gaussian (Mean, StdDev)	0.24971	0.00170				
S23.Arg	Gaussian (Mean, StdDev)	4.85989	0.00842				
S13.Mod	Gaussian (Mean, StdDev)	0.49952	0.00340				
S13.Arg	Gaussian (Mean, StdDev)	4.79054	0.00835				

Correlations

**2. Choose Options**

Number of realizations of the output quantity:

Random number generator seed:

Symmetrical coverage intervals

**3. Write the Definition of Output Quantity**

Definition of output quantity (R expression):

```

S22 = complex(modulus=S22.Mod, argument=S22.Arg)
S12 = complex(modulus=S12.Mod, argument=S12.Arg)
S23 = complex(modulus=S23.Mod, argument=S23.Arg)
S13 = complex(modulus=S13.Mod, argument=S13.Arg)
Gamma = S22 * S12 * S23 / S13
Re(Gamma)

```

Figure 8: **Voltage Reflection Coefficient.** Input Web page of the NIST Uncertainty Machine used for the real and imaginary parts of the complex-valued output quantity  $\Gamma$  discussed in §12.

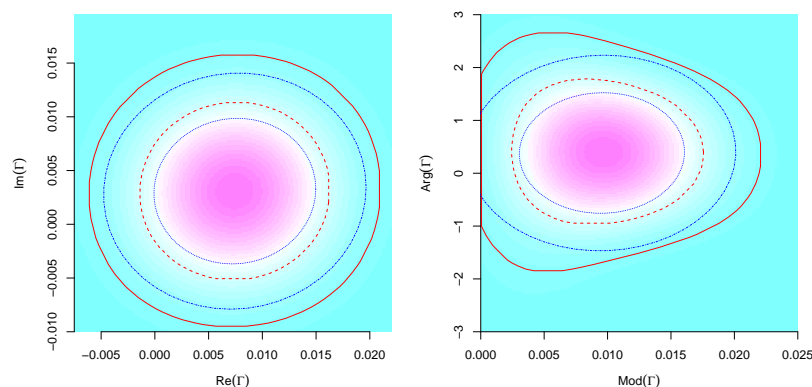


Figure 9: The left panel shows an estimate of the probability density of the joint distribution of the real and imaginary parts of  $\Gamma$ , and the right panel shows its counterpart for the modulus and argument of  $\Gamma$ . The solid (red) curves outline 95 % coverage regions, and the dashed (red) curves outline 68 % coverage regions. Their (blue) counterparts, dotted and dash-dotted, are based on the (obviously erroneous) assumption that the joint bivariate distributions are Gaussian.

#### Listing 1: R code used to characterize the uncertainty associated with $\Gamma$

```
## Read values of output quantities produced in the two runs
## of the NIST Uncertainty Machine, assuming that R's
## current working directory is the same that contains
## the files with the values of the output quantities

Gamma.Re = scan("NUM-Gamma-Real-Results-Values.txt")
Gamma.Im = scan("NUM-Gamma-Imaginary-Results-Values.txt")

Gamma.Mod = Mod(complex(real=Gamma.Re, imaginary=Gamma.Im))
Gamma.Arg = Arg(complex(real=Gamma.Re, imaginary=Gamma.Im))

c(mean(Gamma.Re), sd(Gamma.Re))
c(mean(Gamma.Im), sd(Gamma.Im))
cor(Gamma.Re, Gamma.Im)

require(ash)
require(car)

par(mfrow=c(1,2), mar=c(4.5, 4.5, 1.5, 1.5))

## Estimate the probability density of the bivariate
```



```

## joint distribution of the real and imaginary parts
## of the complex-valued measurand Gamma

ab = cbind(Gamma.Re, Gamma.Im)
abx = matrix(c(-0.0075, -0.0100, 0.0220, 0.0195), 2, 2)
nbin = c(200, 200)
bins = bin2(ab, abx, nbin)
m = c(60,60)
f = ash2(bins,m)
image(f$x, f$y, f$z, col=cm.colors(24), axes=FALSE,
      xlab=expression(plain(Re)(Gamma)),
      ylab=expression(plain(Im)(Gamma)))
axis(1, lwd=0.5); axis(2, lwd=0.5)

## Normalize bivariate probability density estimate
## that has been computed over each cell of a
## 200x200 grid, and determine the order of the cells
## according to decreasing values of their corresponding
## probabilities

w = (f$z[-length(f$z)]*diff(f$x)*diff(f$y)) /
     sum(f$z[-length(f$z)]*diff(f$x)*diff(f$y))
iw = order(w, decreasing=TRUE)

## Determine the boundary of the smallest subset
## of the cells whose total probability is 0.95

iw95 = which.min(abs(cumsum(w[iw]))-0.95))
xx = matrix(rep(f$x, 200), ncol=200)
yy = matrix(rep(f$y, 200), ncol=200, byrow=TRUE)
xx = xx[iw][1:iw95]
yy = yy[iw][1:iw95]
ixy = chull(xx, yy)
lines(c(xx[ixy], xx[ixy][1]),
      c(yy[ixy], yy[ixy][1]), col="Red")

## Determine the boundary of the smallest subset
## of the cells whose total probability is 0.68

iw68 = which.min(abs(cumsum(w[iw]))-0.68))
xx = matrix(rep(f$x, 200), ncol=200)
yy = matrix(rep(f$y, 200), ncol=200, byrow=TRUE)
xx = xx[iw][1:iw68]
yy = yy[iw][1:iw68]
ixy = chull(xx, yy)
lines(c(xx[ixy], xx[ixy][1]),
      c(yy[ixy], yy[ixy][1]), col="Red", lty=2)

## Determine the ellipses that contain 95% or 68% of
## the replicates of Gamma, assuming that the bivariate
## distributions are Gaussian

dataEllipse(Gamma.Re, Gamma.Im, levels=0.68,
            add=TRUE, plot.points=FALSE, center.cex=0,
            col="Blue", lty=3, lwd=0.5)
dataEllipse(Gamma.Re, Gamma.Im, levels=0.95,

```

```

        add=TRUE, plot.points=FALSE, center.cex=0,
        col="Blue", lty=4, lwd=0.5)

## Estimate the probability density of the bivariate
## joint distribution of the modulus and argument of
## the complex-valued measurand Gamma

ab = cbind(Gamma.Mod, Gamma.Arg)
abx = matrix(c(0, -3, 0.025, 3), 2, 2)
nbin = c(200, 200)
bins = bin2(ab, abx, nbin)
m = c(60,60)
f = ash2(bins,m)
image(f$x, f$y, f$z, col=cm.colors(24), axes=FALSE,
      xlab=expression(plain(Mod)(Gamma)),
      ylab=expression(plain(Arg)(Gamma)))
axis(1, lwd=0.5); axis(2, lwd=0.5)

## Normalize bivariate probability density estimate
## that has been computed over each cell of a
## 200x200 grid, and determine the order of the cells
## according to decreasing values of their corresponding
## probabilities

w = (f$z[-length(f$z)]*diff(f$x)*diff(f$y)) /
    sum(f$z[-length(f$z)]*diff(f$x)*diff(f$y))
iw = order(w, decreasing=TRUE)

## Determine the boundary of the smallest subset
## of the cells whose total probability is 0.95

iw95 = which.min(abs(cumsum(w[iw])-0.95))
xx = matrix(rep(f$x, 200), ncol=200)
yy = matrix(rep(f$y, 200), ncol=200, byrow=TRUE)
xx = xx[iw][1:iw95]
yy = yy[iw][1:iw95]
ixy = chull(xx, yy)
lines(c(xx[ixy], xx[ixy][1]),
      c(yy[ixy], yy[ixy][1]), col="Red")

## Determine the boundary of the smallest subset
## of the cells whose total probability is 0.68

iw68 = which.min(abs(cumsum(w[iw])-0.68))
xx = matrix(rep(f$x, 200), ncol=200)
yy = matrix(rep(f$y, 200), ncol=200, byrow=TRUE)
xx = xx[iw][1:iw68]
yy = yy[iw][1:iw68]
ixy = chull(xx, yy)
lines(c(xx[ixy], xx[ixy][1]),
      c(yy[ixy], yy[ixy][1]), col="Red", lty=2)

## Determine the ellipses that contain 95% or 68% of
## the replicates of Gamma, assuming that the bivariate
## distributions are Gaussian

```

---

```
dataEllipse(Gamma.Mod, Gamma.Arg, levels=0.68,
            add=TRUE, plot.points=FALSE, center.cex=0,
            col="Blue", lty=3, lwd=0.5)
dataEllipse(Gamma.Mod, Gamma.Arg, levels=0.95,
            add=TRUE, plot.points=FALSE, center.cex=0,
            col="Blue", lty=4, lwd=0.5)
```

---

### 13 Example — Age of Allende Meteorite

*A blinding blue-white fireball, possibly a meteor, turned night into day across Mexico and the southwestern United States early today, then apparently dropped to earth — Washington Post, February 9, 1969.*

Table 7 lists isotopic ratios and associated uncertainties for several samples drawn from two chondrules of the Allende meteorite [Clarke et al., 1971], to measure their absolute age using a geochronometer based on isotopic ratios of radiogenic lead.

The original data, from Table S4 of Connelly et al. [2012], comprise values of  $R(^{204}\text{Pb}/^{206}\text{Pb})$ ,  $R(^{207}\text{Pb}/^{206}\text{Pb})$ , and relative expanded uncertainties (with coverage factor  $k = 2$ ) expressed as percentages. The isotopic ratios listed in Table 7 were derived from these as  $R(^{206}\text{Pb}/^{204}\text{Pb}) = 1/R(^{204}\text{Pb}/^{206}\text{Pb})$  and  $R(^{207}\text{Pb}/^{204}\text{Pb}) = R(^{207}\text{Pb}/^{206}\text{Pb})R(^{206}\text{Pb}/^{204}\text{Pb})$ .

The standard uncertainties listed in Table 7 were derived from the expanded uncertainties in [Connelly et al., 2012, Table S4], by application of the Monte Carlo method, modeling the isotopic ratios as Gaussian random variables, and taking into account the correlation between  $R(^{204}\text{Pb}/^{206}\text{Pb})$  and  $R(^{207}\text{Pb}/^{206}\text{Pb})$  also listed in the aforementioned Table S4. The standard uncertainties listed are the median absolute deviations from the median, rescaled as per the default definition of R function mad.

Since  $^{206}\text{Pb}$  and  $^{207}\text{Pb}$  both are radiogenic, being the end-products of the decay of  $^{235}\text{U}$  and  $^{238}\text{U}$ , respectively, and  $^{204}\text{Pb}$  is primordial, the isotopic ratios in Table 7 may be used as a geochronometer [White, 2015], under the following assumptions:

- (a) The isotopic ratio  $R(^{238}\text{U}/^{235}\text{U})$  of the parent material is known;
- (b) All atoms of  $^{206}\text{Pb}$  and  $^{207}\text{Pb}$  derive entirely from uranium originally in the parent material, and none have been lost;

SAMPLE	$^{206}\text{Pb}/^{204}\text{Pb}$		$^{207}\text{Pb}/^{204}\text{Pb}$	
	$R$	$u(R)$	$R$	$u(R)$
C20-L4	22.012	0.018	18.223	0.014
C20-L5	33.078	0.043	25.145	0.028
C20-L7	55.066	0.220	38.880	0.140
C20-L8	91.684	0.348	61.765	0.219
C20-L9	217.155	5.695	140.222	3.572
C20-LR	172.028	9.454	112.025	5.969
C30-L2	23.265	0.021	18.996	0.015
C30-L5	31.195	0.056	23.958	0.036
C30-L7	59.726	0.083	41.801	0.050
C30-L8	77.310	0.054	52.799	0.033
C30-L9	97.437	0.156	65.392	0.096
C30-LR	232.829	12.658	150.096	7.929

Table 7: **Allende Meteorite**. Isotopic ratios and associated uncertainties derived from measurements made and reported by [Connolly et al. \[2012\]](#). “ $R$ ” denotes either  $R(^{206}\text{Pb}/^{204}\text{Pb})$  or  $R(^{207}\text{Pb}/^{204}\text{Pb})$ , which refer to ratios of numbers of atoms of the isotopes of lead indicated. The samples listed, from chondrules C20 and C30, are those that [Connolly et al. \[2012\]](#) selected for their age determinations.

- (c) No atoms of  $^{204}\text{Pb}$  have been added or removed from the chondrules since their formation.

The absolute age  $A$  is the root of the equation

$$\frac{\exp(A\lambda_{235}) - 1}{\exp(A\lambda_{238}) - 1} = \beta R(^{238}\text{U}/^{235}\text{U}), \quad (2)$$

where  $\lambda_{235}$  and  $\lambda_{238}$  denote the decay constants of  $^{235}\text{U}$  and  $^{238}\text{U}$ , and  $\beta$  denotes the slope of the line (*isochron*) shown in Figure 10 [[Schoene, 2014](#)].

To compute estimates of the absolute age we use Equation (2) with  $\lambda_{235} = \log 2 / T_{1/2}(^{235}\text{U})$ ,  $\lambda_{238} = \log 2 / T_{1/2}(^{238}\text{U})$ , and  $R(^{238}\text{U}/^{235}\text{U}) = 137.786$  [[Connolly et al., 2012](#), Table 1]. This last value is noticeably different from the value, 137.818, usually accepted for terrestrial materials [[Hiess et al., 2012](#)]. The half-lives are  $T_{1/2}(^{235}\text{U}) = 704 \text{ Ma}$  [[Bé et al., 2010](#)] and  $T_{1/2}(^{238}\text{U}) = 4468.3 \text{ Ma}$  [[Villa et al., 2016](#)].

The isochron has slope  $\beta = 0.6253$ , computed by (Gaussian maximum likelihood) errors-in-variables regression that takes the uncertainty in both isotopic ratios into account, with associated standard uncertainty  $u(\beta) = 0.0028$  (which expresses contributions only from sources (c) and (d) listed below).

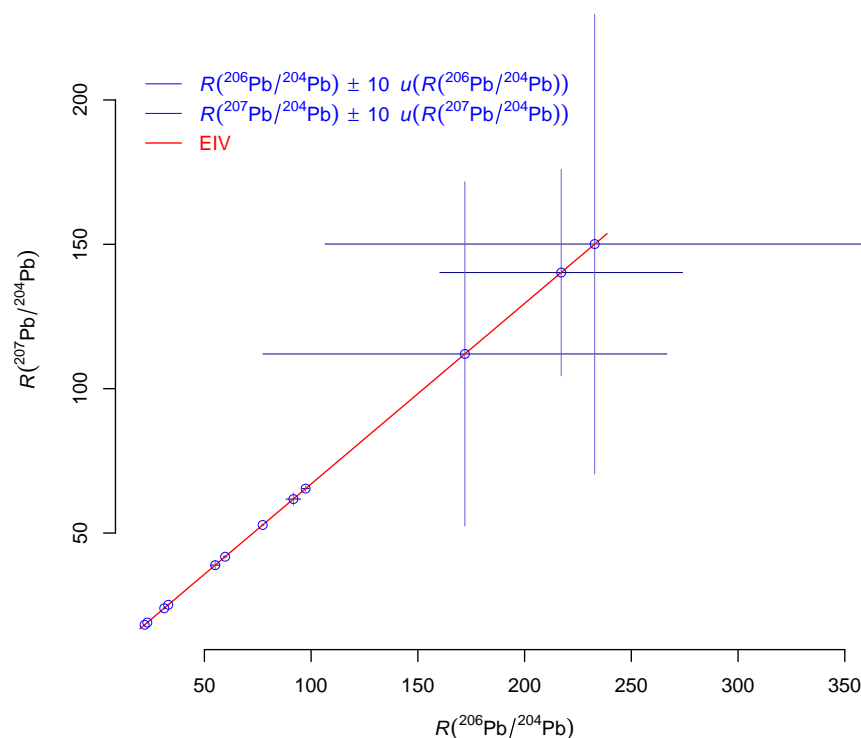


Figure 10: **Allende Isochron.** Measurement results (estimates and standard uncertainties) for lead isotope ratios used to define an isochron for chondrules C20 and C30 from the Allende meteorite. The isochron was fitted to these measurement results using errors-in-variables regression, by the method of maximum likelihood, assuming that the data are outcomes of independent Gaussian random variables with known standard deviations. The standard uncertainties are magnified 10-fold only to facilitate comparing them visually.

The evaluation of uncertainty associated with age estimates needs to recognize contributions from the following sources:

- (a) The uncertainties associated with the half-lives of the relevant uranium isotopes:  $u(T_{1/2}(^{235}\text{U})) = 1 \text{ Ma}$  [Bé et al., 2010] and  $u(T_{1/2}(^{238}\text{U})) = 4.8 \text{ Ma}$  [Villa et al., 2016];
- (b) The uncertainty associated with the isotopic ratio of the same uranium isotopes:  $u(R(^{238}\text{U}/^{235}\text{U})) = 0.013$  [Connelly et al., 2012, Table 1];
- (c) The measurement uncertainties associated with the measured lead isotope ratios  $\{u(R(^{206}\text{Pb}/^{204}\text{Pb}))\}$  and  $\{u(R(^{207}\text{Pb}/^{204}\text{Pb}))\}$ ;
- (d) The sampling uncertainty associated with the selection of the  $n = 12$  samples that were used to define the isochron.

The measurement equation is  $A = f(B, R, T_{235}, T_{238})$ , where the inputs are modeled as random variables:  $B$  denoting the slope of the isochron;  $R$  denoting the value of the isotopic ratio  $R(^{238}\text{U}/^{235}\text{U})$ ;  $T_{235}$  denoting the half-life of  $^{235}\text{U}$ ; and  $T_{238}$  denoting the half-life of  $^{238}\text{U}$ .

To evaluate the uncertainty associated with  $A$ , either by application of Gauss's formula or of the Monte Carlo method, three obstacles must be overcome: (i) computing values of the function  $f$ , which involves solving Equation (2) using numerical methods; (ii) computing the values of the partial derivatives of  $f$  that are needed in Gauss's formula, which requires numerical differentiation; and (iii) representing the probability distribution of  $B$  in a form that the NIST Uncertainty Machine can process.

While (i) would be burdensome and (ii) would be practically insurmountable without recourse to suitably specialized software, for the NIST Uncertainty Machine neither is challenging. Indeed, once  $f$  is determined by specifying  $R$  commands in the appropriate box in the input page, the NIST Uncertainty Machine will have no difficulty addressing (i) or (ii).

$B$  poses a difficulty of a different kind because the corresponding probability distribution is represented by a sample drawn using a previous application of the Monte Carlo method outside of the NIST Uncertainty Machine environment, and none of the parametric distributions available in the NIST Uncertainty Machine fit it adequately.

Therefore, one needs to use the sample itself, which the NIST Uncertainty Machine also allows, as already mentioned in (U-5) on Page 8. In fact, the NIST Uncertainty Machine can read a file with the values of such sample, and then

use it alongside the parametric distributions specified for the other inputs, both when it applies Gauss's formula, and the Monte Carlo method.

For Gauss's formula, the NIST Uncertainty Machine simply uses the average and the standard deviation of the sample of values of  $B$  that is provided. For the Monte Carlo method, it resamples this sample repeatedly, with replacement, thus treating it as if it were an infinite population. (Therefore, when such a sample is provided as input, it need not be of the same size as the number of replicates of the output quantity that are requested. However, the sample should still be of sufficiently large size to provide an accurate representation of the underlying distribution.)

To load the specifications for this example into the NIST Uncertainty Machine, click [here](#).

The probability distribution of  $B$  expresses the contributions from the uncertainties associated with the isotopic ratios, and with the selection of the twelve samples of the two chondrules that were used, from among those that were measured (uncertainty sources (c) and (d) mentioned above). These contributions were evaluated by application of two variants of the statistical bootstrap in tandem: the parametric version for (c), and the non-parametric version for (d) [Efron and Tibshirani, 1993]. Figure 11 shows the graph of an estimate of the probability density of  $B$  that was derived from the input sample.

Figure 12 shows a screenshot of the input page of the NIST Uncertainty Machine with the characterization of the input variables:  $B$  is not assigned any parametric distribution, and only a sample of size 2023 is provided that was drawn from its otherwise unspecified distribution; the other three are modeled as Gaussian random variables with specified means and standard deviations. The input page also includes the definition of the measurement equation, whose R code may more easily be examined in Listing 2.

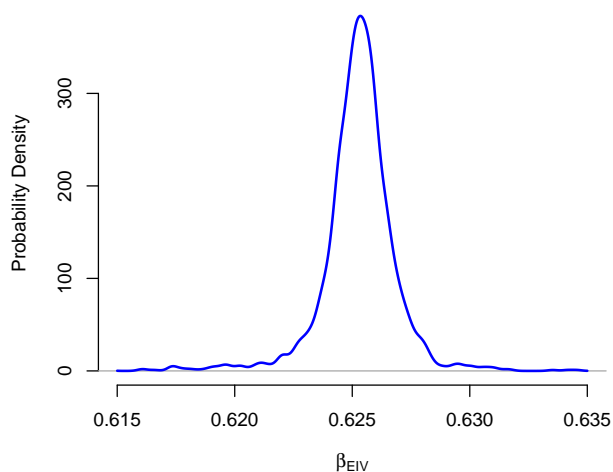


Figure 11: **Slope of Allende Meteorite Isochron.** Kernel estimate [Silverman, 1986] of the probability density of the slope of the isochron depicted in Figure 10, based on a sample of 2023 values, expressing contributions from the uncertainties associated with the isotopic ratios, and with the selection of the twelve samples of the two chondrules that were used, from among those that were measured.

Listing 2: R code used to evaluate the measurement function that computes the age of chondrules in the Allende meteorite.

```
lambda235 = log(2)/T235
lambda238 = log(2)/T238
ageEquation = function(x, beta, lambdaU238, lambdaU235, RU238U235) {
  (exp(x*lambdaU235)-1)/(exp(x*lambdaU238)-1) - RU238U235*beta }
lowerAge = 4e9
upperAge = 5e9
f = function(lambda238,lambda235,R,B) {
  uniroot(ageEquation, lower=lowerAge, upper=upperAge,
    beta=B, lambdaU238=lambda238, lambdaU235=lambda235,
    RU238U235=R)$root }
mapply(f,lambda238,lambda235,R,B)
```

The measurement function  $f$  in  $A = f(B, R, T_{235}, T_{238})$ , which is defined in Listing 2, differs in several essential ways from the measurement functions in other examples in this manual:

- (1) It involves another function, `ageEquation`, that is used to define Equation (2) above, whose root is the value of  $f$ ;



INPUT

1. Select Inputs & Choose Distributions

Number of input quantities: 4

Names of input quantities:

B

R

T235

T238

B

Sample values (between 30 and 100000)

2023 Samples loaded

Drop sample file here or click to upload

R

Gaussian (Mean, StdDev)

137.786

0.013

T235

Gaussian (Mean, StdDev)

704e6

1e6

T238

Gaussian (Mean, StdDev)

4.4683e9

4.8e6

Correlations

2. Choose Options

Number of realizations of the output quantity: 1000000

Random number generator seed: 54

Symmetrical coverage intervals

3. Write the Definition of Output Quantity

Definition of output quantity (R expression):

lambda235 = log(2)/T235  
lambda238 = log(2)/T238  
ageEquation = function(x, beta, lambdaU238, lambdaU235, RU238U235) {  
 (exp(x\*lambdaU235)-1)/(exp(x\*lambdaU238)-1) - RU238U235\*beta}  
lowerAge = 4e9  
upperAge = 5e9  
f = function(lambda238,lambda235,R,B){unifroot(ageEquation, lower=lowerAge, upper=upperAge,  
 beta=B,lambdaU238=lambda238,lambdaU235=lambda235,RU238U235=R)\$root}  
mapply(f,lambda238,lambda235,R,B)

Run the computation

OUTPUT

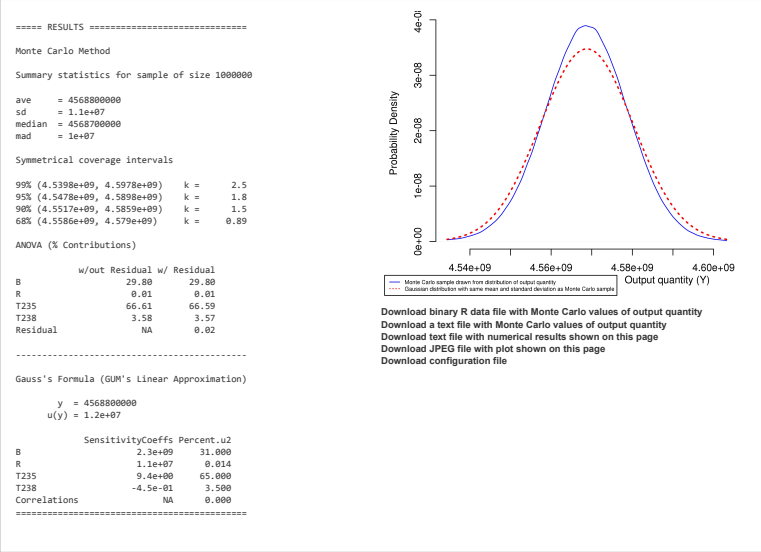


Figure 12: Allende Meteorite. Input and output Web pages for the example discussed in §13.

- (2) It uses a numerical method to find this root, which is implemented in R function `uniroot`;
- (3) A programming device (invoking `mapply`) is required to ensure that  $f$  is *vectorized*: that is, if each of its arguments is a vector of length  $K$ , then the value of  $f$  is a vector of length  $K$  whose  $k$ th element is the root of the `ageEquation` that correspond to the  $k$ th set of values of the inputs.

The NIST Uncertainty Machine always requires that the measurement function  $f$  be vectorized, in the sense just described. However, in all the other examples this is accomplished automatically owing to the evaluation rules of the R language (which govern the interpretation of the code entered in the box where the value of  $f$  is specified, in the input Web page of the NIST Uncertainty Machine). Not in this case, owing to the presence of the root finder `uniroot`, which does not accommodate vectorization.

Figure 12 shows two areas of the output page: the portion that summarizes the results of the GUM calculations, including application of Gauss's formula, and the portion with the results of the Monte Carlo method, including the plot of the estimate of the probability density of the output quantity (which is the age of the chondrules).

It is worth noting, in the portion of the output produced by the Monte Carlo method, that the percentage of the variance of the output quantity attributable to non-linearity of the measurement function (0.02 %) is very small, even though the function clearly is non-linear. This is attributable to the fact that, its overall non-linearity notwithstanding,  $f$  still is approximately linear within a neighborhood of the estimates of the input quantities of size comparable to their associated uncertainties.

The corresponding age estimate is 4569 Ma with associated standard uncertainty 12 Ma according to Gauss's formula, and 11 Ma according to the Monte Carlo method. (Connelly et al. [2012] report 4566 Ma for C20 and 4567 Ma for C30, with much smaller uncertainties.)

These chondrules are truly ancient, frozen remnants of the protoplanetary disk that would evolve to become the solar system. However, Scott [2007] points out that "the Allende chondrite is not a pristine chondrite, as was once believed. It was severely altered by fluid-assisted metamorphism in its parent asteroid." Therefore, an uncertainty even larger than our calculations suggest should surround the age of these chondrules.

## Acknowledgments

The authors are grateful to their colleagues Will Guthrie, Alan Heckert, Narain Krishnamurthy, Adam Pintar, Jolene Splett, and Jack Wang, for the many suggestions that they offered for improvement of the NIST Uncertainty Machine and of this user's manual.

Alan Heckert, Steven Conn, Shawn Winhoven, Walter Rowe, Dale Little, and Del Brockett, greatly facilitated the deployment of this Web-based application for use on the World Wide Web.

The authors will be very grateful to users of the software, and to readers of this manual, for information about errors and other deficiencies, and for suggestions for improvement, which may be sent via eMail to [thomas.lafarge@nist.gov](mailto:thomas.lafarge@nist.gov) and to [antonio.possolo@nist.gov](mailto:antonio.possolo@nist.gov).

## References

- T. W. Anderson and D. A. Darling. Asymptotic theory of certain “goodness-of-fit” criteria based on stochastic processes. *Annals of Mathematical Statistics*, 23:193–212, 1952.
- M.-M. Bé, V. Chisté, C. Dulieu, X. Mougeot, E. Browne, V. Chechev, N. Kuzmenko, F. Kondev, A. Luca, M. Galán, A. L. Nichols, A. Arinc, and X. Huang. *Table of Radionuclides*, volume 5 – A = 22 to 244 of *Monographie BIPM-5*. Bureau International des Poids et Mesures, Sèvres, France, 2010. ISBN 978-92-822-2234-8.
- S. Bell. *A Beginner's Guide to Uncertainty of Measurement*. Number 11 (Issue 2) in Measurement Good Practice Guide. National Physical Laboratory, Teddington, Middlesex, United Kingdom, 1999. URL [www.npl.co.uk/publications/guides/a-beginners-guide-to-uncertainty-of-measurement](http://www.npl.co.uk/publications/guides/a-beginners-guide-to-uncertainty-of-measurement). Amendments March 2001.
- P. Billingsley. *Probability and Measure*. John Wiley & Sons, New York, NY, 1979.
- R. S. Clarke, Jr., E. Jarosewich, B. Mason, J. Nelen, M. Gomez, and J. R. Hyde. *Alende, Mexico, Meteorite Shower*. Number 5 in Smithsonian Contributions to the Earth Sciences. Smithsonian Institution, Washington, DC, February 1971. doi: 10.5479/si.00810274.5.1.
- J. N. Connelly, M. Bizzarro, A. N. Krot, A. Nordlund, D. Wielandt, and M. A. Ivanova. The absolute chronology and thermal processing of solids in the solar protoplanetary disk. *Science*, 338:651–655, November 2012. doi: 10.1126/science.1226919.
- M. H. DeGroot and M. J. Schervish. *Probability and Statistics*. Addison-Wesley, 4th edition, 2011.

- B. Efron and R. J. Tibshirani. *An Introduction to the Bootstrap*. Chapman & Hall, London, UK, 1993.
- D. Freedman, R. Pisani, and R. Purves. *Statistics*. W. W. Norton & Company, New York, NY, fourth edition, 2007.
- K. O. Friedrich. A Berry-Esseen bound for functions of independent random variables. *The Annals of Statistics*, 17(1):170–183, 1989.
- C. Gauss. Theoria combinationis observationum erroribus minimis obnoxiae. In *Werke, Band IV, Wahrscheinlichkeitsrechnung und Geometrie*. Königlichen Gesellschaft der Wissenschaften, Göttingen, 1823. [gdz.sub.uni-goettingen.de/](http://gdz.sub.uni-goettingen.de/).
- P. Gilbert and R. Varadhan. *numDeriv: Accurate Numerical Derivatives*, 2016. URL [CRAN.R-project.org/package=numDeriv](https://CRAN.R-project.org/package=numDeriv). R package version 2016.8-1.
- W. F. Guthrie, H.-k. Liu, A. L. Rukhin, B. Toman, J. C.M. Wang, and N.-f. Zhang. Three statistical paradigms for the assessment and interpretation of measurement uncertainty. In F. Pavese and A. B. Forbes, editors, *Data Modeling for Metrology and Testing in Measurement Science*, Modeling and Simulation in Science, Engineering and Technology, pages 1–45. Birkhäuser Boston, 2009. doi: 10.1007/978-0-8176-4804-6\_3.
- B. D. Hall and D. R. White. *An Introduction to Measurement Uncertainty*. Measurement Standards Laboratory of New Zealand, Lower Hutt, New Zealand, 2018. Also available from [www.lulu.com](http://www.lulu.com).
- J. Hiess, D. J. Condon, N. McLean, and S. R. Noble.  $^{238}\text{U}/^{235}\text{U}$  systematics in terrestrial uranium-bearing minerals. *Science*, 335(6076):1610–1614, 2012. doi: 10.1126/science.1215507.
- Joint Committee for Guides in Metrology. *Evaluation of measurement data — Guide to the expression of uncertainty in measurement*. International Bureau of Weights and Measures (BIPM), Sèvres, France, 2008a. URL [www.bipm.org/en/publications/guides/gum.html](http://www.bipm.org/en/publications/guides/gum.html). BIPM, IEC, IFCC, ILAC, ISO, IUPAC, IUPAP and OIML, JCGM 100:2008, GUM 1995 with minor corrections.
- Joint Committee for Guides in Metrology. *Evaluation of measurement data — Supplement 1 to the “Guide to the expression of uncertainty in measurement” — Propagation of distributions using a Monte Carlo method*. International Bureau of Weights and Measures (BIPM), Sèvres, France, 2008b. URL [www.bipm.org/en/publications/guides/gum.html](http://www.bipm.org/en/publications/guides/gum.html). BIPM, IEC, IFCC, ILAC, ISO, IUPAC, IUPAP and OIML, JCGM 101:2008.
- Joint Committee for Guides in Metrology. *Evaluation of measurement data — Supplement 2 to the “Guide to the expression of uncertainty in measurement” — Extension to any number of output quantities*. International Bureau of Weights and Measures (BIPM), Sèvres, France, 2011. URL [www.bipm.org/en/publications/guides/gum.html](http://www.bipm.org/en/publications/guides/gum.html). BIPM, IEC, IFCC, ILAC, ISO, IUPAC, IUPAP and OIML, JCGM 102:2011.

- S. J. Kline and F. A. McClintock. Describing uncertainties in single-sample experiments. *Mechanical Engineering*, 75(1):3–8, 1953.
- T. Lafarge and A. Possolo. The NIST Uncertainty Machine. *NCSLI Measure Journal of Measurement Science*, 10(3):20–27, September 2015.
- P. J. Mohr, B. N. Taylor, and D. B. Newell. CODATA recommended values of the fundamental physical constants: 2010. *Reviews of Modern Physics*, 84(4):1527–1605, October-December 2012. doi: 10.1063/1.4724320.
- M. G. Morgan and M. Henrion. *Uncertainty — A Guide to Dealing with Uncertainty in Quantitative Risk and Policy Analysis*. Cambridge University Press, New York, NY, first paperback edition, 1992. 10th printing, 2007.
- R. B. Nelsen. *An Introduction to Copulas*. Springer, New York, NY, 2nd edition, 2006. Corrected 2nd. printing, 2007.
- D. B. Newell, F. Cabiati, J. Fischer, K. Fujii, S. G. Karshenboim, H. S. Margolis, E. de Mirandés, P. J. Mohr, F. Nez, and K. Pachucki. The CODATA 2017 values of  $h$ ,  $e$ ,  $k$ , and  $N_A$  for the revision of the SI. *Metrologia*, 55(1):L13–L16, January 2018. doi: 10.1088/1681-7575/aa950a.
- A. Possolo. Copulas for uncertainty analysis. *Metrologia*, 47:262–271, 2010. doi: 10.1088/0026-1394/47/3/017.
- A. Possolo. *Simple Guide for Evaluating and Expressing the Uncertainty of NIST Measurement Results*. National Institute of Standards and Technology, Gaithersburg, MD, 2015. URL <http://dx.doi.org/10.6028/NIST.TN.1900>. NIST Technical Note 1900.
- A. Possolo and C. Elster. Evaluating the uncertainty of input quantities in measurement models. *Metrologia*, 51(3):339–353, June 2014. doi: 10.1088/0026-1394/51/3/339.
- A. Possolo and H. K. Iyer. Concepts and tools for the evaluation of measurement uncertainty. *Review of Scientific Instruments*, 88(1):011301, 2017. doi: 10.1063/1.4974274.
- A. Possolo, B. Toman, and T. Estler. Contribution to a conversation about the Supplement 1 to the GUM. *Metrologia*, 46:L1–L7, 2009.
- R Core Team. *R: A Language and Environment for Statistical Computing*. R Foundation for Statistical Computing, Vienna, Austria, 2015. URL [www.R-project.org/](http://www.R-project.org/).
- F. E. Satterthwaite. An approximate distribution of estimates of variance components. *Biometrics Bulletin*, 2(6):110–114, December 1946.

- B. Schoene. U-Th-Pb Geochronology. In H. D. Holland and K. K. Turekian, editors, *Treatise on Geochemistry*, volume 4 (*The Crust*), chapter 10, pages 341–378. Elsevier, Amsterdam, second edition, 2014. doi: 10.1016/B978-0-08-095975-7.00310-7.
- E. R. D. Scott. Chondrites and the protoplanetary disk. *Annual Review of Earth and Planetary Sciences*, 35:577–620, 2007. doi: 10.1146/annurev.earth.35.031306.140100.
- B. W. Silverman. *Density Estimation*. Chapman and Hall, London, 1986.
- B. N. Taylor and C. E. Kuyatt. *Guidelines for Evaluating and Expressing the Uncertainty of NIST Measurement Results*. NIST Technical Note 1297. National Institute of Standards and Technology, Gaithersburg, MD, 1994. URL [physics.nist.gov/Pubs/guidelines/TN1297/tn1297s.pdf](https://physics.nist.gov/Pubs/guidelines/TN1297/tn1297s.pdf).
- C. M. Tsui, A. Y. K. Yang, and H. W. Li. Software tools for evaluation of measurement models for complex-valued quantities in accordance with Supplement 2 to the GUM. *NCSLI Measure Journal of Measurement Science*, 7(3):48–55, September 2012.
- I. M. Villa, M. L. Bonardi, P. De Bièvre, N. E. Holden, and P. R. Renne. IUPAC-IUGS status report on the half-lives of  $^{238}\text{U}$ ,  $^{235}\text{U}$  and  $^{234}\text{U}$ . *Geochimica et Cosmochimica Acta*, 172:387–392, 2016. doi: 10.1016/j.gca.2015.10.011.
- B. L. Welch. The generalization of ‘Student’s’ problem when several different population variances are involved. *Biometrika*, 34:28–35, January 1947.
- W. M. White. *Isotope Geochemistry*. John Wiley & Sons, New York, NY, 2015.