

Uncertainty Analysis for Uncorrelated Input Quantities and a Generalization of the Welch-Satterthwaite Formula which handles Correlated Input Quantities

White Paper

Abstract—The Guide to the Expression of Uncertainty in Measurement (GUM) has been widely adopted in the different fields of the industry and science. This guide established general rules for evaluating and expressing uncertainty in the measurements. In this paper we will give an overview on how to use it for uncorrelated input quantities. We will also introduce correlated magnitudes and correlation types due to the important issue in the evaluation of measurement uncertainty as a consequence of the correlation between quantities. We will identify situations not included into the GUM, when the measurand can be expressed as a function of quantities with common sources. So the issue appears when we use the typical Welch-Satterthwaite formula used to calculate the effective number of degrees of freedom when the measurement errors are not with finite degrees of freedom and uncorrelated. We will introduce a generalization of the Welch-Satterthwaite formula for correlated components with finite degrees of freedom.

This paper will also include other methods for computing confidence limits and expanded uncertainties such as using Convolution based on mathematical methods or evaluating the measurement uncertainty based on the propagation of distributions using Monte Carlo simulation.

Speaker: Alberto Campillo
Agilent Technologies
Ctra N-VI km 18.200 Las Rozas, Madrid 28230, Spain,
Phone: (34)91-631-3155 Fax: (34)91-631-3001
E-mail: alberto_campillo@agilent.com

Introduction

In general a measurement is not measured directly, but is determined from n other quantities through a functional relationship:

$$Y = f(X_1, X_2, X_3 \dots X_n)$$

In cases where the input quantities are independent, the combined standard uncertainty is the positive square root of the combined variance which is given by:

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

Mutual dependences in the knowledge about the input quantities can be expressed as a covariance or a correlation coefficient and can be used during the propagation.

$$u_c^2(y) = \sum_{i=1}^n \sum_{j=1}^n \frac{\partial f}{\partial x_i} \frac{\partial f}{\partial x_j} u(x_i, x_j) = \sum_{i=1}^n \left(\frac{\partial f}{\partial x_i} \right)^2 u^2(x_i) + 2 \sum_{i=1}^{n-1} \sum_{j=i+1}^n \frac{\partial f}{\partial x_i} \frac{\partial f}{\partial x_j} u(x_i, x_j)$$



The degree of correlation between x_i and x_j is characterized by the estimated correlation coefficient.

$$r(x_i, x_j) = \frac{u(x_i, x_j)}{u(x_i) * u(x_j)}$$

$$u_c^2(y) = \sum_{i=1}^n c_i^2 u^2(x_i) + 2 \sum_{i=1}^{n-1} \sum_{j=i+1}^n c_i c_j u(x_i) u(x_j) r(x_i, x_j)$$

The expanded uncertainty of measurement is obtained by multiplying the standard uncertainty of the output estimate by a coverage factor k which is chosen on the basis of the desired level of confidence to be associated with the interval defined by: $U = k * u_c(y)$

When a Normal distribution can be attributed to the measurand, and the standard uncertainty associated with the output estimate has sufficient reliability, the standard coverage factor $k = 2$ shall be used.

The assumption is that the combined error follows a normal (infinite degrees of freedom) or t-Student distribution (finite degrees of freedom) results from the Central Limit Theorem.

This theorem demonstrates that the combined error distribution converges toward the normal distribution as the number of constituent errors increases, regardless of their underlying distributions (Figure 1).

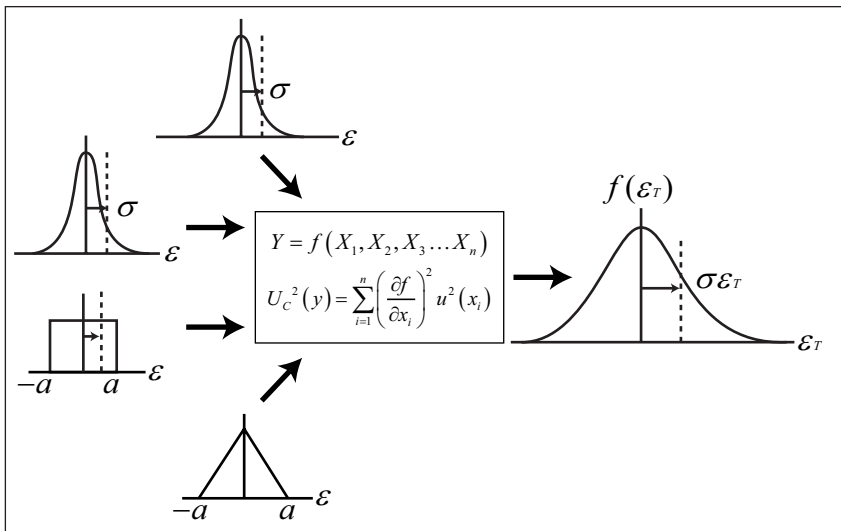


Figure 1. Combined error distribution

A first approach to determine the expanded uncertainty for a confidence level is to use a coverage factor of a normal distribution, k :

$$U = \left[U_A^2 + U_B^2 \right]^{\frac{1}{2}} = k \left[u_A^2 + u_B^2 \right]^{\frac{1}{2}}$$

If the number of random readings is small, so the value of the u_A can be not correct, and the distribution of the random component is better to represent it by a t -Student distribution, but now we could overvalue the uncertainty, especially if the number of measurements is small and the u_A and u_B values are similar in size

$$U = \left[t^2 * u_A^2 + k^2 * u_B^2 \right]^{\frac{1}{2}}$$

So the best way to solve this problem is using the approach of the Welch Satterwaite formula.

If a Normal distribution can be assumed, but the standard uncertainty associated with the output estimate is with insufficient reliability and it is not possible to increase the number of repeated measurements, we will use the Welch Satterthwaite formula. In such a case, the reliability of the standard uncertainty assigned to the output estimate is determined by its effective degrees of freedom.

Considering a direct measurement of n independent measurement errors, the distribution may be approximated by a t -distribution with an effective degrees of freedom ν_{eff} obtained from the Welch Satterthwaite formula:

$$\nu_{eff} = \frac{u_C^4(y)}{\sum_{i=1}^n \frac{u_i^4(y)}{\nu_i}}$$

The coverage factor $k(p)$ will be obtained from the t-student distribution evaluated for a coverage probability of 95.45 %.

Degrees of Freedom	Fraction p in percent					
	68.27 ⁵	90	95	95.45 ⁵	99	99.73 ⁵
1	1.84	6.31	12.71	13.97	63.66	235.80
2	1.32	2.92	4.30	4.53	9.92	19.21
3	1.20	2.35	3.18	3.31	5.84	9.22
4	1.14	2.13	2.78	2.87	4.60	6.62
5	1.11	2.02	2.57	2.65	4.03	5.51
10	1.05	1.81	2.23	2.28	3.17	3.96
20	1.03	1.72	2.09	2.13	2.85	3.42
30	1.02	1.70	2.04	2.09	2.75	3.27
40	1.01	1.68	2.02	2.06	2.70	3.20
50	1.01	1.68	2.01	2.05	2.68	3.16
100	1.005	1.660	1.984	2.025	2.626	3.077
~	1.000	1.645	1.960	2.000	2.576	3.000

t-student distribution table

3. A normal distribution cannot be justified

In cases where the assumption of a normal distribution cannot be justified and it is not possible to apply the Central Limit Theorem, we may find situations where one of the uncertainty contributions in the budget can be identified as a dominant term or situations when two of the uncertainty contributions in the budget can be identified as dominant terms.

Knowing the distribution density $\varphi(y)$ we can determine the coverage probability p , using the following integral relation:

$$p(U) = \int_{y-U}^{y+U} \varphi(y) dy$$

As the coverage factor may be expressed as:

$$k(p) = \frac{U(p)}{u(y)}$$

3.1 Cases where we have a rectangular distribution as a dominant term:

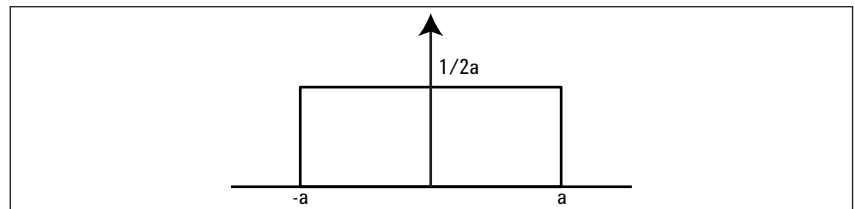


Figure 2. Rectangular distribution

Solving this relation for the Expanded Uncertainty U and inserting the result together with the expression of the Standard Measurement Uncertainty related to a Rectangular Distribution given by:

$$p(U) = \int_{y-U}^{y+U} \varphi(y) dy = \int_{y-U}^{y+U} \frac{1}{2a} dy = \frac{y+U - (y-U)}{2a} = \frac{U}{a}$$

$$u(y)^2 = \frac{a^2}{3}$$

Finally gives the relation:

$$u(y) = \frac{a}{\sqrt{3}} \quad k(p) = \frac{U(p)}{u(y)} = \frac{p \cdot a}{\frac{a}{\sqrt{3}}} = p \cdot \sqrt{3}$$

And for a Coverage Probability $p = 95\%$, the coverage factor k is:

$$k(p) = 0.95 \cdot \sqrt{3} = 1.645 \cong 1.65$$

3.2 Cases where two of the uncertainty contributions in the budget can be identified as dominant terms.

This will involve evaluation of the coverage factor of a stated coverage probability for the convolved distributions.

So depending on the distribution types which are convolved, the coverage factor for a coverage probability of 95.45 % may be obtained from the following Table 1 depending of the stated ratio:

$U(y)$ N/R	$k_{95.45\%}$	$U(y)$ N/U	$k_{95.45\%}$	$U(y)$ R/U	$k_{95.45\%}$	$U(y)$ R/R	$k_{95.45\%}$
0.0	1.65	0.0	1.41	0.0	1.41	0.0	1.65
0.4	1.79	0.4	1.71	0.4	1.73	0.2	1.71
0.8	1.92	0.8	1.89	0.8	1.88	0.4	1.82
1.0	1.95	1.0	1.93	2.0	1.86	0.6	1.89
1.4	1.98	1.4	1.97	6.0	1.70	0.8	1.92
∞	2.00	∞	2.00	∞	1.65	1	1.93

N: Normal, R: Rectangular, U: U-Shaped

Table 1. If two distributions are convolved, the Coverage Factor k is obtained from the following table

4. Distribution for Combined error using convolution

In case where two or more errors are statistically independent, the distribution for the combined errors can be obtained by convolution. This method can be applied for direct measurements where the measurement process errors are statistically independent, so no error correlations.

$$\varphi(y) = (f * g)(y) = \int_{-\infty}^{\infty} f(\tau) g(y - \tau) d\tau$$

4.1 Convolution of two Rectangular Distributions:

If dominant contributions arise from Rectangular Distributions of values, the distribution resulting from convolving then gives a symmetrical Trapezoidal Distribution (Figure 3).

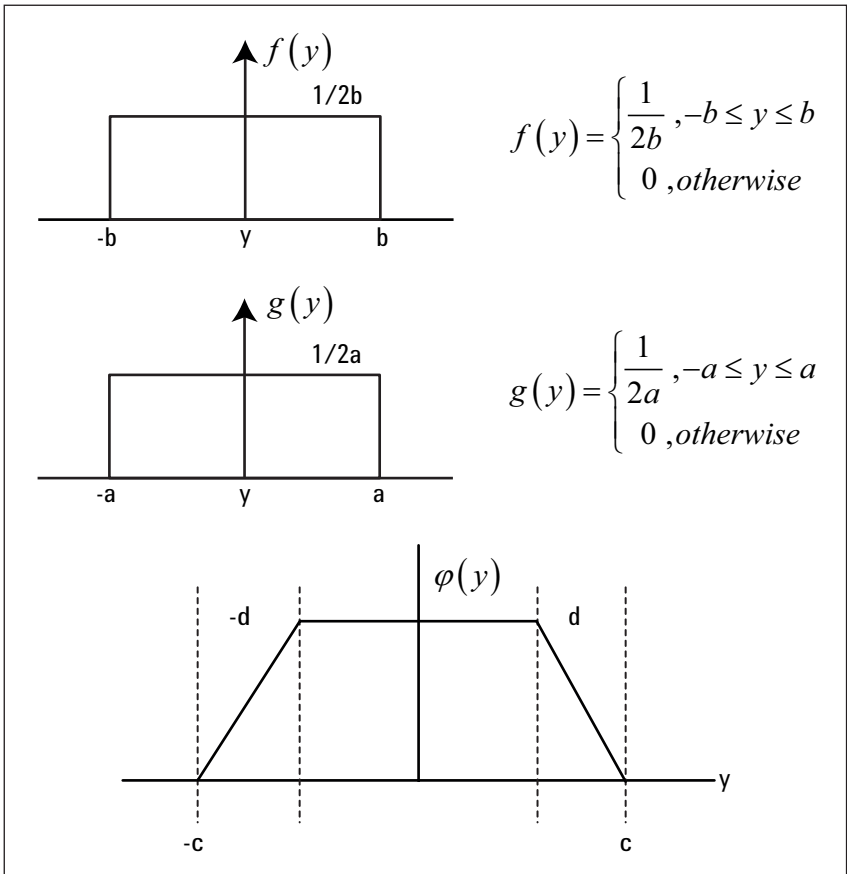


Figure 3. Symmetrical Trapezoidal distribution

Where the half widths of the base and top respectively are: $c = b + a$ and $d = |b - a|$ and the edge parameter:

$$\beta = \frac{d}{c} = \frac{|b - a|}{b + a}$$

Where the distribution density may be conveniently expressed in the form:

$$\varphi(y) = \frac{1}{c(1 + \beta)} * \begin{cases} 1 & \text{if } |y| < \beta.c \\ 0 & \text{if } c < |y| \end{cases}$$

$$\varphi(y) = \frac{1}{c(1 + \beta)} * \frac{1}{1 - \beta} * \left(1 - \frac{|y|}{c}\right) \quad \text{if } \beta.c \leq |y| \leq c$$

The square of the standard measurement uncertainty deduced from the trapezoidal distribution is:

$$u^2(y) = \frac{c^2}{6}(1 + \beta^2)$$

Knowing that the coverage probability is:

$$p(U) = \int_{y-U}^{y+U} \varphi(y) dy$$

And the coverage factor

$$k(p) = \frac{U(p)}{u(y)}$$

So, the coverage factor will be:

$$k(p) = \frac{1}{\sqrt{\frac{1+\beta^2}{6}}} * \begin{cases} \left(1 - \sqrt{(1-p)(1-\beta^2)}\right) & \text{if } \beta \leq \frac{p}{2-p} \\ \frac{p(1+\beta)}{2} & \text{if } \beta > \frac{p}{2-p} \end{cases}$$

Finally, the coverage factor for a coverage probability of 95 % appropriate to a trapezoidal distribution with an edge parameter of $\beta < 0.95$ is calculated from the relation:

$$k(p) = \frac{1}{\sqrt{\frac{1+\beta^2}{6}}} * \left(1 - \sqrt{(1-p)(1-\beta^2)}\right)$$

$k(p)$ can change from 1.645 to 1.93 depending of β . (Table 2 and Figure 4)

Edge Parameter (β)	Coverage Factor (k)
0	1.927
0.1	1.895
0.2	1.8756
0.3	1.8457
0.4	1.8082
0.5	1.706
0.6	1.7246
0.7	1.6862
0.8	1.656
0.9	1.645

Table 2. Edge Parameter vs. Coverage Factor

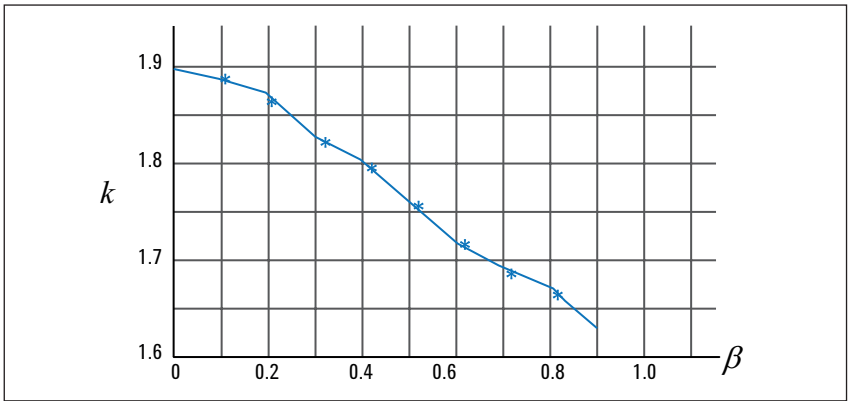


Figure 4. Coverage Factor k vs. Edge Parameter of a trapezoidal distribution

4.2 Convolution of two Gaussian Distributions

The combined error distribution takes on a Gaussian (Figure 5).

$$f(y) = \frac{1}{\sigma_1 \sqrt{2\pi}} * e^{-\frac{1}{2} \left[\frac{(x-\mu_1)}{\sigma_1} \right]^2}$$

$$g(y) = \frac{1}{\sigma_2 \sqrt{2\pi}} * e^{-\frac{1}{2} \left[\frac{(x-\mu_2)}{\sigma_2} \right]^2}$$

$$(f * g)(y) = \frac{1}{\sqrt{2\pi(\sigma_1^2 + \sigma_2^2)}} * e^{-\frac{1}{2} \left[\frac{t - (\mu_1 - \mu_2)}{(\sigma_1^2 + \sigma_2^2)} \right]^2}$$

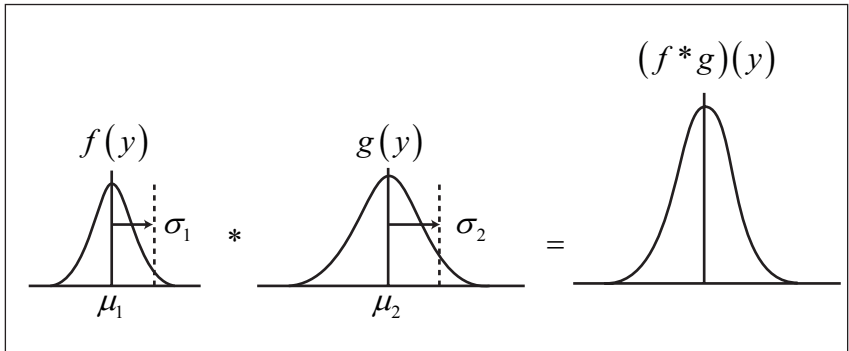


Figure 5. If two Gaussian distributions are convolved, the result is other Gaussian distribution.

5. Welch-Satterthwaite formula for correlated components

The implementation of the GUM exhibits an issue related to the effective degrees of freedom when the measurand is expressible as a function of intermediate quantities that depend on one or more shared inputs. The apparent issue is found in the fact that a linear correlation coefficient of zero does not imply statistical independence. Therefore, the variables cannot be independent unless they are normal, and both degrees of freedom are infinite. It is not specifically associated with the use of the Welch-Satterthwaite formula. It arises from loose and incomplete usage of statistical principles.

We will extend the method described in the GUM to be applicable with correlated components of uncertainty with finite degrees freedom. For this kind of condition, we can use as a generalization of the Welch-Satterthwaite formula the expression proposed by Howard Castrup [2].

So, considering now two measurement errors e_1 and e_2 with uncertainties u_1 and u_2 respectively, and whose correlation coefficient is ρ_{12} , then the variance of the total error is given by:

$$u_c^2 = u_1^2 + u_2^2 + 2\rho_{12}u_1u_2$$

Using the addition rule, we have

$$\begin{aligned} \sigma^2(u_c^2) &= \sigma^2(u_1^2) + \sigma^2(u_2^2) + 4\rho_{12}^2\sigma^2(u_1u_2) + 2\text{cov}(u_1^2, u_2^2) + \\ &4\rho_{12}\text{cov}(u_1^2, u_1u_2) + 4\rho_{12}\text{cov}(u_2^2, u_1u_2) \end{aligned}$$

Working a bit with the cross-product and covariance terms we achieve the following expression:

$$\begin{aligned} \sigma^2(u_c^2) &= 2\frac{u_1^4}{v_1} + 2\frac{u_2^4}{v_2} + \left\{ \left[\sigma^2(u_1) + u_1^2 \right] \left[\sigma^2(u_2) + u_2^2 \right] - u_1^2u_2^2 \right\} + \\ &8u_1u_2\rho_{12} \left[\sigma^2(u_1) + \sigma^2(u_2) \right] \end{aligned}$$

Knowing that $v_{eff} = \frac{2u_c^4}{\sigma^2(u_c^2)}$ and using the before expression for n

measurement errors where two or more are correlated, so the final expression to calculate the Effective Degrees of Freedom for correlated components will be:

$$\begin{aligned} v_{eff} &= u_c^4(y) / \sum_{i=1}^n \frac{u_i^4(y)}{v_i} + 2 \sum_{i=1}^{n-1} \sum_{j>1}^n \rho_{ij}^2 \left(\frac{u_i^2}{v_i} \right) \left(\frac{u_j^2}{v_j} \right) \left(v_i + v_j + \frac{1}{2} \right) + \\ &2 \sum_{i=1}^{n-1} \sum_{j>1}^n \rho_{ij} u_i u_j \left(\frac{u_i^2}{v_i} + \frac{u_j^2}{v_j} \right) \end{aligned}$$

If all the correlation coefficients are zero, this equation simplifies to the Welch-Satterthwaite formula.

6. Propagation of distributions using Monte Carlo simulation

When the model is non-linear or when the probability density function (PDF) for the output quantity departs appreciable from a Gaussian distribution or a scaled and shifted t-student distribution we will also introduce as alternative the Monte Carlo Method (MCM). This method deals with the propagation of probability distribution of the input quantities of a mathematical method of measurements.

MCM provides a method to obtain an appropriate numerical representation of the output quantity Y by means of its distribution function G , given a measurement model equation. G is obtained by sampling of the PDF of the input quantities x_i and applying the model of measurement to obtain sampled values for the output quantity Y . Expectation values, variance and coverage intervals of Y can be extracted from G .

The accuracy of the resulting G increases with the number of trials. An adaptive Monte Carlo procedure can be used instead of using a fixed number of trials to guarantee that the results achieve a required tolerance. This procedure involves carrying out an increasing number of Monte Carlo trials until mean, variance and coverage interval have stabilized. A numerical result can be considered stabilized if twice the standard deviation associated with it is less than the numerical tolerance associated with the standard uncertainty $u(y)$.

7. Learning Objectives

This paper described the method used to estimate the measurement uncertainty in accordance with the principles given in the GUM for uncorrelated input quantities, including cases where it is not possible to apply the Central Limit Theorem. This paper has also extended the method to be applicable with correlated components of uncertainty with finite degree of freedom using a generalization of the Welch-Satterthwaite formula.

Another possibility was finally introduced when all the quantities are correlated and normally distributed. The Monte Carlo Method is a useful tool, to calculate uncertainties when the conditions required applying the GUM are not met, and to validate and gain confidence with the results obtained with GUM.

The last introduced method can handle correlations as long as all quantities which are correlated are distributed normally or are totally correlated. In practice this can be an important limitation in case the distribution of the correlated quantities differs significantly from normal. Often it is not possible to specify the joint PDF for the input variables or the joint PDF may not be in a form that is easy to numerically simulate.

8. References

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