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2.5 Propagation of uncertainty estimates

The interesting quantities for research are often derived from the basic measurements by calculations that combine many measurements into final quantities, transform the measurements, apply filters, or otherwise convert the fundamental measurements into derived quantities. In such cases, the uncertainty characteristics of the derived quantities can become quite complicated and difficult to understand without a prescribed methodology, and serious errors in interpretation can result. For example, some attempts to derive correlations between radar reflectivity (***Z***) and rainfall (***R***) have been distorted by the problem that both are based on different calculations from the same characteristics of the drop size distributions, and hence there is a natural correlation between the two that arises purely from correlated error sources. If data sources are used that provide imprecise estimates of ***Z*** and ***R*** , a correlation will appear that is purely the result of these correlated error contributions and has no connection with a natural correlation between radar reflectivity and rainfall rate. It would be a serious error to use the correlation determined in this way to estimate rainfall from radar reflectivity.

The following develops a consistent approach, often called "error propagation," that makes it possible to determine the uncertainty characteristics in derived quantities if the characteristics of the fundamental measurements are known. Let $\{x\} = \{x_\ell, \ell = 1, L\}$ be a set of measured quantities with known measurement uncertainties.[2.7] Consider derived quantities $\{Y\} = \{Y_m,\ m = 1, M\}$, each of which is a function of the measured quantities $\{x\}$:

$$Y_m = Y_m(x_1, x_2, \ldots x_L) \text{ or } \mathbf{Y} = \mathbf{Y}(\mathbf{x}). \tag{2.15}$$

The mean values of x_ℓ, $\overline{x_\ell}$, are then the "best" values for x_ℓ in the sense that they minimize the squares of the deviations from these best values. In the same sense, the "best" values for Y_m are the values $Y_m(\overline{x_1}, \overline{x_2}, \ldots \overline{x_L})$.[2.8]

The one-standard-deviation uncertainties in $\{Y\}$ are those that represent the range over which $\{Y\}$ can vary while $\{x\}$ remain within one-standard-deviation of their measured values. For small deviations, a first-order Taylor expansion relates deviations in $\{Y\}$ to deviations in $\{x\}$:

$$Y_m(x_1, x_2, \ldots\ x_L) = Y_m(\overline{x_1}, \overline{x_2}, \ldots\ \overline{x_L}) + \sum_{k=1}^{L} \frac{\partial Y_m(x_1, x_2, \ldots\ x_L)}{\partial x_k}\Big|_{\overline{\mathbf{x}}}(x_k - \overline{x_k}). \tag{2.16}$$

The variance in Y_m is then obtained by averaging over the N measurements, indicated by index i :

$$V_{Y_m Y_m} = \frac{1}{N}\sum_{i=1}^{N}\left(Y_m(\{x\}_i) - Y_m(\{\overline{x}\})\right)^2 \tag{2.17}$$

$$= \frac{1}{N}\sum_{i=1}^{N}\left[\left(\sum_{j=1}^{L}\frac{\partial Y_m}{\partial x_j}\Big|_{\overline{\mathbf{x}}}(x_i - x_j)\right)\left(\sum_{k=1}^{L}\frac{\partial Y_m}{\partial x_k}\Big|_{\overline{\mathbf{x}}}(x_k - x_i)\right)\right] \tag{2.18}$$

$$= \sum_j\sum_k \frac{\partial Y_m}{\partial x_j}\Big|_{\overline{\mathbf{x}}}\frac{\partial Y_m}{\partial x_k}\Big|_{\overline{\mathbf{x}}}\left(\frac{1}{N}\sum_i (x_{ji} - \overline{x_j})(x_{ki} - \overline{x_k})\right). \tag{2.19}$$

The matrix elements

$$H_{jk}^{-1} = \frac{1}{N}\sum_{i=1}^{N}(x_{ji} - \overline{x_j})(x_{ki} - \overline{x_k}) \tag{2.20}$$

entering (2.16) are the variances and covariances of the measured quantities, so $\mathbf{H}^{-1}$ is called the ***covariance matrix*** or the ***error matrix.*** If the relationship between $\{Y\}$ and $\{x\}$ is linear or is assumed linear (as in the first-order Taylor expansion) over the range of fluctuations, then this matrix is particularly useful for determining the variances in derived quantities because those variances can be expressed as

$$V_{Y_m Y_n} = \langle (Y_m - \overline{Y_m})(Y_n - \overline{Y_n})\rangle \tag{2.21}$$

$$= \sum_{j=1}^{L}\sum_{k=1}^{L}\frac{\partial Y_m(\mathbf{x})}{\partial x_j}\Big|_{\mathbf{x}=\overline{\mathbf{x}}}\frac{\partial Y_n(\mathbf{x})}{\partial x_k}\Big|_{\mathbf{x}=\overline{\mathbf{x}}}H_{jk}^{-1} \tag{2.22}$$

or, in matrix notation,

$$\mathbf{V} = \mathbf{T}^t \mathbf{H}^{-1} \mathbf{T} \tag{2.23}$$

where $T_{mj} = \partial Y_m / \partial x_j$ is the element of the (column) matrix of derivatives of the derived quantity Y_m with respect to the measured quantity x_j and the superscript t denotes the transpose matrix. This general form is valid for any correlations among the original measurements (which will be represented by off-diagonal elements of $\mathbf{H}$) and properly represents the correlations among dependent variables.

Example 2.1: A thermocouple can be used to measure temperature, because a junction between two metals will produce a voltage difference in the two metals which is dependent on (and nearly proportional to) the temperature of the junction. A common experimental set-up is shown in Fig.2.3.

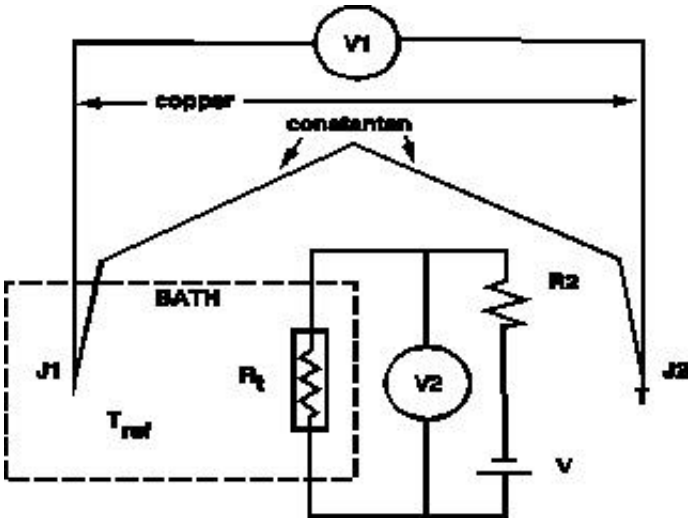

Figure 2.3: ***Experimental configuration for measuring temperature with a thermocouple. Junctions J1 and J2 are junctions between copper and constantan wire, so the voltage V1 is a measure of the temperature difference between T and T_{ref}. A thermistor R_t measures the bath temperature via the voltage V2, and so provides a reference temperature to be added to the temperature difference measured by the thermocouple.***

The thermocouple junctions both produce voltage differences, dependent respectively on the temperature T and on the reference bath temperature T_{ref}. The reason for using this arrangement is that both the wires leading to the instrument measuring the voltage V are then copper wires, and can connect to copper junctions at the voltmeter without introducing additional contact potentials such as would result if the constantan wire were connected directly to the voltmeter. The uncertainty in T is then caused by two sources: (a) the uncertainty in the measurement of $\Delta T = T - T_{ref}$, and (b) the uncertainty in T_{ref}. Often, a

thermistor is used to measure the temperature of the reference bath (or of a metal block used in the same way).

If a thermistor is used to determine the temperature of the reference junction, as shown, there are two voltages that must be measured to determine the unknown temperature T : V_1, produced by the pair of thermocouples, and V_2, produced by the thermistor. These are related to the temperature difference ΔT=(T -T_{ref}) and to T_2, the temperature of the thermistor junction, by functions Y_1 and Y_2, which often are almost linear relationships:

$$\Delta T = Y_1(V_1) = a_1 V_1 \tag{2.24}$$

$$T_2 = Y_2(V_2) = a_2 V_2 . \tag{2.25}$$

Then the first two fundamental quantities affecting the measurement, in the earlier notation, are x_1=V_1 and x_2=V_2.

If V_1 and V_2 are measured by the same voltmeter, part of the uncertainty in V_2 will be correlated with that in V_1because bias in the voltmeter will affect both measurements in the same way. This will be reflected in off-diagonal terms in the error matrix, representing correlations between errors in V_1 and V_2.

There will also be an error in the measurement of T introduced by the assumption that T_{ref} =T_2, because the temperature bath or constant-temperature block may not be uniform in temperature. Another function Y_3=x_3=T_{ref} -T_2 can be introduced to account for this error source, which probably will be a systematic error. The measurement T is then determined from

$$T = \Delta T + (T_{ref} - T_2) + T_2 = Y_1(V_1) + Y_2(V_2) + Y_3. \tag{2.26}$$

Suppose that the voltmeter has a precision of S_i and a systematic error of B_i when measuring V_i , and that the random errors are uncorrelated but the bias errors are always the same (as might occur for a calibration error). If the only sources of error are these random and systematic errors and a non-zero value of Y_3, the error matrix for the random component of the uncertainty is

$$H_r^{-1} = \begin{pmatrix} S_1^2 & 0 & 0 \\ 0 & S_2^2 & 0 \\ 0 & 0 & 0 \end{pmatrix} \tag{2.27}$$

and the bias component is

$$H_s^{-1} = \begin{pmatrix} (B_1^2 & B_1 B_2 & 0 \\ B_1 B_2 & B_2^2 & 0 \\ 0 & 0 & B_3^2 \end{pmatrix} \tag{2.28}$$

when expressed in terms of the fundamental quantities x_1, x_2, and x_3 representing the two measurements and the unmeasured difference between T_{ref} and T_2.

The sum of these matrices can be used in (2.23) to evaluate the variance in the measured temperature:

$$V_{TT} = \begin{pmatrix} a_1 & a_2 & 1 \end{pmatrix} \begin{pmatrix} S_1^2 + B_1^2 & B_1 B_2 & 0 \\ B_1 B_2 & S_2^2 + B_2^2 & 0 \\ 0 & 0 & B_3^2 \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ 1 \end{pmatrix} \tag{2.29}$$

$$= a_1^2 S_1^2 + a_2^2 S_2^2 + (a_1 B_1 + a_2 B_2)^2 + B_3^2 . \tag{2.30}$$

The first two terms show that the random contributions add to the net variance in quadrature, as expected for independent error sources. The next term shows that the bias contributions, however, add linearly. This results because a bias error affects measurements of ΔT and T_2 in the same way, so the error enters the final result additively.

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