Uncertainty and Graphical Analysis

Uncertainties of measured values

All experimental results are uncertain to some degree due to the sensitivity of the measuring instruments and the reproducibility of the experimental conditions. Before using an experimental result, it is necessary to estimate its uncertainty.

Mean and standard deviation of the mean

The goal of most quantitative experiments is to determine the value of a physical quantity. In many experiments, the best estimate of a physical quantity is given by an average. The mean (or average) value of a set of N measurements of x, $(x_1, x_2, x_3, ...x_N)$, is given by

$$x_{avg} = \frac{x_1 + x_2 + x_3 + ... + x_N}{N} = \frac{1}{N}\sum_{i=1}^{N} x_i \tag{14.1}$$

The individual measurements seldom agree exactly. The standard deviation of x, denoted $\sigma(x)$, indicates how far a typical measurement deviates from the mean:

$$\begin{aligned}\sigma(x) &= \sqrt{\frac{(x_1 - x_{avg})^2 + (x_2 - x_{avg})^2 + (x_2 - x_{avg})^2 + (x_3 - x_{avg})^2 + ...(x_N - x_{avg})^2}{N-1}} \\ &= \frac{1}{(N-1)}\left[\sum_{i=1}^{N}(x_1 - x_{avg})^2\right]^{1/2}\end{aligned} \tag{14.2}$$

A small standard deviation indicates that the measurements (x-values) are clustered closely around the mean value, while a large standard deviation indicates that the measurements scatter widely relative to the mean value. Thus a small standard deviation of a repeated measurement indicates that this particular quantity is very reproducible and has a small uncertainty.

The best estimate of the uncertainty of the *average* (our estimate of the physical quantity) is called the standard deviation (or standard error) of the mean, or $\sigma(x_{avg})$. Given a set of N measurements of x, the best estimate of $\sigma(x_{avg})$ is generally given by:

$$\sigma(x_{avg}) = \frac{1}{\sqrt{N(N-1)}} \left[\sum_{i=1}^{N} (x_1 - x_{avg})^2 \right]^{1/2} = \frac{\sigma(x)}{\sqrt{N}} \tag{14.3}$$

The standard deviation function of most spreadsheet programs (Excel, OpenOffice), DataStudio, and calculators gives $\sigma(x)$, from Equation 14.2. To calculate the standard deviation of the mean from this number, you must divide by the square root of N, the number of data points.

On the other hand, the standard error provided by spreadsheet Regression functions and DataStudio's curve fit function corresponds to the standard deviation of the mean, $\sigma(x_{avg})$ from Equation 14.3. Do not divide these numbers by $\sqrt{N}$. These functions have already accounted for the extra factor of $\sqrt{N}$.

Other methods for estimating uncertainty

When several measured quantities are used in a calculation, a relatively crude measurement of one quantity may contribute little to the overall uncertainty. If so, there is little point in improving the measurement. To demonstrate that the uncertainty is small, we must provide an upper bound on the uncertainty and show that the effect of this uncertainty is indeed relatively small.

Smallest division

Most measuring devises have a a smallest division that can be read. In this case, one can use the size of the smallest division as an upper bound on the uncertainty. In some cases, it is appropriate to to use one-half of this smallest division. For instance the smallest division displayed on a meter stick is usually 1 mm. The distance d is read to the nearest mark. Suppose, for example, you look at the meter stick a few times and read d = 85 mm each time. Because you never measured 84 or 86 mm, you are confident that $84.5 \leq d \leq 85.5$. That is, the magnitude of the uncertainty in d is less than 0.5 mm. This is a useful upper bound.

Interpolation

If the uncertainty in such a measurement is not small relative to the other uncertainties in an experiment, a better estimate of the uncertainty is needed. In this case, taking the standard deviation of the mean of multiple measurements is necessary. For instance, you can estimate d to one-tenth of a mm using a meter stick. (Estimating values between the marks is called interpolation.) In this case, repeated estimates, made with care, will disagree, and you can calculate the standard deviation of their mean.

Manufacturer's specification

The user manuals for many instruments (electronic ones in particular) often include the manufacturer's specifications as to the "guaranteed" reliability of the readings. For example, the last digit on the right of digital voltmeters and ammeters is notoriously inaccurate. In this case, it makes sense to use the manufacturer's specifications as a simple upper bound.

Notation for uncertainties

Because we have several methods of estimating uncertainties, it helps to have a separate symbol for uncertainty. We will represent the uncertainty of a quantity x by $u(x)$. If the average and standard deviation of x are available, the best estimate of x is generally x_{avg}, and the best estimate of the uncertainty of x_{avg} is the standard deviation of its mean, $\sigma(x_{avg})$. Then $u(x_{avg}) = \sigma(x_{avg})$. However you estimate an uncertainty, it is important to specify how the estimate was made.

Using error bars to indicate uncertainties on a graph

When plotting points (x, y) with known uncertainties on a graph, we plot the average, or mean, value of each point and indicate its uncertainty by means of "error bars." If for example the uncertainty is primarily in the y quantity, we indicate the upper limit of expected values by drawing a bar at a position y_{max} above y_{avg}, that is, at position $y_{max} = y_{avg} + u(y_{avg})$. Similarly, we we indicate the lower limit of expected values by drawing a bar at position $y_{min} = y_{avg} - u(y_{avg})$. Figure 14.1 shows how the upper error bar at y_{max} and the lower error bar at y_{min} are plotted. If the quantity x also has significant uncertainty, one adds horizontal error bars (a vertical error bar rotated 90°) with rightmost error bar at position x_{max} and the leftmost error bar at position x_{min}.

Occasionally one encounters systems where the upper and lower error bars have different lengths. In this case, the upper uncertainty, $u_{+}(y_{avg})$ does not equal the lower uncertainty, $u_{-}(y_{avg})$. This often happens when the Minimum-Maximum method is used to estimate uncertainties.

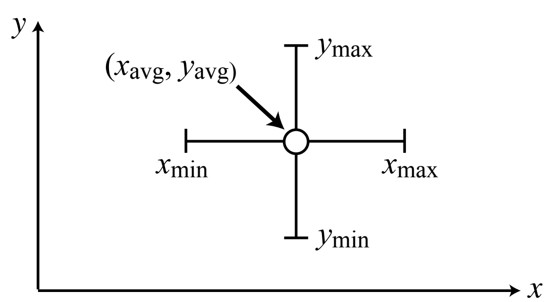

Figure 14.1. Diagram of error bars showing uncertainties in the value of the x- and y-coordinates for point (x_{avg}, y_{avg}).

Uncertainties in calculated quantities

Uncertain measured values are often used to calculate other quantities. These calculated quantities will be uncertain as well, and the degree of uncertainty will depend on the uncertainty of our measurements. We will use two methods of estimating uncertainties in calculated quantities: the Minimum-Maximum method and the Derivative method.

Minimum-Maximum method for propagating uncertainties

Let us start with a simple example. Assume that we have measured the quantity, x, and we need to calculate a value for the function $f(x) = 1/x$. Say that several measurements of x have yielded $x_{avg} = 2.0$, with an uncertainty $u(x_{avg}) = \sigma(x_{avg}) = 0.1$. As long as there is no confusion, this can be reported as $x = 2.0 \pm 0.1$.

The value of $f(x)$ when evaluated at $x = 2.0$ is 0.50, but how does the uncertainty in x (the $\pm$ 0.1) affect our value for $f(x)$ (the 0.50)? For simple functions, the change in $f(x)$ due to a change in x, Δx, can be evaluated directly by calculating $f(x + \Delta x)$ and $f(x - \Delta x)$. Here $\Delta x = u(x_{avg})$ and we have $f(x + \Delta x) = 1/(2.0 + 0.1) = 0.476$. Similarly $f(x - \Delta x) = 1/(2.00.1) = 0.526$. [Note that for $f(x) = 1/x$, $f(x)$ increases as x decreases and vise versa.] To plot error bars for $f(x = 2.0)$, we would put the upper error bar at 0.526 and the lower error bar at 0.476.

The uncertainty in $f(x)$, $u(f(x))$, is just the length of the error bars. The Minimum-Maximum method gives two uncertainties, $u_+(f(x)) = |0.526 - 0.500|$ = 0.026 for the upper error bar and $u_-(f(x)) = |0.476 - 0.500| = 0.24$ for the lower error bar. This can be summarized by saying that $f(x) = 0.50 + 0.026, -0.024$. Since the uncertainty is in the second place to the right of the decimal it would be legitimate to round the uncertainty in $f(x)$ to 0.50 + 0.03, – 0.02. Notice that the plus and minus uncertainties are not equal even after rounding.

In many cases, our goal is to use our uncertainty to compare our measured $f(x)$ with another measurement or prediction. In this case, it is not necessary to calculate both $u_-(f(x))$ and $u_+(f(x))$. If the prediction is greater than $f(x)$, then $u_+(f(x))$ (the length of the upper error bar) is the important quantity. Similar, if the prediction is smaller than $f(x)$, $u_-(f(x))$, the length of the lower error bar, is the important quantity. Your knowledge of how $f(x)$ varies with x will usually allow you to guess whether $(x + \Delta x)$ or $(x - \Delta x)$ is needed. If you guess wrong, you just use the other.

For more complicated functions, say $f(x, y)$, one calculates $u_+(f(x, y))$ by choosing the signs of $\pm\Delta x$ and $\pm\Delta y$ that together maximize the value of the function $f(x, y)$. For instance, if $f(x, y) = x^2/y$, then $f(x, y)$ is maximized by choosing a high value of x and a low value of y. Similarly, the function is minimized by choosing a low value of x and a high value of y. Therefore,

$$u_+(f(x, y)) = \frac{(x_{avg} + \Delta x)^2}{(y - \Delta y)} \qquad \text{and} \qquad u_-(f(x, y)) = \frac{(x_{avg} - \Delta x)^2}{(y + \Delta y)} \tag{14.4}$$

Again, you do not need to compute both $u_+(f(x))$ and $u_-(f(x))$ if your only goal is to compare your measurement with a prediction or another measured value.

The Minimum-Maximum method is relatively easy to use, but it has some drawbacks that are beyond the scope of this introduction. The problems are usually minor as long as the uncertainties are small and $u_+(f(x)) \approx u_-(f(x))$.

Derivative method for propagating uncertainties

Derivatives can be used to estimate the uncertainty associated with a function of the measured quantity, $f(x)$, due to uncertainty in the measured variable, x. We normally have an experimental value of x_{avg}. To see how the uncertainty in x affects $f(x_{avg})$, we can plot $f(x)$ as shown in Figure 14.2. The change due to small variation in x is given by $\Delta f \approx f'(x)\Delta x$, where $f'(x)$ is the slope (and the derivative) of $f(x)$ at x_{avg}.

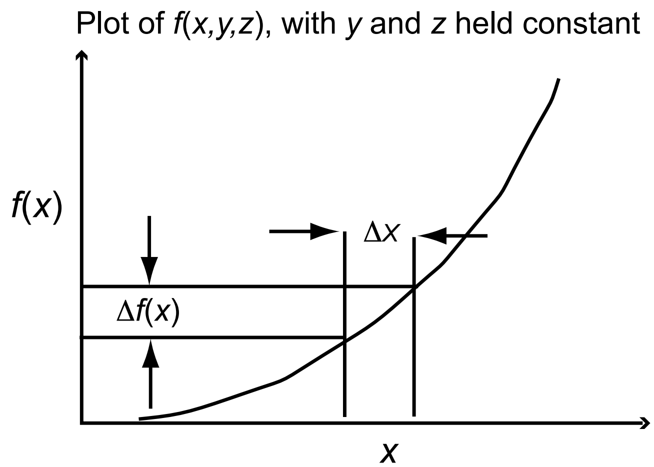

Figure 14.2. Diagram relating the uncertainty in $y = f(x)$ due to the uncertainty in x.

For the simple function $f(x) = 1/x$ used in the example for the Minimum-Maximum method, $x_{avg} = 2.0$ and $u(x_{avg}) = 0.1$, so that the uncertainty in $f(x)$, $u(f(x))$, is

$$u(f(x,y,x)) = \sqrt{\left(\frac{df}{dx}u(x_{avg})\right)^2} = \sqrt{\left(-\frac{1}{x^2}u(x_{avg})\right)^2} = \sqrt{\left(\frac{1}{4.0}\right)^2 (0.1)^2} = 0.25 \tag{14.5}$$

The result $f(x) = 0.50 \pm 0.025$, which we round to $f(x) = 0.50 \pm 0.03$, is essentially the same as the uncertainty from the Minimum-Maximum method. We round up to avoid underestimating the uncertainty.

If f is a function of more than one variable, say (x, y, z), where x, y, and z represent three measured quantities, we can generalize the Derivative method by performing a Taylor series expansion of $f(x, y, z)$ about the point $(x_{avg}, y_{avg}, z_{avg})$:

$$\Delta f \approx \left(\frac{\partial f}{\partial x}\right)\Delta x + \left(\frac{\partial f}{\partial y}\right)\Delta y + \left(\frac{\partial f}{\partial z}\right)\Delta z \tag{14.6}$$

where the symbols $(\partial f/\partial x)$, $(\partial f/\partial y)$, and $(\partial f/\partial z)$ represent the partial derivatives of $f(x, y, z)$ with respect to x, y, and z respectively. The partial derivative is simply the derivative of a function with respect to the indicated variable only: all the other variables are treated as constants. For example, when you take the partial derivative of $f(x, y, z)$ with respect to x, y and z are treated as constants. Partial differential equations will be treated in detail in your differential equations course. *Calculating* a partial derivative is simple using what you learned in first-semester calculus.

The three terms on the right side of the equation for Δf represent the contribution to the deviation of f from its mean value due to the uncertainties x, y, and z respectively. The uncertainty of $f(x, y, z)$, denoted $u(f)$, can be expressed as[1]

$$u(f(x, y, x)) = \sqrt{\left(\frac{\partial f}{\partial x}\right)^2 u(x_{avg})^2 + \left(\frac{\partial f}{\partial y}\right)^2 u(y_{avg})^2 + \left(\frac{\partial f}{\partial z}\right)^2 u(z_{avg})^2} \tag{14.7}$$

where $u(f(x, y, z))$ is the estimated uncertainty in $f(x, y, z)$; $u(x_{avg})$, $u(y_{avg})$, and $u(z_{avg})$ are the uncertainties in the measured values of x_{avg}, y_{avg}, and z_{avg}, respectively, all evaluated at $(x_{avg}, y_{avg}, z_{avg})$. This technique can be generalized to account for as many measured parameters as necessary.

Consider the function $f(x, y, z) = x^{1/2} y^2 \sin(z)$. By way of contrast, the regular (or total) derivative of $f(x, y, z)$ with respect to x can be calculated using the product rule for derivatives.

$$\frac{df}{dx} = \frac{y^2 \sin(z)}{2x^{1/2}} + x^{1/2} 2y \sin(z) \frac{dy}{dx} + x^{1/2} y^2 \cos(z) \frac{dz}{dx} \tag{14.8}$$

However, if x, y, and z are independent variables, $dy/dx = dz/dx = 0$. For the purposes of calculating the contribution of $u(x_{avg})$ to the uncertainty of f, y and z might as well be constants. That is, we want the partial, not total derivative of $f(x, y, z)$ with respect to x. The three partial derivatives of $f(x, y, z)$ from Equation 14.7 are:

$$\frac{\partial f}{\partial x} = \frac{y^2 \sin(z)}{2x^{1/2}} \qquad \frac{\partial f}{\partial y} = 2x^{1/2} y \sin(z) \qquad \frac{\partial f}{\partial z} = x^{1/2} y^2 \cos(z) \tag{14.9}$$

In practice, calculating these partial derivatives directly can be a lot of work. However, many of the calculations we do in real life are simplified by taking the natural logarithm of the calculated quantity. Since

$$\frac{\partial}{\partial x}\left[\ln(f)\right] = \frac{1}{f}\frac{\partial f}{\partial x} \quad , \tag{14.10}$$

we can calculate the partial derivatives we need from the partial derivatives of the logarithm. Since the logarithm function splits our function into terms with simple (partial) derivatives, they are easy to compute. In our example, $\ln(f) = (1/2)\ln(x) + 2\ln(y) + \ln(\sin z)$, so

[1]John R. Taylor, *An Introduction to Error Analysis—The Study of Uncertainties in Physical Measurements* (University Science, South Orange, New Jersey, 1982, 1992).

$$
\begin{aligned}
\frac{\partial}{\partial x}\left[\ln(f)\right] &= \frac{\partial}{\partial x}\left[\frac{\ln(x)}{2}\right] = \frac{1}{2x} \\
\frac{\partial}{\partial y}\left[\ln(f)\right] &= \frac{\partial}{\partial y}\left[2\ln(y)\right] = \frac{2}{y} \\
\frac{\partial}{\partial z}\left[\ln(f)\right] &= \frac{\partial}{\partial y}\left[2\ln(\sin z)\right] = \frac{\cos z}{\sin z} = \cot(z)
\end{aligned}
\tag{14.11}
$$

Substituting these partial derivatives into Equation 14.7 yields

$$
\frac{u(f(x,y,z))}{f(x,y,z)} = \sqrt{\left[\frac{u(x_{avg})}{2x_{avg}}\right]^2 + \left[\frac{2u(y_{avg})}{y_{avg}}\right]^2 + \left[\cot(z_{avg})u(z_{avg})\right]^2} \tag{14.12}
$$

While this expression is not pretty, it is much simpler than the one obtained by substituting the partial derivatives of Equation 14.9 directly into Equation 14.7.

Using uncertainties to compare to measurements or calculations

Uncertainties are used to determine whether two measurements or calculations of the same quantity are consistent. For instance, you may have estimated an objects mass, $m_{F/a}$, from force and acceleration measurements and the relation *F* = *ma*. You must decide whether this mass is consistent with the value m_{bal} you measure using an electronic balance.

Under some rather general conditions, you can use the uncertainties $u(m_{F/a})$ and $u(m_{bal})$ to calculate the probability that two sets of measurements disagree. For the purposes of this course, we will assume that the measurements disagree if their difference is greater than three times the calculated uncertainty. If the two mass values are exactly the same, then $m_{dif} = (m_{F/a} - m_{bal}) = 0$. The uncertainty in this difference, $u(m_{dif})$, can be expressed in terms of $u(m_{F/a})$ and $u(m_{bal})$ using Equation 14.7.

$$
u(m_{dif}) = \sqrt{u(m_{F/a})^2 + u(m_{bal})^2} \tag{14.13}
$$

If the two values of mass are consistent, we expect that, most of the time, $\left|m_{F/a} - m_{bal}\right| < u(m_{dif})$. Random variations being what they are, there will be exceptions. Assuming that you have made a large number of measurements (typically $N \geq 20$), it is fair to say that there is a 95% probability that that the measurements disagree if $\left|m_{F/a} m_{bal}\right| > 2u(m_{dif})$. If $\left|m_{F/a} - m_{bal}\right| > 3u(m_{dif})$, the probability that the two measurement disagree is over 99%. While the conclusion is not so strong if you make fewer measurements, the probability of disagreement is usually greater than 95% if $N > 4$. (Taking more data generally increases the confidence that can be placed in the result, although the effect is small for $N > 30$). In this laboratory, you should conclude that two measurements do not agree when they differ by more than three times the uncertainty of their difference.

When the difference between two quantities (that should agree) differ by more than three times the uncertainty in their difference, systematic errors are usually to blame. Uncertainties cannot (and should not) account for systematic errors. You should carefully review your calculations and measurements procedures for errors. If systematic errors appear to be significant, and you know what they might be, you should describe them in your lab notes. If time permits, repeating a portion of the experiment may be in order. Whatever your conclusion, your lab notes need to indicate how you estimated your uncertainties.

In the United States, the best general authority on the reporting of uncertainties is the National Institute of Standards and Technology.[2] Their standards have been developed in consultation with international standards bodies. That said, when the potential consequences of a decision are critical or when the data are unusual in some way, it is wise to consult a qualified statistician.[3]

Determining functional relationships from graphs

Linear relations are simple to identify visually after graphing and are easy to analyze because straight lines are described by simple mathematical functions. It is often instructive to plot quantities with unknown relationships on a graph to determine how they relate to one another. Since data points have not only measurement uncertainties but also plotting uncertainties (especially when drawn by hand), slopes and such should not be determined by using individual data points but by using a "best-fit line" that appears to fit the data most closely as determined visually. If graphing software is used, then the slope of the line can usually be determined by a computer using a "least squares" technique. We won't go into detail about these methods here.

Linear functions $(y = mx + b)$

If x and y are related by a simple linear function such as $y = mx+b$ (where m and b are constants), then a graph of y (on the vertical axis) versus x (on the horizontal axis) will be a straight line whose slope ("rise" over "run") is equal to m and whose y-axis intercept is b. Both m and b can be determined once the graph is made and the "best-fit" line through the data is drawn. if $x = 0$ does not appear on your graph, b can be found by determining m and finding a point (x, y) lying on the "best-fit" line; then equation $y = mx + b$ can be solved for b.

Simple power functions $(y = ax^n)$

In nature we often find that quantities are related by simple power functions with $n = \pm 0.5, \pm 1, \pm 1.5, \pm 2$, etc., where a is a constant. Except for $n = +1$, making a simple graph of y (vertical axis) and x (horizontal axis) for simple power functions will yield a curved line rather than a straight line.

[2] Barry N. Taylor and Chris E. Kuyatt, "Guidelines for Evaluating and Expressing the Uncertainty of NIST Measurement Results," NIST Technical Note 1297, 1996 edition (National Institute of Standards and Technology, Gaithersburg, Maryland, 1994).

[3] W. Edwards Deming, *Out of the Crisis* (MIT Press, Cambridge, Massachusetts, 1982). Some authors attribute the ability of Japanese automakers to break into the U.S. market to their skillful application of principles popularized by W. Edwards Deming and Joseph Juran.

From the curve it is difficult to determine what the actual functional dependence is. Fortunately it is possible to plot simple power functions in such a way that they become linear.

Starting with the equation $y = ax^n$, we take the natural logarithm of each side to show

$$\ln(y) = \ln(ax^n) = \ln(a) + \ln(x^n) = \ln(a) + n\ln(x) \tag{14.14}$$

If $\ln(y)$ is plotted on the vertical axis of a graph with $\ln(x)$ plotted on the horizontal axis (This is often called a doubly logarithmic, or log-log graph.), then Equation 14.14 leads us to expect that the result is a straight line with a slope equal to n and a vertical axis intercept equal to $\ln(a)$. If the relationship between y and x is a simple power law function, then a graph of $\ln(y)$ as a function of $\ln(x)$ will be linear, where the slope is n, the power of x, and the intercept is the natural logarithm of the coefficient a. This is quite useful, because it is easy to determine whether a graph is linear. If we suspect a simple power function relationship between two quantities, we can make a log-log graph. If the graph turns out to be linear, then we are correct in thinking that it should be a simple power function and can characterize the relationship by finding values for n and a.

Exponential functions $(y = ae^{bx})$

Radioactive decay, the temperature of a hot object as it cools, and chemical reaction rates are often exponential in character. However, plotting a simple graph of y (on the vertical axis) and x (on the horizontal axis) does not generate a straight line and therefore will not be readily recognizable. A simple graphical method remedies this problem. Starting with an equation for the exponential function, $(y = ae^{bx})$. We can take the natural logarithm of each side to show

$$\ln(y) = \ln(ae^{bx}) = \ln(a) + \ln(e^{bx}) = \ln(a) + bx \tag{14.15}$$

If $\ln(y)$ is plotted on the vertical axis and x is plotted on the horizontal axis (This is called a semi-log graph.), Equation 14.15 takes the form of a straight line with a slope equal to b and a vertical axis intercept equal to $\ln(a)$. Thus any relationship between two variables of this simple exponential form will appear as a straight line on a semi-log graph. We can test functions to check whether they are exponential by making a semi-log graph and seeing whether it is a straight line when plotted this way. If so, the values of a and b that characterize the relationship can be found.