Resources for Uncertainty Analysis

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Overview

Comparison of experimental results from different experiments or comparison of data with models/theory is only meaningful when uncertainty estimates for data are made.

International organizations publish and periodically revise documents that define best practices and common terminology.

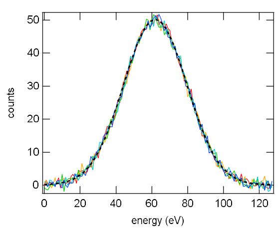
The top level international document of this type is the "GUM", the Guide to the Expression of Uncertainty in Measurement,
https://www.bipm.org/en/publications/guides/gum.html

The National Institute of Standards and Technology is the national metrology institute for the United States and publishes additional resources for uncertainty analysis.
https://www.nist.gov/pml/nist-technical-note-1297
The NIST Uncertainty Machine: https://uncertainty.nist.gov/

Student presenters at the Electronic Materials Conference may apply for the NIST Student Award by documenting an uncertainty analysis of a numerical result in their presentation due August 31, 2018.
https://www.mrs.org/60th-emc-nist-student-award

And about 200 + more …

Example: Spectroscopy Peak Location



Position
63
63
61
62
64
59
59
61

(a) Mean = 61.5 eV
$u_p = \sigma / \sqrt{N}$
= 0.65 eV

(b) Curve fit
61.9 ± 0.088 eV
Standard uncertainty
u_p = 0.088 eV

Spectrum is a Gaussian peak with noise.
Method (a): Acquire 8 spectra and locate peak value in each one, as listed in table. Take mean and uncertainty of the mean.
Method (b) Curve fit (dashed line in figure) with program that returns the uncertainty of parameters for each fit. This method of locating the peak is significantly more accurate, but not infinitely so.

A Few Definitions

Uncertainty components are classified into two categories:
Type A: those which are evaluated by statistical methods
Type B: those which are evaluated by other means, such as: experience with, or general knowledge of, the behavior of relevant materials and instruments, manufacturer's specifications, data provided in calibration and other reports
Type A is loosely referred to "random error" and Type B to "systematic error," but this nomenclature depends on the measurement process and is not absolute.

Example: Measuring the temperature *T* of a liquid bath

- Type A uncertainty: Make ten measurements of the bath temperature with a thermometer and calculate the standard deviation σ_T of those measurements; σ_T is a Type A component
- Type B uncertainty: Look up the manufacturer's specified accuracy for the thermometer u_{TM}; u_{TM} is a Type B component

Terminology relating to confidence intervals in a data distribution
Standard uncertainty (*k*=1) : one standard deviation, 68.3% confidence interval
Expanded uncertainty (*k*=2): two standard deviations, 95.5% confidence interval

Combining Uncertainties Propagation of Error

Uncertainty components to a numerical result calculated from data inputs are typically combined by one of two methods:

- Calculated with partial derivatives of the result on the data input variables (see Chapter 5 of the GUM for many examples)
- Monte Carlo simulation varying the input parameters over the uncertainty range of those parameters

Example for Statistically Independent Measurements:
Current I calculated from a set of voltage measurements of that current through a resistor with resistance R
$I = V / R$, where V is the mean value of the voltage measurements

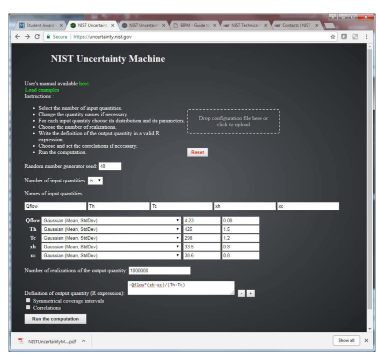
Because errors/variations in V and R are uncorrelated, these two variables are statistically independent and the combined uncertainty u_I for $I = f(V)$ is calculated as:
$(u_I)^2 = (1/R)^2 (u_V)^2 + (V/R^2)^2 (u_R)^2$

$$u_c^2(y) = \sum_{i=1}^{N} \left(\frac{\partial f}{\partial x_i} \right)^2 u^2(x_i)$$

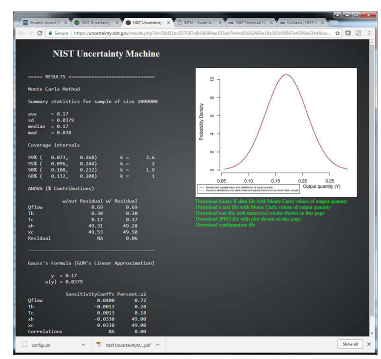
Or if we multiply both sides by $(R/V)^2 = (1/I)^2$,
$(u_I/I)^2 = (u_V/V)^2 + (u_R/R)^2$

Example for Correlated Error in Measurements: (taken from GUM, pg. 22)
Ten resistors, each of nominal resistance R_i = 1 000 Ω, are calibrated with the same 1 000 Ω standard resistor R_s characterized by a standard uncertainty $u(R_s)$ = 100 mΩ as given in its calibration certificate. The resistors are connected in series in order to obtain a reference resistance R_{ref} of nominal value 10 kΩ. The uncertainty in R_{ref} is the sum of the uncertainties in each R_i, that is $u(R_{ref})$ = 10 * 100 mΩ = 1 Ω because the same standard resistor was used in each calibration and therefore the errors in the sum are perfectly correlated and will add linearly.

Monte Carlo Example: The NIST Uncertainty Machine



Enter calculation of thermal conductivity of a bar of homogeneous material carrying a heat flow of 4.23 W with temperatures in K and distances in meters. Estimates of uncertainty are entered for each input variable and a distribution format for the deviations (Gaussian above).



The NIST Uncertainty Machine returns a value of 0.17 W K^{-1} m^{-1} ± 0.038 W K^{-1} m^{-1} based on the entered standard deviations for each input quantity.