NIST Uncertainty Machine — User's Manual

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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 give them names if desired.
- Select a probability distribution for each of the input quantities, and enter values for the parameters (in the absence of cogent reason to do otherwise, assign Gaussian distributions to them with means equal to their values and with standard deviations equal to their standard uncertainties);
- 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 in version 1.3 of the `NIST Uncertainty Machine`).
- 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 10 for the case when the output quantity is a vector.)
- If there are correlations between the input quantities, then check the box marked **`Correlations`**, enter the values of the non-zero correlations, and select a copula to apply them with (*cf.* Figure 6 on Page 23).
- 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 $y = f(x_1, \ldots, x_n)$, where the real-valued function f is specified fully and explicitly, and the input quantities are modeled as random variables whose joint probability distribution also is specified fully.

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], which is described in the *Guide to the Evaluation of Uncertainty in Measurement* (GUM) [Joint Committee for Guides in Metrology, 2008a] and also by Taylor and Kuyatt [1994];
- The Monte Carlo method described by Morgan and Henrion [1992] and specified in the Supplement 1 to the GUM (GUM-S1) [Joint Committee for Guides in Metrology, 2008b].

Section 11, beginning on Page 24, 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 (or, vectorial) measurand.

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, and it requires:

(a) Estimates $x_1, \ldots, x_n$ of the input quantities;

(b) Standard measurement uncertainties $u(x_1), \ldots, u(x_n)$;

(c) Correlations $\{r_{ij}\}$ between every pair of different input quantities (by default these are all assumed to be zero);

(d) Values of the partial derivatives of f evaluated at $x_1, \ldots, x_n$.

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. However, this also holds for some markedly non-Gaussian probability distributions, including many Student's t, lognormal, gamma, and Weibull distributions [Freedman et al., 2007].

The GUM also considers the case where the distribution of the output quantity 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 modeled adequately as Gaussian random variables.

The GUM suggests that the Central Limit Theorem (CLT) from Probability Theory 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 of 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].

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 to compute the standard uncertainty associated with the output quantity, and to compute and to interpret coverage intervals probabilistically.

> 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 5 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 you may assign Gaussian (or, normal) distributions to them:

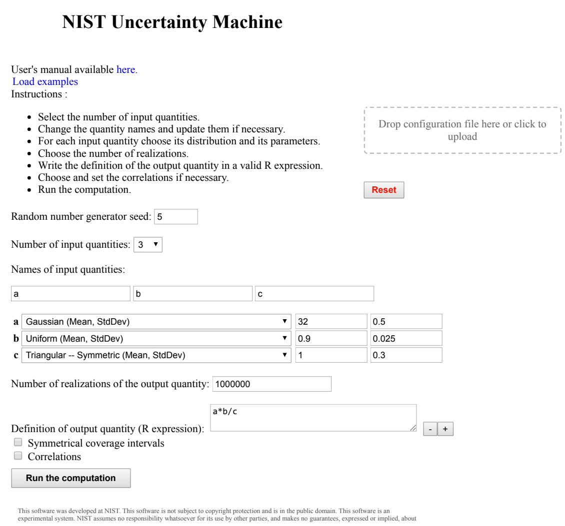
- If the input quantities are uncorrelated, then this amounts to assigning a Gaussian distribution to each one of them, with mean and standard deviation equal to the corresponding estimate and standard uncertainty;
- If the input quantities are correlated, then besides assigning Gaussian distributions to them as in the previous case, then you will also need to check the box 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 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 $f(x_1, \ldots, x_n)$ 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 $\widehat{c}$ is its estimate, and $u(c)/\widehat{c}$ is less than 5 %, say, then c may be assigned a lognormal

INPUT



OUTPUT

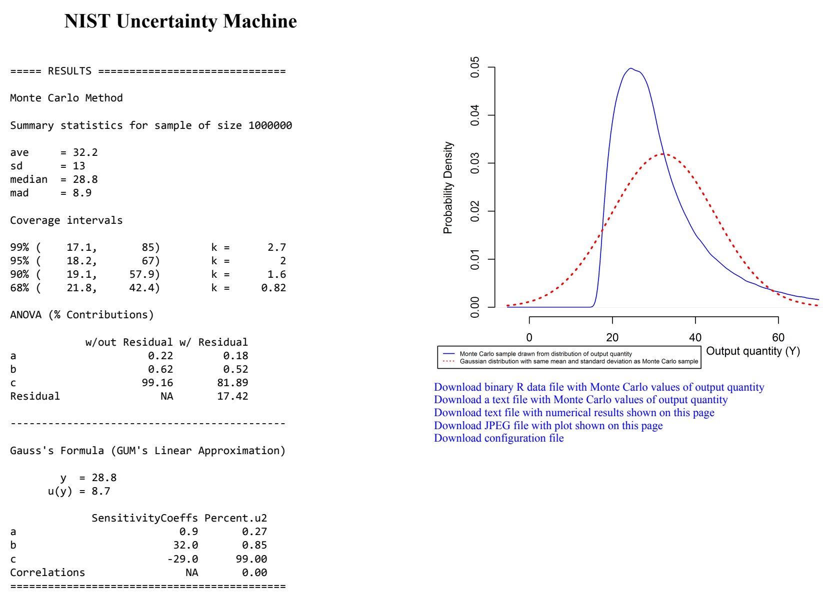


Figure 1: **ABC.** Entries in the Web page correspond to the example discussed in §3. In each numerical result, only the digits that the `NIST Uncertainty Machine` deems to be significant are printed. Estimate of the probability density of the output quantity (solid blue line), and probability density (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 $\widehat{c}$ 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. Possolo and Elster [2014] provide detailed guidance for how to assign probability distributions to input quantities, and illustrate this guidance with examples.

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. If at any point you wish to clear all the entries in the input page, just reload the page and the browser will display a fresh input page.

(U-1) If you wish 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 it 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`**. It will update the labels that appear immediately below and that are used to assign probability distributions to 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.

Table 2 on Page 12 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. Such specification would be equivalent to specifying the value of a constant: this may be done either by entering this value as a numerical constant in the expression that defines the output quantity (*cf.* the example in Section 10 that begins on Page 22), or by selecting `Constant` as distribution type and entering the value of the constant in the corresponding box.

(U-5) Starting with version 1.3, 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 **`Provide Sample (of size 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 writen 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 be written as `1.98376e3` or `1.98376E3`. Once the file has been parsed the number of values loaded will be shown for easy reviewing. The total number of sample values provided in this way, shared across all input quantities, cannot exceed 2 400 000 approximately. In case this limit is reached, an error message appears once the computation starts.

When samples are provided, the modus operandi of the `NIST Uncertainty Machine` is quite similar to the normal use case. The main difference is that instead of drawing a random sample from a particular parametric distribution, it resamples the values in the sample that was provided repeatedly, uniformly at random with replacement. §12 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, 1×10^6, is the minimum recommended sample size (currently the `NIST Uncertainty Machine` is able to generate samples of size from 1×10^5 to 5×10^6).

(U-7) Enter a valid R expression into the box labeled **`Value of output quantity (R expression)`** that represents $f(x_1, \ldots, x_n)$, 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.)

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

+	-	*	^	%%	%/%
/	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`.

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 $A = (L_1 - L_0)/\big(L_0(T_1 - T_0)\big)$, 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` always 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 kth element of this vector is the value of f at the kth values of all the input quantities. This may not happen automatically for some intricate measurement equations that involve optimizations, root-finding, or solutions of differencial equations, among others. In the case of the example described in §12, vectorization may be achieved by merely invoking `mapply`.

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` and `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 check the box 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 $\widehat{y} \pm ku(y)$ where $\widehat{y}$, 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.

(U-10) If there are correlations between input quantities that need to be taken into account, then check the box 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. The `NIST Uncertainty Machine` makes sure that the values entered do define a positive definite correlation matrix, and issues an error message (`Illegal correlation matrix`) if they do not.

(U-11) If the box marked **`Correlations`** has been checked, 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. 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 sample size than what was specified 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 5.

Below this plot there are five clickable lines of green text: 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 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 of a plot, and it is divided into two sections. The top section lists the results from the application of the Monte Carlo method. The bottom section lists the 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, and likewise MAD may be a reasonable, and in some cases a preferable alternative to the

NAME	PARAMETERS	CONSTRAINTS
Bernoulli	Prob. of success	0 < Prob. of success < 1
Beta	Mean, StdDev	0 < Mean < 1, 0 < StdDev < ½
	Shape1, Shape2	Shape1 > 0, Shape2 > 0
Beta – Shifted & Rescaled	Mean, StdDev, Left, Right	0 < Mean < 1, 0 < StdDev < ½, Left < Right
	Shape1, Shape2, Left, Right	Shape1 > 0, Shape2 > 0, Left < Right
Chi-Squared	DF	DF > 0
Constant	Value	—
Exponential	Mean	Mean > 0
Gamma	Mean, StdDev	Mean > 0, StdDev > 0
	Shape, Scale	Shape > 0, Scale > 0
Gaussian	Mean, StdDev	StdDev > 0
Gaussian – Truncated	Mean, StdDev, Left, Right	StdDev > 0, Left < Right
Lognormal	Mean, StdDev	Mean > 0, StdDev > 0
Rectangular	Mean, StdDev	StdDev > 0
	Left, Right	Left < Right
Student's t	Mean, StdDev, DF	StdDev > 0, DF > 2
	Center, Scale, DF	Scale > 0, DF > 0
Triangular – Symmetric	Mean, StdDev	StdDev > 0
	Left, Right	Left < Right
Triangular – Asymmetric	Left, Right, Mode	Left ⩽ Mode ⩽ Right; Left ≠ Right
Uniform	Mean, StdDev	StdDev > 0
	Left, Right	Left < Right
Weibull	Mean, StdDev	Mean > 0, StdDev > 0
	Shape, Scale	Shape > 0, 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.

standard deviation as evaluation of $u(y)$. It behooves the user to state, when reporting measurement results, 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.

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).

If the box mentioned in (U-9) above is checked 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 it is responsible for, computed under the assumption that the output quantity is a *linear* function of the input quantities.

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: in the one headed "`w/out Residual`" the proportions are 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 GUM results appear 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, both computed according to the GUM.

Finally, a table shows the sensitivity coefficients that are 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 %: 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 graphical output on the output Web page is a plot with a kernel estimate [Silverman, 1986] of the probability density of the output quantity (drawn in a solid blue line), and with 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 (drawn as a red dotted line).
- Below this plot there are five clickable lines of green text 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 $p \geqslant 2$ components, as contemplated in (U-8), the `NIST Uncertainty Machine` will produce p tabs with output, labeled `Output 1`, `Output 2`, ... A download request initiated by clicking the green text just mentioned *on any of the output tabs* 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 $p \geqslant 2$ components, as contemplated in (U-8), the `NIST Uncertainty Machine` will produce p tabs with output, labeled `Output 1`, `Output 2`, ... A download request initiated by clicking the green text just mentioned *on any of the output tabs* 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 suffix `.um` that specifies the inputs that were used and that may be reused as explained in (U-1).

6 Example — Thermal Expansion Coefficient

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

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 $u(L_0) = 0.0001\,\mathrm{m}$, $u(L_1) = 0.0002\,\mathrm{m}$, $u(T_0) = 0.02\,\mathrm{K}$, and $u(T_1) = 0.05\,\mathrm{K}$.

This assignment of distributions to the four input quantities would be appropriate if their estimates were averages of four replicated readings each, and these were outcomes of independent Gaussian random variables with unknown common mean and standard deviation. To load the specifications for this example into the `NIST Uncertainty Machine`, click **here**.

The GUM's approach yields $\alpha = 1.727 \times 10^{-5}\,\mathrm{K}^{-1}$ and $u(\alpha) = 2 \times 10^{-6}\,\mathrm{K}^{-1}$, and the Monte Carlo method reproduces these results. Figure 2 on Page 16 reflects these facts, and lists the results.

INPUT

NIST Uncertainty Machine

User's manual available here.
Load examples
Instructions :

- Select the number of input quantities.
- Change the quantity names and update them if necessary.
- For each input quantity choose its distribution and its parameters.
- Choose the number of realizations.
- Write the definition of the output quantity in a valid R expression.
- Choose and set the correlations if necessary.
- Run the computation.

Drop configuration file here or click to upload

Reset

Random number generator seed: 5

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

Number of realizations of the output quantity: 1000000

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

- +

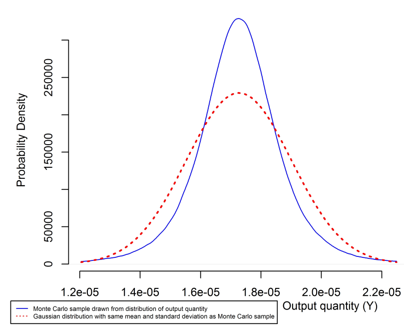
Symmetrical coverage intervals
Correlations

Run the computation

OUTPUT

NIST Uncertainty Machine

```
===== RESULTS ==============================

Monte Carlo Method

Summary statistics for sample of size 1000000

ave     = 1.727e-05
sd      = 1.7e-06
median  = 1.727e-05
mad     = 1.2e-06

Coverage intervals

99% ( 1.2e-05,  2.3e-05)       k =      3.2
95% ( 1.4e-05, 2.05e-05)       k =      1.9
90% (1.48e-05, 1.97e-05)       k =      1.4
68% ( 1.6e-05, 1.86e-05)       k =     0.75

ANOVA (% Contributions)

            w/out Residual w/ Residual
L0                   20.48       20.48
T0                    0.00        0.00
L1                   79.52       79.52
T1                    0.00        0.00
Residual                NA        0.00

--------------------------------------------

Gauss's Formula (GUM's Linear Approximation)

        y  = 1.727e-05
      u(y) = 1.8e-06

             SensitivityCoeffs Percent.u2
L0                    -7.9e-03    2.0e+01
T0                     2.0e-07    5.4e-04
L1                     7.8e-03    8.0e+01
T1                    -2.0e-07    3.4e-03
Correlations                NA    0.0e+00
============================================
```



Download binary R data file with Monte Carlo values of output quantity
Download a text file with Monte Carlo values of output quantity
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Figure 2: **Thermal Expansion Coefficient.** Input and output Web pages for the example discussed in §6.

7 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 $\delta\theta$ denote single 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**.

QUANTITY	x	$u(x)$
l_S	50 000 623 nm	25 nm
d	215 nm	9.7 nm
$\delta\alpha$	0 °C^{-1}	0.58×10^{-6} °C^{-1}
θ	−0.1 °C	0.41 °C
α_S	11.5×10^{-6} °C^{-1}	1.2×10^{-6} °C^{-1}
$\delta\theta$	0 °C	0.029 °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.

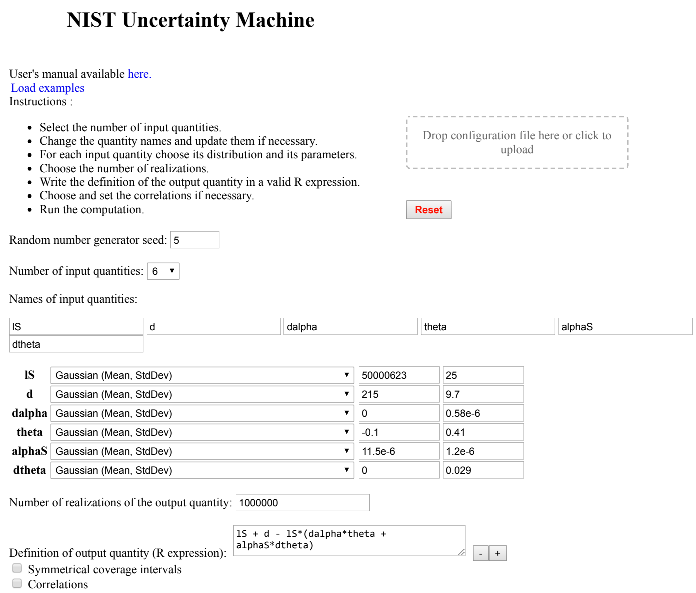
The GUM's approach yields $l = 50\,000\,838$ nm and $u(l) = 32$ nm, while the Monte Carlo method reproduces the value for l but evaluates $u(l) = 34$ nm. Refer to Figure 3 on Page18.

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 you choose a coverage interval that is probabilistically 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 (and this is not quite centered at the estimate of y).

8 Example — Dynamic Viscosity

The dynamic viscosity μ_M of a solution of sodium hydroxide in water at 20 °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 $\mu_C =$

INPUT



OUTPUT

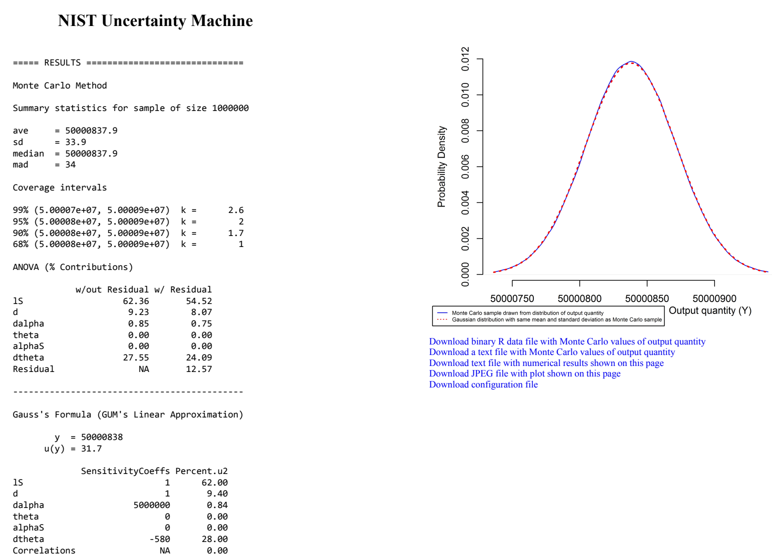


Figure 3: **End-Gauge Calibration.** Input and output Web pages for the example discussed in §7. Note that the value of α_S, $11.5 \times 10^{-6}\,°\mathrm{C}^{-1}$, was entered as `11.5e-6`.

4.63 mPa s, $\rho_C = 810\,\mathrm{kg/m^3}$, and $t_C = 36.6\,\mathrm{s}$ denote the viscosity, mass density, and ball travel time for the calibration liquid, and $\rho_M = 1180\,\mathrm{kg/m^3}$ and $t_M = 61\,\mathrm{s}$ 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 $u(\mu_C) = 0.01\mu_C$, $u(\rho_B) = u(\rho_C) = u(\rho_M) = 0.5\,\mathrm{kg/m^3}$, $u(t_C) = 0.15t_C$, and $u(t_M) = 0.10t_M$, then the Monte Carlo method of the GUM-S1 as implemented in the `NIST Uncertainty Machine` produces: $\widehat{\mu}_M = 5.8\,\mathrm{mPa\,s}$, $u(\mu_M) = 1.12\,\mathrm{mPa\,s}$, and $[4.05\,\mathrm{mPa\,s},\ 8.4\,\mathrm{mPa\,s}]$ as an approximate 95 % coverage interval for μ_M. This interval is asymmetric relative to the estimate $\widehat{\mu}_M$.

If, instead, the estimates of the input quantities were substituted into the measurement equation, the resulting estimate of μ_M would have been 5.69 mPa s. And if the approximate method described by Taylor and Kuyatt [1994] and in the GUM, and which also is implemented in the `NIST Uncertainty Machine`, 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 20.

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 21 shows the corresponding input and output Web pages of the `NIST Uncertainty Machine`.

9 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 20.

For the Monte Carlo method, we model the input quantities as correlated Gaus-

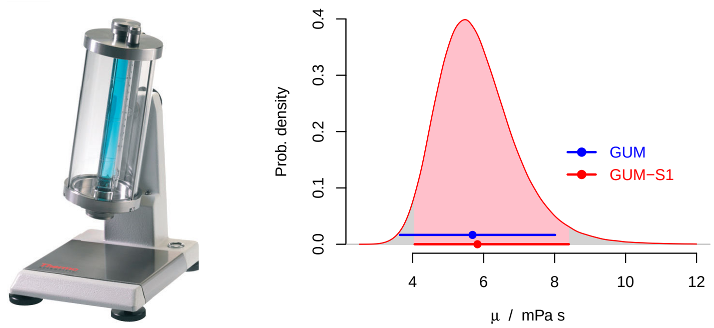


Figure 4: HAAKE™ falling ball viscometer from Thermo Fisher Scientific, Inc., (left panel), and probability density (right panel) corresponding to a Monte Carlo sample of size 1×10^6, also showing 95 % coverage intervals for the value of the dynamic viscosity of the liquid, one corresponding to the prescription 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.

sian random variables with means and standard deviations equal to the estimates 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 listed.

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	19.6610×10^{-3} A	0.0095×10^{-3} A
ϕ	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

INPUT

NIST Uncertainty Machine

User's manual available here.
Load examples
Instructions :

- Select the number of input quantities.
- Change the quantity names and update them if necessary.
- For each input quantity choose its distribution and its parameters.
- Choose the number of realizations.
- Write the definition of the output quantity in a valid R expression.
- Choose and set the correlations if necessary.
- Run the computation.

Drop configuration file here or click to upload

Reset

Random number generator seed: 5

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

Number of realizations of the output quantity: 1000000

Definition of output quantity (R expression):
```
muC * ((rhoB-rhoM)/(rhoB-rhoC)) *
(tM/tC)
```
- +

Symmetrical coverage intervals
Correlations

Run the computation

OUTPUT

NIST Uncertainty Machine

```
===== RESULTS ==============================

Monte Carlo Method

Summary statistics for sample of size 1000000

ave     = 5.82
sd      = 1.1
median  = 5.69
mad     = 1

Coverage intervals

99% (    3.65,      9.7)       k =      2.7
95% (    4.05,      8.4)       k =      1.9
90% (    4.27,     7.84)       k =      1.6
68% (    4.77,     6.86)       k =     0.94

ANOVA (% Contributions)

            w/out Residual w/ Residual
muC                   0.28        0.26
rhoB                  0.00        0.00
rhoM                  0.00        0.00
rhoC                  0.00        0.00
tM                   28.54       27.22
tC                   71.18       67.88
Residual                NA        4.64

--------------------------------------------

Gauss's Formula (GUM's Linear Approximation)

        y  = 5.69
      u(y) = 1

             SensitivityCoeffs Percent.u2
muC                     1.2000    3.1e-01
rhoB                    0.0014    4.9e-05
rhoM                   -0.0055    7.1e-04
rhoC                    0.0040    3.9e-04
tM                      0.0930    3.1e+01
tC                     -0.1600    6.9e+01
Correlations                NA    0.0e+00
============================================
```

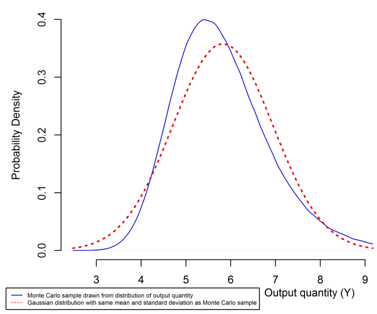


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Figure 5: **Viscosity.** Input and output Web pages for the example discussed in §8.

95 % coverage interval for the resistance without invoking any additional assumptions about R. Figure 6 on Page 23 reflects these facts, and lists the results.

10 Example — Stefan-Boltzmann Constant

The functional relation used to define the Stefan-Boltzmann constant σ involves the Planck constant h, the molar gas constant R, Rydberg's constant R_∞, 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 α:

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

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 "σ" refer to the Stefan-Boltzmann constant.

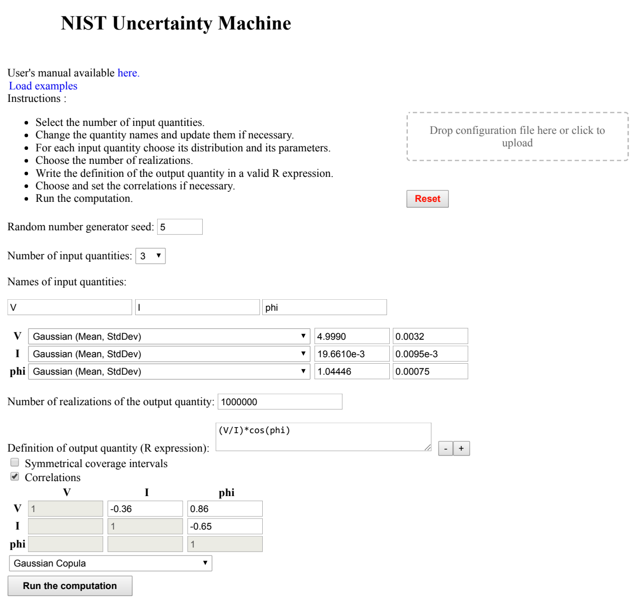
Table 5 lists the 2010 CODATA [Mohr et al., 2012] recommended values of the quantities that determine the value of the Stefan-Boltzmann constant, and the measurement uncertainties associated with them. To load the specifications for this example into the `NIST Uncertainty Machine`, click **here**.

	VALUE	STD. MEAS. UNC.	UNIT
h	$6.626\,069\,57 \times 10^{-34}$	$0.000\,000\,29 \times 10^{-34}$	J s
R	$8.314\,462\,1$	$0.000\,007\,5$	$\mathrm{J\,mol^{-1}\,K^{-1}}$
R_∞	$10\,973\,731.568\,539$	$0.000\,055$	$\mathrm{m^{-1}}$
$A_r(e)$	$5.485\,799\,094\,6 \times 10^{-4}$	$0.000\,000\,002\,2 \times 10^{-4}$	u
M_u	1×10^{-3}	0	kg/mol
c	$299\,792\,458$	0	m/s
α	$7.297\,352\,569\,8 \times 10^{-3}$	$0.000\,000\,002\,4 \times 10^{-3}$	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.

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 $\sigma = 5.670\,37 \times 10^{-8}\,\mathrm{W\,m^{-2}\,K^{-4}}$. Both the GUM's approximation and the Monte Carlo method produce the same evaluation of $u(\sigma) = 2 \times 10^{-13}\,\mathrm{W\,m^{-2}\,K^{-4}}$.

INPUT



OUTPUT

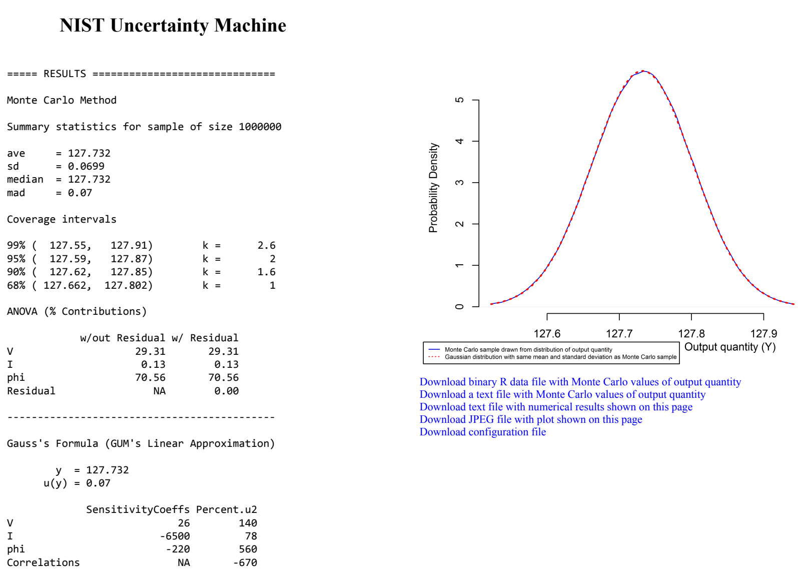


Figure 6: **Resistance.** Input and output Web pages for the example discussed in §9. Note that, in this case, the `NIST Uncertainty Machine` reconfigured its graphical user interface automatically to accommodate the correlations that had to be specified.

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 additional assumptions, it is impossible to interpret an expression like $\sigma \pm u(\sigma)$ probabilistically. The assumptions that are needed to apply the Monte Carlo method of the GUM-S1 deliver not only an evaluation of uncertainty, but also enable a probabilistic interpretation.

If the measurement uncertainties associated with h, R, R_∞, $A_r(e)$, and α 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 gaged by the Anderson-Darling test of Gaussian shape [Anderson and Darling, 1952].

Figure 7 on Page 25 reflects these facts and shows the results, which imply that the interval from $5.670\,332 \times 10^{-8}\,\mathrm{W\,m^{-2}\,K^{-4}}$ to $5.670\,412\,6 \times 10^{-8}\,\mathrm{W\,m^{-2}\,K^{-4}}$ is a coverage interval for σ 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, you 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 25.

11 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 Γ (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 Γ.

The `NIST Uncertainty Machine` does handle vectorial output quantities. Additional outputs fields can be added by clicking the "+" button as explained in

INPUT

NIST Uncertainty Machine

User's manual available here.
Load examples
Instructions :

- Select the number of input quantities.
- Change the quantity names and update them if necessary.
- For each input quantity choose its distribution and its parameters.
- Choose the number of realizations.
- Write the definition of the output quantity in a valid R expression.
- Choose and set the correlations if necessary.
- Run the computation.

Drop configuration file here or click to upload

Reset

Random number generator seed: 5

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-

Number of realizations of the output quantity: 1000000

Definition of output quantity (R expression):

```
N = 32 * (pi^5) * h * (R^4) * (Rinf^4)
D = 15 * (e^4) * ((1e-3)^4) *
(299792458^6) * (alpha^8)
N / D
```

- +

Symmetrical coverage intervals
Correlations

Run the computation

OUTPUT

NIST Uncertainty Machine

```
===== RESULTS ==============================

Monte Carlo Method

Summary statistics for sample of size 1000000

ave     = 5.6703725e-08
sd      = 2.05e-13
median  = 5.6703725e-08
mad     = 2e-13

Coverage intervals

99% (5.67032e-08, 5.67043e-08)  k =      2.6
95% (5.67033e-08, 5.67041e-08)  k =        2
90% (5.67034e-08, 5.67041e-08)  k =      1.6
68% (5.67035e-08, 5.67039e-08)  k =        1

ANOVA (% Contributions)

            w/out Residual w/ Residual
R                      100       99.99
Residual                NA        0.01

--------------------------------------------

Gauss's Formula (GUM's Linear Approximation)

      y  = 5.6703725e-08
    u(y) = 2.05e-13

             SensitivityCoeffs Percent.u2
h                      8.6e+25    1.5e-02
R                      2.7e-08    1.0e+02
Rinf                   2.1e-14    3.1e-09
e                     -4.1e-04    2.0e-05
alpha                 -6.2e-05    5.3e-05
Correlations                NA    0.0e+00
============================================
```

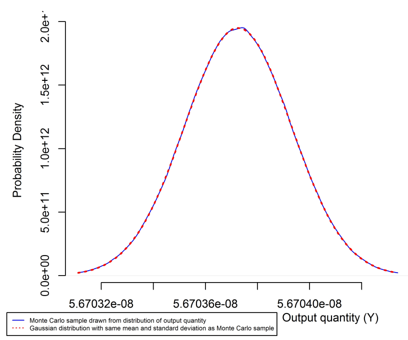


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Figure 7: **Stefan-Boltzmann Constant.** Input and output Web pages for the example discussed in §10.

	Mod(S)	u(Mod(S))	Arg(S)	u(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(Arg(S)) expressed in radian.

(U-8) on Page 10. 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. If $\boldsymbol{y} = \boldsymbol{f}(x_1, \dots, x_n)$ is the measurement model for a p-dimensional output quantity $\boldsymbol{y} = (y_1, \dots, y_p)$, then the model may be re-written as a system of p simultaneous measurement equations $y_1 = f_1(x_1, \dots, x_n)$, ..., $y_p = f_p(x_1, \dots, x_n)$, where $\boldsymbol{f} = (f_1, \dots, f_p)$.

The 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, ..., y_p of the vectorial output quantity; (ii) read this file into some statistical analysis computing environment, for example R, and complete the uncertainty analysis for the output quantity inside 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 Γ 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 27 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**.

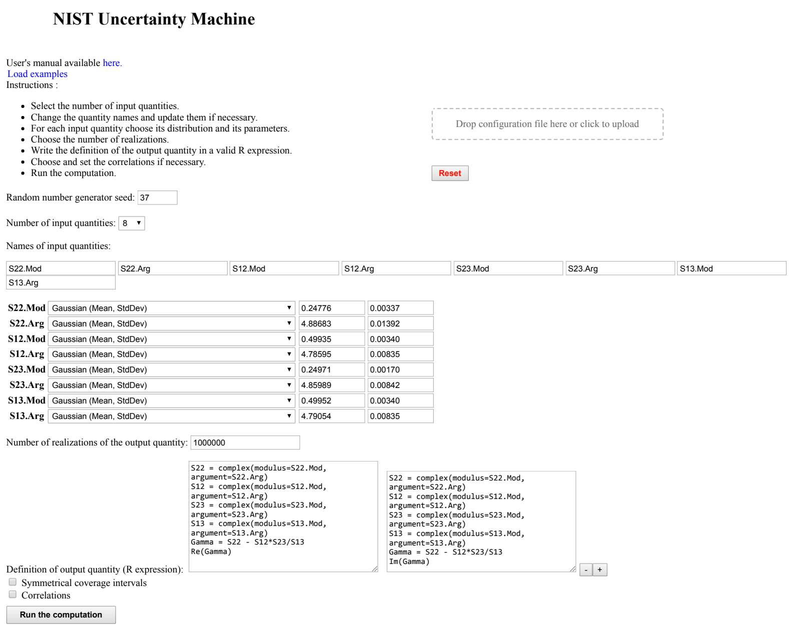


Figure 8: **Voltage Reflection Coefficient.** Input Web page of the `NIST Uncertainty Machine` used for the real and imaginary parts of the complex-valued output quantity Γ discussed in §11.

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 Γ, for example as depicted in Figure 9 on Page 28, 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 $u(\Re(\Gamma)) = 0.0045$. The correlation between $\Re(\Gamma)$ and $\Im(\Gamma)$ is 0.0311.

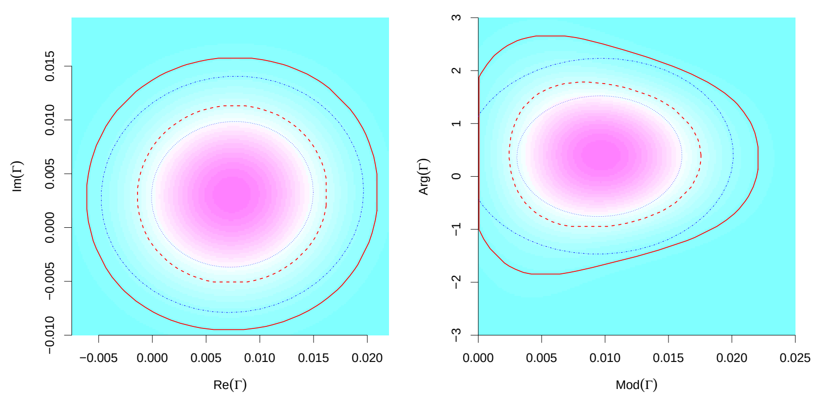


Figure 9: The left panel shows an estimate of the probability density of the joint distribution of the real and imaginary parts of Γ, and the right panel shows its counterpart for the modulus and argument of Γ. The solid (red) curves outline 95 % coverage regions, and the dashed (red) curves outline 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 Γ

```
## 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)
```

12 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 [R. S. 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`.

	^{206}Pb/^{204}Pb		^{207}Pb/^{204}Pb	
SAMPLE	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 uncertaintites derived from measurements made and reported by Connelly 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 Connelly et al. [2012] selected for their age determinations.

Since ^{206}Pb and ^{207}Pb both are radiogenic, being the end-products of the decay of ^{235}U and ^{238}U, respectively, and ^{204}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}Pb and ^{207}Pb derive entirely from uranium originally in the parent material, and none have been lost;

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

The absolute age A is the root of the equation

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

where λ_{235} and λ_{238} denote the decay constants of ^{235}U and ^{238}U, and β denotes the slope of the line (*isochron*) shown in Figure 10 [Schoene, 2014].

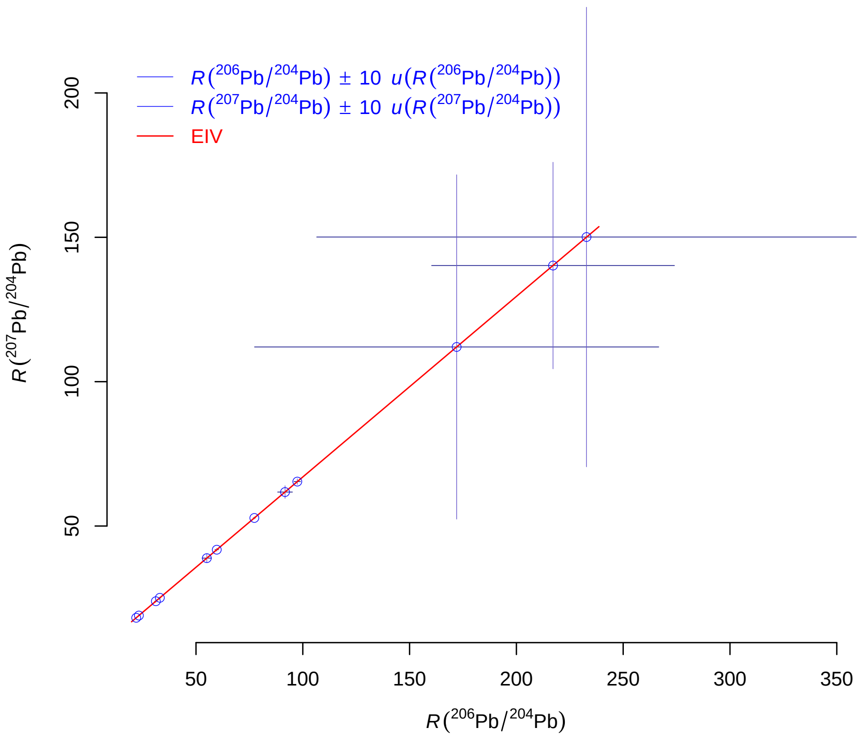


Figure 10: **Allende Isochron.** Measurement results (estimates and standard uncertainties) for lead isotope ratios used to define an isochron for chondrules C20 and C30 from the Allende meteorite. The isochron was fitted to these measurement results using errors-in-variables regression, by the method 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.

To compute estimates of the absolute age we use Equation (2) with $\lambda_{235} = \log 2/T_{½}(^{235}\mathrm{U})$, $\lambda_{238} = \log 2/T_{½}(^{238}\mathrm{U})$, and $R(^{238}\mathrm{U}/^{235}\mathrm{U}) = 137.786$ [Connelly 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 $T_{½}(^{235}\mathrm{U}) = 704\,\mathrm{Ma}$ [Bé et al., 2010] and $T_{½}(^{238}\mathrm{U}) = 4468.3\,\mathrm{Ma}$ [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).

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: $u(T_{1/2}(^{235}\mathrm{U})) = 1\,\mathrm{Ma}$ [Bé et al., 2010] and $u(T_{1/2}(^{238}\mathrm{U})) = 4.8\,\mathrm{Ma}$ [Villa et al., 2016];

(b) The uncertainty associated with the isotopic ratio of the same uranium isotopes: $u(R(^{238}\mathrm{U}/^{235}\mathrm{U})) = 0.013$ [Connelly et al., 2012, Table 1];

(c) The measurement uncertainties associated with the measured lead isotope ratios $\{u(R(^{206}\mathrm{Pb}/^{204}\mathrm{Pb}))\}$ and $\{u(R(^{207}\mathrm{Pb}/^{204}\mathrm{Pb}))\}$;

(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 $R(^{238}\mathrm{U}/^{235}\mathrm{U})$; T_{235} denoting the half-life of $^{235}\mathrm{U}$; and T_{238} denoting the half-life of $^{238}\mathrm{U}$.

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` fits 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 7. 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.

To load the specifications for this example into the `NIST Uncertainty Machine`, click **here**.

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 that 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.)

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.

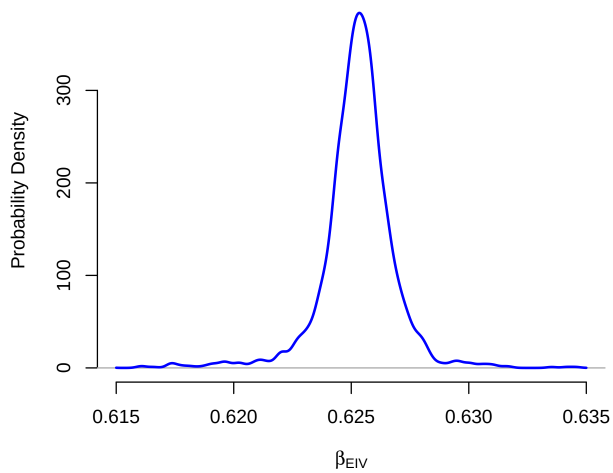


Figure 11: **Slope of Allende Meteorite Isochron.** Kernel estimate [Silverman, 1986] of the probability density of the slope of the isochron depicted in Figure 10, based on a sample of 2023 values, expressing contributions from the uncertainties associated with the isotopic ratios, and with the selection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

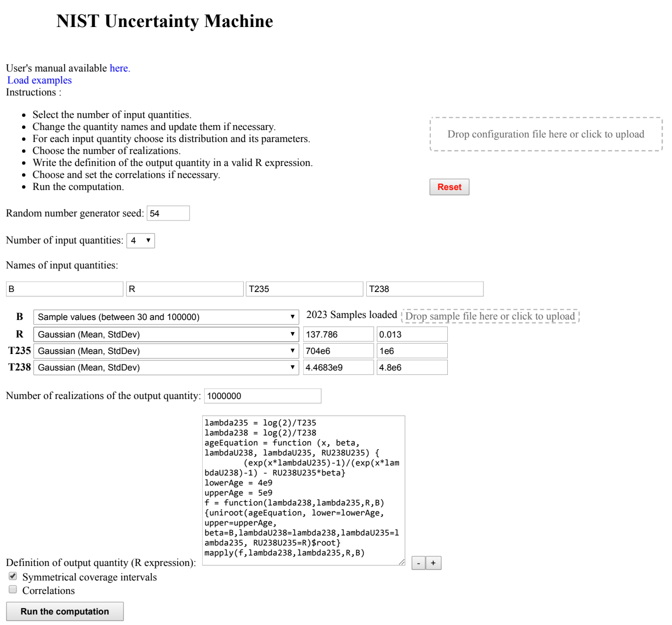
Listing 2: R code used to evaluate the measurement function that computes the age of chondrules in the Allende meteorite.

```
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 an equation (Equation (2) above) whose root is the value of f;

INPUT



NIST Uncertainty Machine

User's manual available here.
Load examples
Instructions :

- Select the number of input quantities.
- Change the quantity names and update them if necessary.
- For each input quantity choose its distribution and its parameters.
- Choose the number of realizations.
- Write the definition of the output quantity in a valid R expression.
- Choose and set the correlations if necessary.
- Run the computation.

Drop configuration file here or click to upload

Reset

Random number generator seed: 54

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

Number of realizations of the output quantity: 1000000

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*lam
bdaU238)-1) - RU238U235*beta}
lowerAge = 4e9
upperAge = 5e9
f = function(lambda238,lambda235,R,B)
{uniroot(ageEquation, lower=lowerAge,
upper=upperAge,
beta=B,lambdaU238=lambda238,lambdaU235=l
ambda235, RU238U235=R)$root}
mapply(f,lambda238,lambda235,R,B)
```

- +

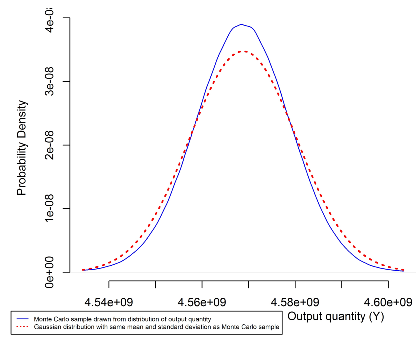
Symmetrical coverage intervals
Correlations

Run the computation

OUTPUT

NIST Uncertainty Machine

```
===== RESULTS ==============================

Monte Carlo Method

Summary statistics for sample of size 1000000

ave     = 4568800000
sd      = 1.1e+07
median  = 4568700000
mad     = 1e+07

Symmetrical coverage intervals

99% (4.5398e+09, 4.5978e+09)    k =      2.5
95% (4.5478e+09, 4.5898e+09)    k =      1.8
90% (4.5517e+09, 4.5859e+09)    k =      1.5
68% (4.5586e+09, 4.579e+09)     k =     0.89

ANOVA (% Contributions)

           w/out Residual w/ Residual
B                   29.80       29.80
R                    0.01        0.01
T235                66.61       66.59
T238                 3.58        3.57
Residual               NA        0.02

-------------------------------------------

Gauss's Formula (GUM's Linear Approximation)

       y  = 4568800000
      u(y) = 1.2e+07

             SensitivityCoeffs Percent.u2
B                      2.3e+09     31.000
R                      1.1e+07      0.014
T235                   9.4e+00     65.000
T238                  -4.5e-01      3.500
Correlations                NA      0.000
===========================================
```



Download binary R data file with Monte Carlo values of output quantity
Download a text file with Monte Carlo values of output quantity
Download text file with numerical results shown on this page
Download JPEG file with plot shown on this page
Download configuration file

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

(2) It uses a numerical method to find this root, which is implemented in R function `uniroot`;

(3) A special 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 kth element is the root of the `ageEquation` that correspond to the set of kth values of the four 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 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.

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