The Uncertainty Derivation Demystified (or maybe more mystified)

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Consider the general case of a function f of one or more measured parameters (3 are shown here):

$$f = f(x, y, z) \tag{1.1}$$

If the function f is known, then the measured values for x, y, z can be plugged into the function to produce a value for f. But whenever we speak of measured values, the issue of uncertainty arises.

The variance, σ_a^2, of a set of n measured values of the parameter a is defined by

$$\sigma_a^2 \equiv \frac{1}{n-1}\sum_{i=1}^{n}\left[\left(a_i - \bar{a}\right)^2\right]. \tag{1.2}$$

The standard deviation, σ_a, a commonly used parameter in the field of statistics and uncertainty analysis, is defined as the square root of the variance.

In order to determine a value for f, the parameters x, y, z must be measured. For systems that follow a Gaussian or normal distribution, when the system is held in a constant condition, the measured value of each parameter will not be the same for each measurement iteration. In general, the value of the i^{th} measurement of the parameter a will deviate from the average measured value. The standard deviation is a relative indication of the average deviation of each measurement from the mean measured value. In engineering, we write:

$$a_i = \bar{a} \pm \Delta a \tag{1.3}$$

where Δa is called the uncertainty. In general, (1.3) is thought of as stating that each measurement of a at constant conditions will fall within a range of $2\Delta a$, centered at $\bar{a}$.

The value of f resulting from the i^{th} measurement of each of the measured parameters can be written as:

$$f_i = f(x_i, y_i, z_i) \tag{1.4}$$

We can also speak of the mean value of f, which is determined by the mean values of all the measured parameters.

$$\bar{f} = f(\bar{x}, \bar{y}, \bar{z}) \tag{1.5}$$

The objective here is to examine how deviations of the functional parameters of f propagate through the function, resulting in a deviation of f about its mean value. Performing a first-order Taylor series expansion of f around the point $\bar{f}$:

$$f_i = \overline{f} + \left.\frac{\partial f}{\partial x}\right|_{\bar{x}} \left(x_i - \overline{x}\right) + \left.\frac{\partial f}{\partial y}\right|_{\bar{y}} \left(y_i - \overline{y}\right) + \left.\frac{\partial f}{\partial z}\right|_{\bar{z}} \left(z_i - \overline{z}\right) \tag{1.6}$$

Rearranging slightly…

$$f_i - \overline{f} = \left.\frac{\partial f}{\partial x}\right|_{\bar{x}} \left(x_i - \overline{x}\right) + \left.\frac{\partial f}{\partial y}\right|_{\bar{y}} \left(y_i - \overline{y}\right) + \left.\frac{\partial f}{\partial z}\right|_{\bar{z}} \left(z_i - \overline{z}\right) \tag{1.7}$$

From the definition of the variance:

$$\sigma_f^2 = \frac{1}{n-1} \sum_{i=1}^{n} \left[\left(f_i - \overline{f} \right)^2 \right]. \tag{1.8}$$

Plugging in the RHS of (1.7) we obtain:

$$\sigma_f^2 = \frac{1}{n-1} \sum_{i=1}^{n} \left[\left(\left.\frac{\partial f}{\partial x}\right|_{\bar{x}} \left(x_i - \overline{x}\right) + \left.\frac{\partial f}{\partial y}\right|_{\bar{y}} \left(y_i - \overline{y}\right) + \left.\frac{\partial f}{\partial z}\right|_{\bar{z}} \left(z_i - \overline{z}\right) \right)^2 \right] \tag{1.9}$$

Expanding the square of the expression in parenthesis…

$$\sigma_f^2 = \frac{1}{n-1} \sum_{i=1}^{n} \left[\begin{array}{l} \left.\frac{\partial f}{\partial x}\right|_{\bar{x}}^2 \left(x_i - \overline{x}\right)^2 + \left.\frac{\partial f}{\partial y}\right|_{\bar{y}}^2 \left(y_i - \overline{y}\right)^2 + \left.\frac{\partial f}{\partial z}\right|_{\bar{z}}^2 \left(z_i - \overline{z}\right)^2 \\ +2 \left.\frac{\partial f}{\partial x}\right|_{\bar{x}} \left.\frac{\partial f}{\partial y}\right|_{\bar{y}} \left(x_i - \overline{x}\right)\left(y_i - \overline{y}\right) + 2 \left.\frac{\partial f}{\partial x}\right|_{\bar{x}} \left.\frac{\partial f}{\partial z}\right|_{\bar{z}} \left(x_i - \overline{x}\right)\left(z_i - \overline{z}\right) \\ +2 \left.\frac{\partial f}{\partial y}\right|_{\bar{y}} \left.\frac{\partial f}{\partial z}\right|_{\bar{z}} \left(y_i - \overline{y}\right)\left(z_i - \overline{z}\right) \end{array} \right] \tag{1.10}$$

and now splitting the RHS into separate summations…

$$\sigma_f^2 = \left\{ \begin{array}{l} \frac{1}{n-1} \sum_{i=1}^{n} \left[\left.\frac{\partial f}{\partial x}\right|_{\bar{x}}^2 \left(x_i - \overline{x}\right)^2 \right] + \frac{1}{n-1} \sum_{i=1}^{n} \left[\left.\frac{\partial f}{\partial y}\right|_{\bar{y}}^2 \left(y_i - \overline{y}\right)^2 \right] + \frac{1}{n-1} \sum_{i=1}^{n} \left[\left.\frac{\partial f}{\partial z}\right|_{\bar{z}}^2 \left(z_i - \overline{z}\right)^2 \right] \\ \quad + \frac{1}{n-1} \sum_{i=1}^{n} \left[2 \left.\frac{\partial f}{\partial x}\right|_{\bar{x}} \left.\frac{\partial f}{\partial y}\right|_{\bar{y}} \left(x_i - \overline{x}\right)\left(y_i - \overline{y}\right) \right] \\ \quad + \frac{1}{n-1} \sum_{i=1}^{n} \left[2 \left.\frac{\partial f}{\partial x}\right|_{\bar{x}} \left.\frac{\partial f}{\partial z}\right|_{\bar{z}} \left(x_i - \overline{x}\right)\left(z_i - \overline{z}\right) \right] \\ \quad + \frac{1}{n-1} \sum_{i=1}^{n} \left[2 \left.\frac{\partial f}{\partial y}\right|_{\bar{y}} \left.\frac{\partial f}{\partial z}\right|_{\bar{z}} \left(y_i - \overline{y}\right)\left(z_i - \overline{z}\right) \right] \end{array} \right\} \tag{1.11}$$

Since all of the partial derivatives are evaluated at mean values, they do not change with *i*, and can be pulled out of the summations:

$$\sigma_f^2 = \left\{ \begin{aligned} &\left.\frac{\partial f}{\partial x}\right|_{\bar{x}}^2 \frac{1}{n-1}\sum_{i=1}^{n}\left[\left(x_i-\bar{x}\right)^2\right] + \left.\frac{\partial f}{\partial y}\right|_{\bar{y}}^2 \frac{1}{n-1}\sum_{i=1}^{n}\left[\left(y_i-\bar{y}\right)^2\right] + \left.\frac{\partial f}{\partial z}\right|_{\bar{z}}^2 \frac{1}{n-1}\sum_{i=1}^{n}\left[\left(z_i-\bar{z}\right)^2\right] \\ &\quad + 2\left.\frac{\partial f}{\partial x}\right|_{\bar{x}}\left.\frac{\partial f}{\partial y}\right|_{\bar{y}} \frac{1}{n-1}\sum_{i=1}^{n}\left[\left(x_i-\bar{x}\right)\left(y_i-\bar{y}\right)\right] \\ &\quad + 2\left.\frac{\partial f}{\partial x}\right|_{\bar{x}}\left.\frac{\partial f}{\partial z}\right|_{\bar{z}} \frac{1}{n-1}\sum_{i=1}^{n}\left[\left(x_i-\bar{x}\right)\left(z_i-\bar{z}\right)\right] \\ &\quad + 2\left.\frac{\partial f}{\partial y}\right|_{\bar{y}}\left.\frac{\partial f}{\partial z}\right|_{\bar{z}} \frac{1}{n-1}\sum_{i=1}^{n}\left[\left(y_i-\bar{y}\right)\left(z_i-\bar{z}\right)\right] \end{aligned} \right\} \tag{1.12}$$

The first 3 terms on the RHS can be simplified using the definition of the variance:

$$\sigma_f^2 = \left[\begin{aligned} &\left.\frac{\partial f}{\partial x}\right|_{\bar{x}}^2 \sigma_x^2 + \left.\frac{\partial f}{\partial y}\right|_{\bar{y}}^2 \sigma_y^2 + \left.\frac{\partial f}{\partial z}\right|_{\bar{z}}^2 \sigma_z^2 \\ &\quad + 2\left.\frac{\partial f}{\partial x}\right|_{\bar{x}}\left.\frac{\partial f}{\partial y}\right|_{\bar{y}} \frac{1}{n-1}\sum_{i=1}^{n}\left[\left(x_i-\bar{x}\right)\left(y_i-\bar{y}\right)\right] \\ &\quad + 2\left.\frac{\partial f}{\partial x}\right|_{\bar{x}}\left.\frac{\partial f}{\partial z}\right|_{\bar{z}} \frac{1}{n-1}\sum_{i=1}^{n}\left[\left(x_i-\bar{x}\right)\left(z_i-\bar{z}\right)\right] \\ &\quad + 2\left.\frac{\partial f}{\partial y}\right|_{\bar{y}}\left.\frac{\partial f}{\partial z}\right|_{\bar{z}} \frac{1}{n-1}\sum_{i=1}^{n}\left[\left(y_i-\bar{y}\right)\left(z_i-\bar{z}\right)\right] \end{aligned} \right] \tag{1.13}$$

If all of the measured parameters are independent from one another, each of the last 3 terms on the RHS will approach zero as the number of samples, *n*, in the data set increases. In this event, the expression for the variance of f reduces to:

$$\sigma_f^2 = \left.\frac{\partial f}{\partial x}\right|_{\bar{x}}^2 \sigma_x^2 + \left.\frac{\partial f}{\partial y}\right|_{\bar{y}}^2 \sigma_y^2 + \left.\frac{\partial f}{\partial z}\right|_{\bar{z}}^2 \sigma_z^2 \tag{1.14}$$

We often define the uncertainty, Δa, of a parameter a as

$$\Delta a \equiv k\sigma_a, \tag{1.15}$$

where k is usually a positive integer such as 1, 2, or 3. (For a normally distributed system, 68.3% of measurements will be within one sigma (i.e. standard deviation) from the mean. For 2 and 3-sigma uncertainties, the percentages are 95.5% and 99.7%, respectively. Substituting (1.15) into (1.14), we obtain:

$$\left(\frac{\Delta f}{k_f}\right)^2 = \left.\frac{\partial f}{\partial x}\right|_{\bar{x}}^2 \left(\frac{\Delta x}{k_x}\right)^2 + \left.\frac{\partial f}{\partial y}\right|_{\bar{y}}^2 \left(\frac{\Delta y}{k_y}\right)^2 + \left.\frac{\partial f}{\partial z}\right|_{\bar{z}}^2 \left(\frac{\Delta z}{k_z}\right)^2 \tag{1.16}$$

If the uncertainties of all the measured parameters and of f are defined with the same value of k (e.g. 1-sigma or 3-sigma), then $1/k^2$ is a common factor, and can be cancelled. Then, (1.16) simplifies to:

$$\left(\Delta f\right)^2 = \left.\frac{\partial f}{\partial x}\right|_{\bar{x}}^2 \left(\Delta x\right)^2 + \left.\frac{\partial f}{\partial y}\right|_{\bar{y}}^2 \left(\Delta y\right)^2 + \left.\frac{\partial f}{\partial z}\right|_{\bar{z}}^2 \left(\Delta z\right)^2 \qquad (1.17)$$

Solving for Δf and grouping squared terms:

$$\Delta f = \sqrt{\left(\left.\frac{\partial f}{\partial x}\right|_{\bar{x}} \Delta x\right)^2 + \left(\left.\frac{\partial f}{\partial y}\right|_{\bar{y}} \Delta y\right)^2 + \left(\left.\frac{\partial f}{\partial z}\right|_{\bar{z}} \Delta z\right)^2} \qquad (1.18)$$

This is the most general form of the expression of the uncertainty of f. Depending upon the form of the functional relationship between the measured parameters and f, expression (1.18) can be simplified further. For example, consider the case where f is of the following form:

$$f\left(x, y, z, ...\right) = Kx^a y^b z^c \qquad (1.19)$$

where *K*, *a*, *b*, and *c* are constants (positive or negative). Then the partial derivatives are given by,

$$\frac{\partial f}{\partial x} = Kax^{a-1} y^b z^c \quad ; \quad \frac{\partial f}{\partial y} = Kbx^a y^{b-1} z^c \quad ; \quad \frac{\partial f}{\partial z} = Kcx^a y^b z^{c-1} \qquad (1.20)$$

Plugging these into (1.18), we obtain,

$$\Delta f = \sqrt{\left(Ka\bar{x}^{a-1}\bar{y}^b\bar{z}^c\Delta x\right)^2 + \left(Lb\bar{x}^a\bar{y}^{b-1}\bar{z}^c\Delta y\right)^2 + \left(Kc\bar{x}^a\bar{y}^b\bar{z}^{c-1}\Delta z\right)^2} \qquad (1.21)$$

We can divide both sides by $\bar{f}$ to get,

$$\frac{\Delta f}{\bar{f}} = \sqrt{\left(\frac{Ka\bar{x}^{a-1}\bar{y}^b\bar{z}^c}{K\bar{x}^a\bar{y}^b\bar{z}^c}\Delta x\right)^2 + \left(\frac{Kb\bar{x}^a\bar{y}^{b-1}\bar{z}^c}{K\bar{x}^a\bar{y}^b\bar{z}^c}\Delta y\right)^2 + \left(\frac{Kc\bar{x}^a\bar{y}^b\bar{z}^{c-1}}{K\bar{x}^a\bar{y}^b\bar{z}^c}\Delta z\right)^2} \qquad (1.22)$$

which simplifies to

$$\frac{\Delta f}{\bar{f}} = \sqrt{\left(a\frac{\Delta x}{\bar{x}}\right)^2 + \left(b\frac{\Delta y}{\bar{y}}\right)^2 + \left(c\frac{\Delta z}{\bar{z}}\right)^2} \qquad (1.23)$$

Note that the signs of *a*, *b*, and *c* do not matter, due to the squaring of each term.

A brief example illustrating all the principles described so far is the calculation of the electrical resistance of a piece wire. The general equation for wire resistance is given by:

$$R = \frac{\rho L}{A}, \qquad (1.24)$$

where L and A denote the wire's length and cross-sectional area, and ρ denotes the wire resistivity, which is a property of the material of the wire. Let us assume our wire has a circular cross-section of diameter D, allowing us to write the wire resistance in terms of its diameter:

$$R = \frac{4\rho L}{\pi D^2} \tag{1.25}$$

In this example, we already have the wire resistance expressed as a function of three variables – two of which (D and A) can be measured, and one (ρ) can be looked up in a material properties database. The aim here is to determine how the uncertainties of each of the three variables combine to yield the overall uncertainty in our calculation of the wire resistance.

Let us suppose we will measure the wire's diameter using a vernier caliper, which is a standard tool used to measure lengths on the order of a few inches and smaller. The particular caliper we have available is marked on its back side with "±0.001," which tells us it is accurate to within ±0.001 inches.

Supposing the wire's length is on the order of several feet, we decide to measure its length using a simple tape measure. Our rusty old tape measure doesn't have a convenient "measurement uncertainty" marking on it, so we decide to assume one of $1/8^{th}$ of an inch, due to the noticeable amount of wiggle present at the hook at the end of the tape.

Finally, we consult a material properties online database to determine the proper value for the resistivity of copper, which is what our wire is made of. Luckily for us, the database specifies an uncertainty up front, but in a weird format: "±1%." This is a common way for uncertainties to be expressed (when it makes physical sense). It means the uncertainty of the number is proportional to the number itself. In our case, the resistivity is quoted as 6.73e-7 Ohm-inches, so the uncertainty would be ±0.01*6.73e-7 = ±6.73e-9 Ohm-inches. As we'll see later, this calculation isn't even necessary, which is why the "±?%." form of uncertainty specification is so commonly used.

Now that we have figured out the uncertainties of each of the 3 variables (albeit all in different ways), we are ready to calculate the total uncertainty of our resistance calculation. Although we could use (1.18) to do this, we note that our expression for wire resistance in (1.25) is in the general form shown by (1.19):

$$R = \left(\frac{4}{\pi}\right)\rho^1 L^1 D^{-2} \tag{1.26}$$

We can now attempt to apply (1.23) directly:

$$\frac{\Delta R}{\bar{R}} = \sqrt{\left(\frac{\Delta\rho}{\bar{\rho}}\right)^2 + \left(\frac{\Delta L}{\bar{L}}\right)^2 + \left(-2\frac{\Delta D}{\bar{D}}\right)^2} \tag{1.27}$$

There are several points to note here. First, we have not yet said anything about the actual size of our wire, so we don't have the values of $\bar{L}$, $\bar{D}$, or $\bar{R}$. This means we can't solve for the wire resistance uncertainty until we've made those measurements. This is not too surprising, but let's go back to the weird way in which the resistivity uncertainty was initially specified:

$$\Delta\rho = 0.01 \cdot \bar{\rho} \tag{1.28}$$

We can simply divide by $\bar{\rho}$ to get

$$\frac{\Delta\rho}{\bar{\rho}} = 0.01 \quad . \tag{1.29}$$

This allows us to fill in the entire first term under the radical in (1.27) whether we have an actual value for $\bar{\rho}$ or not. Say, for example, that the materials database stated that resistivity data for any material had an uncertainty of ±1%. We would still be able to plug in a value of 0.01 into the first term under the radical, without even knowing the material of the wire or the value of its resistivity. If all of the uncertainties had been specified as percentages, we would have been able to plug values into the entire right hand side of (1.27)! This would in turn yield the wire resistance uncertainty, also specified as a percentage.

Getting back on track, let's suppose we measured the wire to be 14.8" long, with a diameter of 0.063". Plugging the variable values and uncertainties into (1.27), we obtain

$$\frac{\Delta R}{\bar{R}} = \sqrt{(0.01)^2 + \left(\frac{0.125}{14.8}\right)^2 + \left(-2\frac{0.001}{0.063}\right)^2} = 0.0343 \tag{1.30}$$

Interpreted as a percentage uncertainty, this corresponds to ±3.4%. We can also plug the variable values into (1.25) to obtain $\bar{R}$,

$$\bar{R} = \frac{4\left(6.73x10^{-7}\right)14.8}{(0.063)^2} = 0.0100 \text{ Ohms} , \tag{1.31}$$

and solve for the actual resistance uncertainty in Ohms:

$$\Delta R = 0.0343\bar{R} = 0.0343(0.0100) = 3.43x10^{-4} \text{ Ohms} \tag{1.32}$$

In the end, we are able to state that the electrical resistance of our wire is 0.0100±0.0003 Ohms.