

## Calculating Propagated Uncertainties Using Higher Order Taylor Terms In the Uncertainty Analysis

Speaker/Author: Dennis W. Dubro, Ph. D.  
Pacific Gas & Electric Company  
Technical and Land Services  
3400 Crow Canyon Road  
San Ramon, CA 94583  
Telephone: (925) 866-5239  
Fax : (925) 866-5681  
Email: [dwd8@pge.com](mailto:dwd8@pge.com)

Author: Howard Castrup, Ph. D.  
President, Integrated Sciences Group

### Abstract

Most metrologists can easily calculate the variance in a multi-variate uncertainty analysis using the Law of Propagation of Uncertainties in their sleep. However, the G.U.M. (Guide to the Expression of Uncertainty in Measurement) alludes to the possibility that a measurement model might be sufficiently non-linear in the measurement parameters, that the usual method of calculation may not be adequate. This paper investigates the difficulty and properties of such a non-linear calculation by extending a measurement model out to three orders of a Taylor series expansion in two variables and compares the results with the G.U.M.'s mysterious suggestion of what the next most significant terms might look like. We come to the conclusion that the paucity of additional treatment in the G.U.M. is a clear suggestion that a metrologist would probably not want to venture there if (s)he could possibly avoid it.

The intended audience is practical metrologists who routinely perform uncertainty analyses. Almost all uncertainty analyses are based upon linear approximations of the measurement model. This paper investigates the extension of existing theory to a non-linear model and will help metrologists decide if such a model might be of benefit to their particular work.

Any experienced metrologist is long familiar with the process for calculating uncertainties propagated through a mathematical model of an experiment. The formula is known as the Law of Propagation of Uncertainty and is presented without derivation in countless books on uncertainty analysis and in the United States Guide to the Expression of Uncertainty in Measurement (G.U.M.) [1].

Equation (10) in Chapter 5 of the G.U.M. states that when dealing with several independent random uncertainties, the combined standard uncertainty  $\sigma_c(z)$  is the positive square root of the combined variance  $\sigma_c^2(z)$  obtained from

$$\sigma_c^2(z) = \sum_{i=1}^N \left( \frac{\delta f}{\delta x_i} \right)^2 \sigma^2(x_i)$$

where  $\sigma(x_i)$  is a standard uncertainty and  $f()$  is the appropriate measurement model. Later in Chapter 5 (5.2.2), the G.U.M. states that when dealing with dependent random uncertainties, the correlation term --

$$2 \sum_{i=1}^{N-1} \sum_{j=i+1}^N \frac{\delta f}{\delta x_i} \frac{\delta f}{\delta x_j} \sigma(x_i, x_j)$$

needs to be added to the above equation where

$\sigma(x_i, x_j)$  is the estimated covariance of  $x_i$  and  $x_j$ .

In a note, the G.U.M. states that the above formulae, based upon a first-order Taylor series approximation of  $z = f(x_1, x_2, \dots, x_n)$  expresses the *law of propagation of uncertainty* and that when the non-linearity of  $f()$  is significant, higher-order terms in the Taylor series expansion must be included in the calculation. And in such a case, when the distribution of each  $x_i$  is symmetric about its mean, the G.U.M. presents a mysterious formula for the most important terms of next highest order --

$$\sum_{i=1}^N \sum_{j=1}^N \left( \frac{1}{2} \left( \frac{\delta^2 f}{\delta x_i \delta x_j} \right)^2 + \frac{\delta f}{\delta x_i} \frac{\delta^3 f}{\delta x_i \delta x_j^2} \right) * \sigma^2(x_i) * \sigma^2(x_j),$$

which to an inquiring metrologist, who wonders when (s)he might have to do the hard work and carry out a non-linear analysis, begs to be investigated further to see what is involved.

For two variables,  $x$  and  $y$ , and  $N=2$ , the above expression can be expanded to

$$\begin{aligned} & [ 0.5 * f_{xx} * f_{xx} + f_x * f_{xxx} ] * (\sigma_x^2)^2 + \\ & [ 0.5 * f_{xy} * f_{xy} + f_x * f_{xyy} ] * \sigma_x^2 \sigma_y^2 + \\ & [ 0.5 * f_{xy} * f_{xy} + f_y * f_{xxy} ] * \sigma_x^2 \sigma_y^2 + \\ & [ 0.5 * f_{yy} * f_{yy} + f_y * f_{yyy} ] * (\sigma_y^2)^2 . \end{aligned}$$

In this notation, partial derivatives are represented by an "f" with suffixes of the variables to which the function f is differentiated.  $f_{xx}$  is the second partial derivative with respect to x.

As developed below in this paper, the first term in each bracket is derived from a second-order Taylor expansion, and the second term in each bracket is from a third-order expansion.

But the process is not as simple as just sharpening one's pencil and multiplying out a series of expansions. In the process, we encountered three pitfalls:

1. On beginning higher order analysis, one needs to re-investigate all one's usual assumptions regarding distributions and statistical formulae for their validity in non-linear work.
2. The G.U.M.'s mysterious formula only applies to Normal distributions, which might have been assumed, but was not explicitly stated. The G.U.M. simply says the formula applies to independent and symmetric error distributions.
3. After beginning the investigation, we came to the awareness that any analysis involving higher order terms, is most probably, going to require attention paid to correlated (non-independent) errors. This is true from the practical side in which a real calibration problem will probably have some type of correlated errors. And it is also true from a mathematical perspective in that the mathematical form of a correlation can produce higher order cross-product expectation values which do not reduce to zero even if the errors are not correlated.

In addressing Pitfall #1, it is important to go back to the definition of a variance and work through the derivation of the Law of the Propagation of Uncertainties because there are a number of subtleties involved. "The Law", is almost intuitively acceptable to most people. And it is statistically valid for a first-order Taylor series. In that case, it follows immediately from the statistical identity that the variance of a sum of independent random variables is equal to the sum of the variances of those random variables:

$$\text{var}(x_1 + x_2 + \dots + x_n) = \text{var}(x_1) + \text{var}(x_2) + \dots + \text{var}(x_n)$$

If the random variables are not independent, then the addition of the covariance terms is needed. One can easily see, that a first-order Taylor approximation of errors is simply a sum of random errors, each scaled by its partial derivative, and this fits the statistical identity above.

However, when a higher order Taylor series is used, you no longer have a simple linear sum of random variables. You have a sum of mixed powers of random variables and to calculate a variance, we need to return to the rigorous definition of a variance of a random variable, z, which is the second moment minus the first moment squared --

$$\sigma_z^2 = E[z^2] - E[z]^2.$$

In a higher order expansion of z, the expectation value of z is not zero even if the component errors are symmetric about their origins.

To illustrate this, we begin with a general Taylor series expansion where

$$z = f(x_1, x_2, \dots, x_n)$$

To calculate the error,  $\Delta z$ , the zeroth order term is subtracted from the function so that it appears on the left side of the equation and the rest of the expansion appears on the right.

$\Delta z =$

$$f(x_1, x_2, \dots, x_k) - f(x_{10}, x_{20}, \dots, x_{k0}) = \sum_{j=1}^n \frac{1}{j!} \left( \sum_{i=1}^k (x_i - x_{i0}) \frac{\partial}{\partial x_i} \right)^j f(x_1, x_2, \dots, x_k) \Big|_o + R_n$$

where  $R_n$  is the usual remainder term. For a second-order Taylor expansion in two variables, the error looks like --

$$\Delta z = \left( \Delta x \frac{\partial f}{\partial x} + \Delta y \frac{\partial f}{\partial y} \right) + \left( \Delta x^2 \frac{\partial^2 f}{\partial x^2} + 2\Delta x \Delta y \frac{\partial^2 f}{\partial x \partial y} + \Delta y^2 \frac{\partial^2 f}{\partial y^2} \right)$$

and even if the x and the y variables are normally distributed, the expectation value of  $\Delta z$  is not equal to zero because of the squared terms in the x and the y errors.

The results for a second order expansion in two variables are shown below, to illustrate the process and the symbolic notation. The results for a third order expansion in two variables are shown in Appendix A.

For symmetric distributions many of the expectation values calculated will be zero. For the sake of generality, the calculation will assume that the variables are correlated and all terms are retained, even if their expectation values will later be set to zero, but non-zero expectation values (for symmetric distributions) will be shown in **boldface** type. Of special interest are expectation values containing cross-products. They are interesting with regard to Pitfall #3 because not all of them are zero, even though the variables are not correlated. These expectation values are shown indented and in *italics*.

It is a unique property of statistics that even though we do not know the probability density function of joint random variables, we can still represent various formulae and functions with the expectation values of the sums of powers of the variables.

For a second order Taylor expansion of the function  $z = f(x, y)$ , the error in z,  $\Delta z$ , is equal to the sum of the Error terms shown in Table 1, below. The results of the further stages of the variance calculation are shown in the tables following.

Table 1 -- Error terms of Taylor expansion (to 2nd order)

Coef	Error	Coef	E[Error]
1st Order			
1	$\Delta X * f_x$	1	$E[X] * f_x$
1	$\Delta Y * f_y$	1	$E[Y] * f_y$
2nd Order			
0.5	$\Delta X^2 * f_{xx}$	0.5	$E[X^2] * f_{xx}$
1.0	$\Delta X * \Delta Y * f_{xy}$	1.0	$E[XY] * f_{xy}$
0.5	$\Delta Y^2 * f_{yy}$	0.5	$E[Y^2] * f_{yy}$

The next table, Table 2, shows squared error terms from a 2nd order Taylor expansion.

Table 2 -- Error<sup>2</sup> terms from Table 1

Coef	Error <sup>2</sup>	Coef	E[Error <sup>2</sup> ]
Terms from 1st order expansion			
1	$\Delta X^2 * f_x^2$	1	$E[X^2] * f_x^2$
2	$\Delta X * \Delta Y * f_x * f_y$	2	$E[XY] * f_x * f_y$
1	$\Delta Y^2 * f_y^2$	1	$E[Y^2] * f_y^2$
Terms from 2nd order expansion			
1	$\Delta X^3 * f_x * f_{xx}$	1	$E[X^3] * f_x * f_{xx}$
2	$\Delta X^2 * \Delta Y * f_x * f_{xy}$	2	$E[X^2Y] * f_x * f_{xy}$
1	$\Delta X * \Delta Y^2 * f_x * f_{yy}$	1	$E[XY^2] * f_x * f_{yy}$
1	$\Delta X^2 * \Delta Y * f_{xx} * f_y$	1	$E[X^2Y] * f_{xx} * f_y$
2	$\Delta X * \Delta Y^2 * f_{xy} * f_y$	2	$E[XY^2] * f_{xy} * f_y$
1	$\Delta Y^3 * f_y * f_{yy}$	1	$E[Y^3] * f_y * f_{yy}$
0.25	$\Delta X^4 * f_{xx}^2$	0.25	$E[X^4] * f_{xx}^2$
1	$\Delta X^3 * \Delta Y * f_{xx} * f_{xy}$	1	$E[X^3Y] * f_{xx} * f_{xy}$
0.5	$\Delta X^2 * \Delta Y^2 * f_{xx} * f_{yy}$	0.5	$E[X^2Y^2] * f_{xx} * f_{yy}$
1	$\Delta X^2 * \Delta Y^2 * f_{xy}^2$	1	$E[X^2Y^2] * f_{xy}^2$
1	$\Delta X * \Delta Y^3 * f_{xy} * f_{yy}$	1	$E[XY^3] * f_{xy} * f_{yy}$
0.25	$\Delta Y^4 * f_{yy}^2$	0.25	$E[Y^4] * f_{yy}^2$

And finally terms of the variance are shown in Table 3 before expectation values are calculated. It uses the expectation values from Table 1 and Table 2.

Table 3 -- Variance terms summed from the formula  $E[\text{Error}^2] - E[\text{Error}]^2$

Coef	$E[\text{Error}^2]$	Coef	$E[\text{Error}]^2$
Terms from 1st order expansion			
1	$E[X^2] * f_x^2$	-1	$E[X]^2 * f_x^2$
2	$E[XY] * f_x * f_y$	-2	$E[X] * E[Y] * f_x * f_y$
1	$E[Y^2] * f_y^2$	-1	$E[Y]^2 * f_y^2$
Terms from 2nd order expansion			
1	$E[X^3] * f_x * f_{xx}$	-1	$E[X^2] * E[X] * f_x * f_{xx}$
2	$E[X^2Y] * f_x * f_{xy}$	2	$E[XY] * E[X] * f_x * f_{xy}$
1	$E[XY^2] * f_x * f_{yy}$	-1	$E[X] * E[Y^2] * f_x * f_{yy}$
1	$E[X^2Y] * f_{xx} * f_y$	-1	$E[X^2] * E[Y] * f_{xx} * f_y$
2	$E[XY^2] * f_{xy} * f_y$	-2	$E[XY] * E[Y] * f_{xy} * f_y$
1	$E[Y^3] * f_y * f_{yy}$	-1	$E[Y^2] * E[Y] * f_y * f_{yy}$
0.25	$E[X^4] * f_{xx}^2$	-0.25	$E[X^2]^2 * f_{xx}^2$
1	$E[X^3Y] * f_{xx} * f_{xy}$	-1	$E[X^2] * E[XY] * f_{xx} * f_{xy}$
0.5	$E[X^2Y^2] * f_{xx} * f_{yy}$	-0.5	$E[X^2] * E[Y^2] * f_{xx} * f_{yy}$
1	$E[X^2Y^2] * f_{xy}^2$	-1	$E[XY]^2 * f_{xy}^2$
1	$E[XY^3] * f_{xy} * f_{yy}$	-1	$E[XY] * E[Y^2] * f_{xy} * f_{yy}$
0.25	$E[Y^4] * f_{yy}^2$	-0.25	$E[Y^2]^2 * f_{yy}^2$

One thing the G.U.M. doesn't say is that when determining which of the next higher order terms are relevant, they are assuming Normal distributions. The G.U.M only says it assumes independent and symmetric distributions, but in order to get the same terms as shown in the G.U.M., the distributions must also be Normal and the following relations apply.

$$E[X^2] = \sigma_x^2$$

$$E[Y^2] = \sigma_y^2$$

$$E[XY] = \rho\sigma_x\sigma_y$$

$$E[X^4] = 3\sigma_x^4$$

$$E[Y^4] = 3\sigma_y^4$$

$$E[X^2Y] = 0 \text{ and } E[XY^2] = 0$$

$$E[X^3] = 0 \text{ and } E[Y^3] = 0$$

$$E[X^2Y^2] = (1+2\rho^2) \sigma_x^2\sigma_y^2 \quad \text{Note: this is the illustration of Pitfall \#3. If correlation terms are dropped too soon, before the expectation values are calculated, this term disappears.}$$

However, from this equivalent formula, it is seen that part of the term remains even when  $\rho = 0$ .

$$E[X^3Y] = 3\rho\sigma_x^3\sigma_y$$

$$E[XY^3] = 3\rho\sigma_x\sigma_y^3$$

The final terms of the variance for the special case of symmetric independent errors are shown in Table 4. With simple re-arrangement and combination, it is easily seen that the terms from the 2nd order expansion can be converted into the first terms in the G.U.M.'s mysterious formula.

Table 4 -- Variance terms for independent Normal errors

Terms from 1st order expansion

1.00	$E[X^2] * f_x^2$	$= f_x * f_x * \sigma_x^2$
1.00	$E[Y^2] * f_y^2$	$= f_y * f_y * \sigma_y^2$

Terms from 2nd order expansion

0.25	$E[X^4] * f_{xx}^2$	$= 0.25 * 3 * f_{xx} * f_{xx} * \sigma_x^4$
-0.25	$E[X^2]^2 * f_{xx}^2$	$= -0.25 * f_{xx} * f_{xx} * \sigma_x^4$
1.00	$E[X^2] * E[Y^2] * f_{xy}^2$	$= 2 * (0.5 * f_{xy} * f_{xy} * \sigma_x^2 \sigma_y^2)$
0.25	$E[Y^4] * f_{yy}^2$	$= 0.25 * 3 * f_{yy} * f_{yy} * \sigma_y^4$
-0.25	$E[Y^2]^2 * f_{yy}^2$	$= -0.25 * f_{yy} * f_{yy} * \sigma_y^4$

A review of Appendix A and all the terms generated up to a third order expansion leads one to quickly appreciate the work involved -- especially if many of the terms do not go to zero. Table 5, below, lists the number of terms proceeding from each order of expansion for two variables, including a 4th order expansion whose results are not shown. To the extent investigated by this paper, of four orders (fourth order not shown) of expansion in two variables, the terms stemming from one order of expansion did not mix with terms stemming from a different order. The number of terms proliferate as a power as you allow the expansions to include three and more variables.

Table 5 -- Terms generated from each order of expansion

	Initial terms in expansion	Final terms in variance
1st order expansion	2	3
2nd order expansion	5	15
3rd order expansion	9	45
4th order expansion (not shown)	14	105

### Example

An example should serve to illustrate the practical side of such a calculation. Suppose that we seek the volume V of a right cylinder by measuring its length L (x) and diameter D (y). Imagine that these measurements are made by the same person (operator) using the same device, e.g., a micrometer, which will illustrate the realistic occasion of dealing with non-independent parameters. The "system equation" is

$V = \pi L \left( \frac{D}{2} \right)^2$  which for ease of interpretation with the algebra used, can be rewritten as

$$V = \pi x \left( \frac{y}{2} \right)^2$$

The relevant partial derivatives in a 2nd order Taylor series expansion are shown below.

$$f_x = \frac{\delta V}{\delta x} = \pi \left( \frac{D}{2} \right)^2 \quad f_y = \frac{\delta V}{\delta y} = \pi L \left( \frac{D}{2} \right) \quad f_{xy} = \frac{\delta^2 V}{\delta x \delta y} = \pi \left( \frac{D}{2} \right) = f_{yx}$$

$$f_{yy} = \frac{\delta^2 V}{\delta y^2} = \pi \left( \frac{L}{2} \right) \quad f_{xx} = 0$$

Assume that the error in the length measurement is normally distributed and is equal to  $\sigma_L$  and the error in the diameter measurement is also normally distributed and equal to  $\sigma_D$ . Allowing for correlation and symmetric error distribution functions, the variance of the volume can be calculated using the boldface terms for the variance from Table 3.

$$\begin{aligned} \sigma_V^2 = & \sigma_x^2 * f_x^2 && + 2 * \rho \sigma_x \sigma_y * f_x * f_y \\ & + \sigma_y^2 * f_y^2 && + 0.25 * 3 * \sigma_x^4 * f_{xx}^2 \\ & - 0.25 * \sigma_x^4 * f_{xx}^2 && + 3 * \rho \sigma_x^3 \sigma_y * f_{xx} * f_{xy} \\ & - \sigma_x^2 \rho \sigma_x \sigma_y * f_{xx} * f_{xy} && + 0.5 * (1 + \rho^2) \sigma_x^2 \sigma_y^2 * f_{xx} * f_{yy} \\ & - 0.5 * \sigma_x^2 \sigma_y^2 * f_{xx} * f_{yy} && + (1+2\rho^2) \sigma_x^2 \sigma_y^2 * f_{xy}^2 \\ & - \rho^2 \sigma_x^2 \sigma_y^2 * f_{xy}^2 && + 3 * \rho \sigma_x \sigma_y^3 * f_{xy} * f_{yy} \\ & - \rho \sigma_x \sigma_y \sigma_y^2 * f_{xy} * f_{yy} && + 0.25 * 3 * \sigma_y^4 * f_{yy}^2 \\ & - 0.25 * \sigma_y^4 * f_{yy}^2 \end{aligned}$$

where  $\rho$  is the correlation coefficient between the errors in L and D. Since the measurements of L and D were made by the same person using the same micrometer, this coefficient is not zero, that is to say that there are micrometer bias and operator bias correlations between the measurements of L and D. The expression for the correlation coefficient is

$$\rho = \frac{1}{\sigma_L \sigma_D} \sum_{i=1}^{n_L} \sum_{j=1}^{n_D} \rho_{L,D,i,j} \sigma_{L,i} \sigma_{D,j}$$

where  $\rho_{L,D,i,j}$  is the correlation between the *i*th error component of L and the *j*th error component of D. Let  $\sigma_{L,b}$  and  $\sigma_{L,op}$  represent the uncertainty due to micrometer bias and operator bias in the length measurement and let  $\sigma_{D,b}$  and  $\sigma_{D,op}$  represent the uncertainty due to micrometer bias and operator bias in the diameter measurement. Then

$$\rho = 1/\sigma_L \sigma_D ( \rho_{L,D,b,b} \sigma_{L,b} \sigma_{D,b} + \rho_{L,D,op,op} \sigma_{L,op} \sigma_{D,op} )$$



Imagine that micrometer bias and operator bias are the only measurement errors present. (Ordinarily, uncertainties due to random error, micrometer resolution and environment would be included in  $\sigma_L$  and  $\sigma_D$ . The analysis presented here is for purposes of illustration only.)

$$\begin{aligned}\sigma_{L,b} &= 0.0045 \text{ cm} \\ \sigma_{L,op} &= 0.0030 \text{ cm} \\ \sigma_{D,b} &= 0.0045 \text{ cm} \\ \sigma_{D,op} &= 0.0030 \text{ cm}\end{aligned}$$

$$\sigma_L = \sqrt{\sigma_{L,b}^2 + \sigma_{L,op}^2} = 0.0054 \text{ cm}$$

$$\sigma_D = \sqrt{\sigma_{D,b}^2 + \sigma_{D,op}^2} = 0.0054 \text{ cm}$$

Suppose that the only error sources in these measurements are those due to operator bias and device parameter bias. We can estimate the correlation coefficients between x and y to be

$$\begin{aligned}\rho_{L,D,b,b} &= 1.0 \\ \rho_{L,D,op,op} &= 0.5\end{aligned}$$

$$\rho = [(1.0)(0.0045)(0.0045) + (0.5)(0.0030)(0.0030)] / [(0.0054)(0.0054)] = 0.849$$

Consider a 1 cc cylinder with L= 0.65 cm and D= 1.4 cm. We can then substitute for the  $\sigma$ 's,  $\rho$  and partial derivatives in the above equation and obtain --

$$\begin{aligned}\sigma_V^2 = & (0.0054)^2 * (\pi(D/2)^2)^2 & + 2(0.849)(0.0054)(0.0054)\pi(D/2)^2\pi(L/2) \\ & + (0.0054)^2 * (\pi(L/2))^2 & + 0 \\ & + 0 & + 0 \\ & + 0 & + 0 \\ & + 0 & + (1+2(0.849)^2) (0.0054)^2(0.0054)^2 * (\pi(D/2))^2 \\ & - (0.849)^2(0.0054)^2(0.0054)^2 * (\pi(D/2))^2 & \\ & & + 3(0.849)(0.0054)(0.0054)^3 * \pi(D/2) * \pi(L/2) \\ & - (0.849)(0.0054)(0.0054)(0.0054)^2 * \pi(D/2) * \pi(L/2) & \\ & & + 0.25 * 3(0.0054)^4 * (\pi(L/2))^2 \\ & - (0.25)(0.0054)^4 * (\pi(L/2))^2\end{aligned}$$

With a final substitution for L and D, the result is  $\sigma_V^2 = 0.00024 \text{ cm}^2$  and  $\sigma_V = 0.015 \text{ cm}$ .

If the correlation coefficient is not taken into account  $\sigma_V = 0.011 \text{ cm}$ . This calculation was carried out with a 2nd order Taylor series. If a 3rd order Taylor series was used (using the terms from Appendix A) the result is not significantly different, since the extra odd terms tend to zero.

## Conclusion

The primary purpose of this paper has been to address the questions raised by the complex formula in the G.U.M. on the propagation of uncertainties in a non-linear uncertainty analysis. The authors have done the hard and intimidating work of expanding the mathematics and analyzing the resultant terms for their significance. That level of work shows the tremendous number of questions that would have to be analyzed and answered in terms of correlations, cross-correlations and symmetry of probability density functions. The work presented should deter the metrologist from trying to carry out a higher order Taylor analysis unless it is absolutely necessary. Even in this simple examination of two variables carried out to three orders of expansion, it was necessary to write a symbolic manipulator to carry out the expansions and accumulate the terms for this analysis. Such programs can be purchased, but the difficulty would still lie in evaluating each of the potentially hundreds of terms, unless the errors are independent and symmetric, and even then, the numbers of terms can be intimidating.

In carrying out the analysis, some "not so apparent" properties of a variance (a pitfall) have come forth which have produced the opportunity to address them by returning to the full definition of the variance, completing the calculation using higher order terms, and thereby increasing our understanding of it. A similar pitfall was discovered and addressed by elimination of correlation terms prematurely in the analysis. There are many cases in statistics where the full formula is not used because of simplifying assumptions, and this can lead to distorted results in the mathematics.

It appears that the message of the G.U.M., in presenting an intimidating formula for higher order analysis is, "Are you sure you want to go there?"

## References

1. U.S. Guide to the Expression of Uncertainty in Measurement, ANSI/NCLS Z540-2-1997

Appendix A -- Variance calculated for a measurement error model in two parameters carried out to a third order Taylor expansion.

If a given parameter, z, is calculated as a function several variables

$$z = f(x_1, x_2, \dots, x_N)$$

an estimate of uncertainty in z can be obtained by expanding the function in a Taylor series of different orders, depending upon the judgment of the experimentalist, and a variance can be calculated, as discussed in the paper, from --

$$\sigma_z^2 = E[Z^2] - E[Z]^2$$

For a third order Taylor expansion of the function  $z = f(x, y)$ , the error in z,  $\Delta z$ , is equal to the sum of the Error terms shown in Table A-1, below. The results of the further stages of the variance calculation are shown in the tables following. For symmetric distributions many of the expectation values calculated will be zero. For the sake of generality, the calculation will assume that the variables are correlated and all terms are retained, even if their expectation values will later be set to zero but non-zero expectation values (for symmetric distributions) will be shown in **boldface** type. Of special interest, as explained in the text, are expectation values containing cross-products. These expectation values are shown indented and in *italics*.

Table A-1 -- Error terms of Taylor expansion (to 3rd order)

Coef	Error	Coef	E[Error]
<b>1st Order</b>			
1	$\Delta X * f_x$	1	$E[X] * f_x$
1	$\Delta Y * f_y$	1	$E[Y] * f_y$
<b>2nd Order</b>			
0.5	$\Delta X^2 * f_{xx}$	0.5	<b><math>E[X^2] * f_{xx}</math></b>
1.0	$\Delta X * \Delta Y * f_{xy}$	1.0	<i><math>E[XY] * f_{xy}</math></i>
0.5	$\Delta Y^2 * f_{yy}$	0.5	<b><math>E[Y^2] * f_{yy}</math></b>
<b>3rd Order</b>			
0.1667	$\Delta X^3 * f_{xxx}$	0.1667	$E[X^3] * f_{xxx}$
0.5	$\Delta X^2 * \Delta Y * f_{xxy}$	0.5	<i><math>E[X^2Y] * f_{xxy}</math></i>
0.5	$\Delta X * \Delta Y^2 * f_{xyy}$	0.5	<i><math>E[XY^2] * f_{xyy}</math></i>
0.1667	$\Delta Y^3 * f_{yyy}$	0.1667	$E[Y^3] * f_{yyy}$

The next table, Table A-2, shows squared error terms from the Taylor expansion.

Table A-2 -- Error<sup>2</sup> terms from Table A-1

Coef	Error <sup>2</sup>	Coef	E[Error <sup>2</sup> ]
<b>Terms from 1st order expansion</b>			
1	$\Delta X^2 * fx^2$	1	$E[X^2] * fx^2$
2	$\Delta X * \Delta Y * fx * fy$	2	$E[XY] * fx * fy$
1	$\Delta Y^2 * fy^2$	1	$E[Y^2] * fy^2$
<b>Terms from 2nd order expansion</b>			
1	$\Delta X^3 * fx * fxx$	1	$E[X^3] * fx * fxx$
2	$\Delta X^2 * \Delta Y * fx * fxy$	2	$E[X^2Y] * fx * fxy$
1	$\Delta X * \Delta Y^2 * fx * fyy$	1	$E[XY^2] * fx * fyy$
1	$\Delta X^2 * \Delta Y * fxx * fy$	1	$E[X^2Y] * fxx * fy$
2	$\Delta X * \Delta Y^2 * fxy * fy$	2	$E[XY^2] * fxy * fy$
1	$\Delta Y^3 * fy * fyy$	1	$E[Y^3] * fy * fyy$
0.25	$\Delta X^4 * fxx^2$	0.25	$E[X^4] * fxx^2$
1	$\Delta X^3 * \Delta Y * fxx * fxy$	1	$E[X^3Y] * fxx * fxy$
0.5	$\Delta X^2 * \Delta Y^2 * fxx * fyy$	0.5	$E[X^2Y^2] * fxx * fyy$
1	$\Delta X^2 * \Delta Y^2 * fxy^2$	1	$E[X^2Y^2] * fxy^2$
1	$\Delta X * \Delta Y^3 * fxy * fyy$	1	$E[XY^3] * fxy * fyy$
0.25	$\Delta Y^4 * fyy^2$	0.25	$E[Y^4] * fyy^2$
<b>Terms from 3rd order expansion</b>			
0.3334	$\Delta X^4 * fx * fxxx$	0.3334	$E[X^4] * fx * fxxx$
1	$\Delta X^3 * \Delta Y * fx * fxxxy$	1	$E[X^3Y] * fx * fxxxy$
1	$\Delta X^2 * \Delta Y^2 * fx * fxxy$	1	$E[X^2Y^2] * fx * fxxy$
0.3334	$\Delta X * \Delta Y^3 * fx * fyyy$	0.3334	$E[XY^3] * fx * fyyy$
0.3334	$\Delta X^3 * \Delta Y * fxxx * fy$	0.3334	$E[X^3Y] * fxxx * fy$
1	$\Delta X^2 * \Delta Y^2 * fxxxy * fy$	1	$E[X^2Y^2] * fxxxy * fy$
1	$\Delta X * \Delta Y^3 * fxxy * fy$	1	$E[XY^3] * fxxy * fy$
0.3334	$\Delta Y^4 * fy * fyyy$	0.3334	$E[Y^4] * fy * fyyy$
0.1667	$\Delta X^5 * fxx * fxxx$	0.1667	$E[X^5] * fxx * fxxx$
0.5	$\Delta X^4 * \Delta Y * fxx * fxxxy$	0.5	$E[X^4Y] * fxx * fxxxy$
0.5	$\Delta X^3 * \Delta Y^2 * fxx * fxxy$	0.5	$E[X^3Y^2] * fxx * fxxy$
0.1667	$\Delta X^2 * \Delta Y^3 * fxx * fyyy$	0.1667	$E[X^2Y^3] * fxx * fyyy$
0.3334	$\Delta X^4 * \Delta Y * fxxx * fxy$	0.3334	$E[X^4Y] * fxxx * fxy$
1	$\Delta X^3 * \Delta Y^2 * fxxxy * fxy$	1	$E[X^3Y^2] * fxxxy * fxy$
1	$\Delta X^2 * \Delta Y^3 * fxy * fxxy$	1	$E[X^2Y^3] * fxy * fxxy$
0.3334	$\Delta X * \Delta Y^4 * fxy * fyyy$	0.3334	$E[XY^4] * fxy * fyyy$
0.1667	$\Delta X^3 * \Delta Y^2 * fxxx * fyy$	0.1667	$E[X^3Y^2] * fxxx * fyy$
0.5	$\Delta X^2 * \Delta Y^3 * fxxxy * fyy$	0.5	$E[X^2Y^3] * fxxxy * fyy$
0.5	$\Delta X * \Delta Y^4 * fxxy * fyy$	0.5	$E[XY^4] * fxxy * fyy$

Table A-2 (cont.) -- Error<sup>2</sup> terms from Table A-1

Coef	Error <sup>2</sup>	Coef	E[Error <sup>2</sup> ]
0.1667	$\Delta Y^5 * f_{yy} * f_{yyy}$	0.1667	$E[Y^5] * f_{yy} * f_{yyy}$
0.0278	$\Delta X^6 * f_{xxx}^2$	0.0278	$E[X^6] * f_{xxx}^2$
0.1667	$\Delta X^5 * \Delta Y * f_{xxx} * f_{xxy}$	0.1667	$E[X^5 Y] * f_{xxx} * f_{xxy}$
0.1667	$\Delta X^4 * \Delta Y^2 * f_{xxx} * f_{xyy}$	0.1667	$E[X^4 Y^2] * f_{xxx} * f_{xyy}$
0.0556	$\Delta X^3 * \Delta Y^3 * f_{xxx} * f_{yyy}$	0.0556	$E[X^3 Y^3] * f_{xxx} * f_{yyy}$
0.25	$\Delta X^4 * \Delta Y^2 * f_{xxy}^2$	0.25	$E[X^4 Y^2] * f_{xxy}^2$
0.5	$\Delta X^3 * \Delta Y^3 * f_{xxy} * f_{xyy}$	0.5	$E[X^3 Y^3] * f_{xxy} * f_{xyy}$
0.1667	$\Delta X^2 * \Delta Y^4 * f_{xxy} * f_{yyy}$	0.1667	$E[X^2 Y^4] * f_{xxy} * f_{yyy}$
0.25	$\Delta X^2 * \Delta Y^4 * f_{xyy}^2$	0.25	$E[X^2 Y^4] * f_{xyy}^2$
0.1667	$\Delta X * \Delta Y^5 * f_{xyy} * f_{yyy}$	0.1667	$E[XY^5] * f_{xyy} * f_{yyy}$
0.0278	$\Delta Y^6 * f_{yyy}^2$	0.0278	$E[Y^6] * f_{yyy}^2$

And finally, terms of the variance are shown in Table A-3 before expectation values are calculated. It uses the expectation values from Table A-1 and Table A-2.

Table A-3 -- Variance terms summed from the formula  $E[\text{Error}^2] - E[\text{Error}]^2$

Coef	E[Error <sup>2</sup> ]	Coef	E[Error] <sup>2</sup>
Terms from 1st order expansion			
1	$E[X^2] * f_x^2$	-1	$E[X]^2 * f_x^2$
2	$E[XY] * f_x * f_y$	-2	$E[X] * E[Y] * f_x * f_y$
1	$E[Y^2] * f_y^2$	-1	$E[Y]^2 * f_y^2$
Terms from 2nd order expansion			
1	$E[X^3] * f_x * f_{xx}$	-1	$E[X^2] * E[X] * f_x * f_{xx}$
2	$E[X^2 Y] * f_x * f_{xy}$	2	$E[XY] * E[X] * f_x * f_{xy}$
1	$E[XY^2] * f_x * f_{yy}$	-1	$E[X] * E[Y^2] * f_x * f_{yy}$
1	$E[X^2 Y] * f_{xx} * f_y$	-1	$E[X^2] * E[Y] * f_{xx} * f_y$
2	$E[XY^2] * f_{xy} * f_y$	-2	$E[XY] * E[Y] * f_{xy} * f_y$
1	$E[Y^3] * f_y * f_{yy}$	-1	$E[Y^2] * E[Y] * f_y * f_{yy}$
0.25	$E[X^4] * f_{xx}^2$	-0.25	$E[X^2]^2 * f_{xx}^2$
1	$E[X^3 Y] * f_{xx} * f_{xy}$	-1	$E[X^2] * E[XY] * f_{xx} * f_{xy}$
0.5	$E[X^2 Y^2] * f_{xx} * f_{yy}$	-0.5	$E[X^2] * E[Y^2] * f_{xx} * f_{yy}$
1	$E[X^2 Y^2] * f_{xy}^2$	-1	$E[XY]^2 * f_{xy}^2$
1	$E[XY^3] * f_{xy} * f_{yy}$	-1	$E[XY] * E[Y^2] * f_{xy} * f_{yy}$
0.25	$E[Y^4] * f_{yy}^2$	-0.25	$E[Y^2]^2 * f_{yy}^2$
Terms from 3rd order expansion			
0.3334	$E[X^4] * f_x * f_{xxx}$	-0.3334	$E[X^3] * E[X] * f_x * f_{xxx}$
1	$E[X^3 Y] * f_x * f_{xxy}$	-1	$E[X^2 Y] * E[X] * f_x * f_{xxy}$

Table A-3 (cont.) -- Variance terms summed from the formula  $E[\text{Error}^2] - E[\text{Error}]^2$

Coef	$E[\text{Error}^2]$	Coef	$E[\text{Error}]^2$
1	$E[X^2Y^2] * fx * fxyy$	-1	$E[XY^2] * E[X] * fx * fxyy$
0.3334	$E[XY^3] * fx * fyyy$	-0.3334	$E[X] * E[Y^3] * fx * fyyy$
0.3334	$E[X^3Y] * fxxx * fy$	-0.3334	$E[X^3] * E[Y] * fxxx * fy$
1	$E[X^2Y^2] * fxyy * fy$	-1	$E[X^2Y] * E[Y] * fxyy * fy$
1	$E[XY^3] * fxyy * fy$	-1	$E[XY^2] * E[Y] * fxyy * fy$
0.3334	$E[Y^4] * fy * fyyy$	-0.3334	$E[Y^3] * E[Y] * fy * fyyy$
0.1667	$E[X^5] * fxx * fxxx$	-0.1667	$E[X^2] * E[X^3] * fxx * fxxx$
0.5	$E[X^4Y] * fxx * fxyy$	-0.5	$E[X^2Y] * E[X^2] * fxx * fxyy$
0.5	$E[X^3Y^2] * fxx * fxyy$	-0.5	$E[X^2] * E[XY^2] * fxx * fxyy$
0.1667	$E[X^2Y^3] * fxx * fyyy$	-0.1667	$E[X^2] * E[Y^3] * fxx * fyyy$
0.3334	$E[X^4Y] * fxxx * fxy$	-0.3334	$E[X^3] * E[XY] * fxxx * fxy$
1	$E[X^3Y^2] * fxyy * fxy$	-1	$E[X^2Y] * E[XY] * fxyy * fxy$
1	$E[X^2Y^3] * fxy * fxyy$	-1	$E[XY^2] * E[XY] * fxy * fxyy$
0.3334	$E[XY^4] * fxy * fyyy$	-0.3334	$E[XY] * E[Y^3] * fxy * fyyy$
0.1667	$E[X^3Y^2] * fxxx * fyy$	-0.1667	$E[X^3] * E[Y^2] * fxxx * fyy$
0.5	$E[X^2Y^3] * fxyy * fyy$	-0.5	$E[X^2Y] * E[Y^2] * fxyy * fyy$
0.5	$E[XY^4] * fxyy * fyy$	-0.5	$E[XY^2] * E[Y^2] * fxyy * fyy$
0.1667	$E[Y^5] * fyy * fyyy$	-0.1667	$E[Y^2] * E[Y^3] * fyy * fyyy$
0.0278	$E[X^6] * fxxx^2$	-0.0278	$E[X^3]^2 * fxxx^2$
0.1667	$E[X^5Y] * fxxx * fxyy$	-0.1667	$E[X^2Y] * E[X^3] * fxxx * fxyy$
0.1667	$E[X^4Y^2] * fxxx * fxyy$	-0.1667	$E[X^3] * E[XY^2] * fxxx * fxyy$
0.0556	$E[X^3Y^3] * fxxx * fyyy$	-0.0556	$E[X^3] * E[Y^3] * fxxx * fyyy$
0.25	$E[X^4Y^2] * fxyy^2$	-0.25	$E[X^2Y]^2 * fxyy^2$
0.5	$E[X^3Y^3] * fxyy * fxyy$	-0.5	$E[X^2Y] * E[XY^2] * fxyy * fxyy$
0.1667	$E[X^2Y^4] * fxyy * fyyy$	-0.1667	$E[X^2Y] * E[Y^3] * fxyy * fyyy$
0.25	$E[X^2Y^4] * fxyy^2$	-0.25	$E[XY^2]^2 * fxyy^2$
0.1667	$E[XY^5] * fxyy * fyyy$	-0.1667	$E[XY^2] * E[Y^3] * fxyy * fyyy$
0.0278	$E[Y^6] * fyyy^2$	-0.0278	$E[Y^3]^2 * fyyy^2$

When expectation values are calculated and parameters for independent Normal errors, as discussed in the text are substituted into the terms of Table A-3, the final terms of the variance are shown in Table A-4, and with a little re-arrangement, can be shown to match the terms "of next higher significance" in the G.U.M.. From the 3rd order expansion, there are an additional six terms, but they are raised to the sixth power and presumably are too small to be considered as significant.

Table A-4 -- Variance terms for independent Normal errors

Terms from 1st order expansion

1.00	$E[X^2] * f_x^2$	$= f_x * f_x * \sigma_x^2$
1.00	$E[Y^2] * f_y^2$	$= f_y * f_y * \sigma_y^2$

Terms from 2nd order expansion

0.25	$E[X^4] * f_{xx}^2$	$= 0.25 * 3 * f_{xx} * f_{xx} * \sigma_x^4$
-0.25	$E[X^2]^2 * f_{xx}^2$	$= -0.25 * f_{xx} * f_{xx} * \sigma_x^4$
1.00	$E[X^2] * E[Y^2] * f_{xy}^2$	$= 2 * (0.5 * f_{xy} * f_{xy} * \sigma_x^2 \sigma_y^2)$
0.25	$E[Y^4] * f_{yy}^2$	$= 0.25 * 3 * f_{yy} * f_{yy} * \sigma_y^4$
-0.25	$E[Y^2]^2 * f_{yy}^2$	$= -0.25 * f_{yy} * f_{yy} * \sigma_y^4$

Terms from 3rd order expansion

0.3334	$E[X^4] * f_x * f_{xxx}$	$= 0.333 * f_x * f_{xxx} * 3\sigma_x^4$
1	$E[X^2Y^2] * f_x * f_{xyy}$	$= f_x * f_{xyy} * \sigma_x^2 \sigma_y^2$
1	$E[X^2Y^2] * f_{xxy} * f_y$	$= f_y * f_{xxy} * \sigma_x^2 \sigma_y^2$
0.3334	$E[Y^4] * f_y * f_{yyy}$	$= 0.333 * f_y * f_{yyy} * 3\sigma_y^4$
0.0278	$E[X^6] * f_{xxx}^2$	Higher terms -- not significant
0.1667	$E[X^4Y^2] * f_{xxx} * f_{xyy}$	Higher terms -- not significant
0.25	$E[X^4Y^2] * f_{xxy}^2$	Higher terms -- not significant
0.1667	$E[X^2Y^4] * f_{xxy} * f_{yyy}$	Higher terms -- not significant
0.25	$E[X^2Y^4] * f_{xyy}^2$	Higher terms -- not significant
0.0278	$E[Y^6] * f_{yyy}^2$	Higher terms -- not significant