Data Collection and Error Analysis

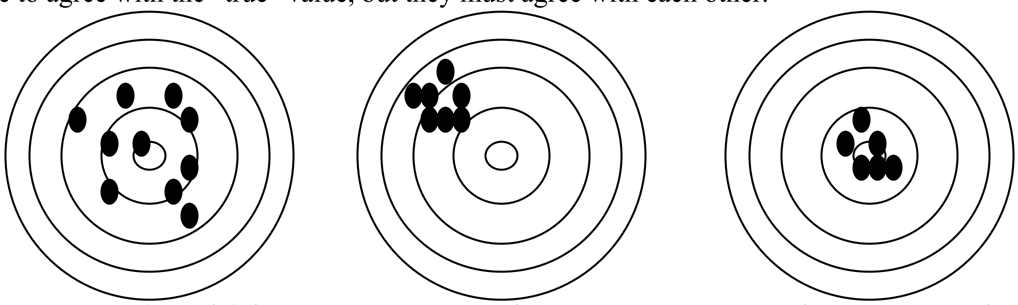
There is error associated with all data. Even the most carefully and professionally collected experimental data has some level of uncertainty, even if it is very small. The most important aspect of experimentation is understanding the error associated with the measurements you take. To have a productive discussion of data and error handling, it is necessary to define some terms.

True/Correct/Known Value – Because all measurements contain error, the concept of a "true", "correct" or "known" value can be tricky. For our purposes, the value that we will accept as "true" has been measured and is known to be accurate with an error significantly smaller than can be measured in subsequent experiments.

Average – Usually the most reliable experimentally determined value. The average of a set of repeated measurements *should* give a value that is reasonably close to the "true" value.

Accuracy – Accurate measurements are those that closely match the "true" value.

Precision – Precise measurements are those that are reliably reproducible. Precise measurements do not necessarily have to agree with the "true" value, but they must agree with each other.



Accurate (poorly) but not precise | *Precise but not accurate* | *Both accurate and precise*

Types of Error:

Random Error – This is error that misses the "true" value by varying amounts in varying directions with no obvious pattern. If multiple *accurate* measurements are taken and averaged, the average will be reliably close to the "true" value. Random error is an indication of the *precision* of a given set of data and *cannot be avoided in any measurement* because it is not possible to make measurements with absolute perfect precision.

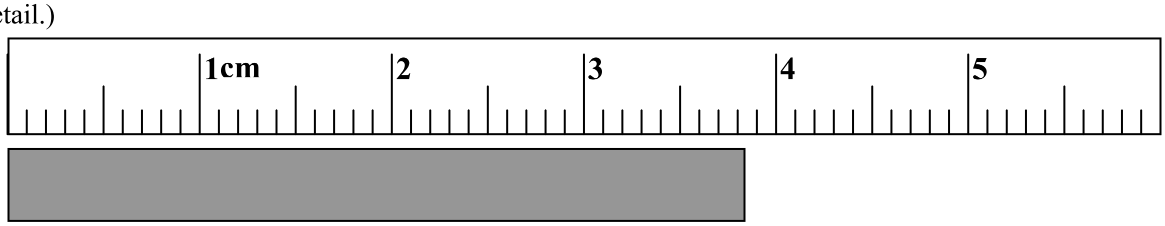
Systematic Error – This is error that misses the "true" value by similar amounts but always in the same direction. The average of a set of data with systematic error will miss the "true" value by some amount that *might* be correctable by addition or subtraction of a correction factor. Systematic error will affect the *accuracy* of the data you are collecting and can typically be eliminated (or at least minimized) by the use of proper laboratory technique.

Taking a Measurement:

All of the measuring devices we use in the lab can be categorized as either digital or analog. Both have their advantages, but they require careful attention to the error involved in each type of device.

Analog Devices:

Measuring devices with analog scales require some degree of interpretation to determine their ultimate accuracy. All of the glassware we use can be considered to be analog. As an example of an analog approach to measurement, consider a simple ruler used to measure the length of a bar as shown below. (The scale of the "ruler" is exaggerated to show detail.)



The length of the grey bar, according to the ruler, is 3.8cm. While this is not an incorrect measurement, upon closer examination it is obvious that the bar is a little longer than 3.8cm. In fact, by reporting the length as "3.8cm", what you are really saying is that the bar is greater than 3.7cm and less than 3.9cm in length. Because the tick marks on the ruler are sufficiently far apart, the observer can quite legitimately estimate a more accurate length of the bar. Estimating, the length of the bar can be reported as 3.83cm with an error of ±0.02cm. When using analog scales, <u>always use your best</u>

judgment in determining the amount of error present in your measurement. The last digit recorded is always assumed to contain some error, include this error whenever you report a number.

Digital Devices:
Many of the modern devices we will use are digital. These include lab balances, temperature probes, pH meters, spectrophotometers, etc. Digital devices remove some of the responsibility for error analysis from the experimenter by eliminating the opportunity for estimation in measurements. In that sense, a digital device is similar to the initial reading of the ruler in the above analog example. If a mass being measured on a digital balance is found to be 1.284g, then it is reasonable to assume the mass is somewhere between 1.283g and 1.285g.

Reporting and Calculating Error:
Significant Figures:
The error present in your reported answers can be implied by correct use of significant figures. If no other error notation is used, it can be assumed that the number is accurate to the last significant figure ±1. For example, the number 1.28 has three significant figures and is implied to be accurately between 1.27 and 1.29. Be aware of this when you report any numbers measured in the lab!! If you use a volumetric pipette to measure 2.00mL of a solution, but you report this as 2mL, then you have only implied that the volume is in the range 1mL to 3mL. If you have trouble with leading and trailing zeros in your sig. figs., try expressing all numbers in scientific notation. This eliminates non-significant zeros from the numbers.

Propagation of Error:
Propagation of error refers to the procedure by which you combine errors from various measurements during a calculation. As an example, say you have weighed out two samples with masses of 1.358g and 1.836g, each of these with absolute errors of +/- 0.001g. If you add those masses together you get 3.194g, but what about the error? The first sample could weigh as much as 1.359g and the second 1.837g, so the total possible mass *could* be as high as 3.196g. Alternatively, the samples could weigh as little as 1.357g and 1.835g, so the total could be as low as 3.192g. The error in the sum (or difference) is, therefore, equal to the sum of the individual errors, or +/- 0.002g. When the quantities are multiplied (or divided), the situation is a little different. Rather than using the absolute amount of the error, the *fractional or relative error* is used. Fractional error is the uncertainty divided by the absolute value of the measured amount. The fractional error of the multiplied (or divided) values are added together to give the error of the result. For example, the area of an 8 +/- 1 cm by 4 +/- 1 cm piece of paper is 32cm^2, but the error is +/- (1/8+1/4)x32 = +/-12cm^2. The area should be reported as 32 +/- 12 cm^2.

Significant figures (sig figs)
Note that the example above follow the rules for significant figures. When adding or subtracting, the number of decimal places in your least accurate measurement is used. When multiplying or dividing, the number of significant figures in your least accurate measurement is used. Thus, since 8 and 4 only have 1 sig fig, the answer, 32, should probably be rounded to 30 (with the 0 not significant) if we are using sig fig rules. Because this is a real measurement with error, we can (and should) use the error to determine where to round the answer. The error, 12, is rounded to the "ones" place; a reported value should be rounded to the same decimal place that its error is rounded, so this value should be reported to the "ones" place, just like the error.

Standard Deviation:
How is error determined with multiple measurements of the same quantity? The best answer is probably the average, so we could treat this as a series of additions and division, but that would give a rather large (and unrealistic) error. A better estimate of the error is to use the *standard deviation*.

$$\sigma_x = \sqrt{\frac{1}{N}\sum(x_i - \bar{x})^2}$$

where: N = number of repeat measurements
x_i = measurement number i
$\bar{x}$ = average measurement

By definition, for a series of repeated measurements, the standard deviation can be considered a 68% confident limit; that is, for a series of measurements with random error, 68% of the measurements should fall within the range (average +/- σ). Most calculators and spreadsheets can calculate the standard deviation, but you should work through the math at least once in a while to remind yourself how it is calculated. The standard deviation implies a rather large sample size and is of questionable validity for fewer than 6-10 repeat measurements (depending upon the quantity being measured). For many of the measurements we will make, it is more proper to refer to the *sample deviation* which has nearly the same mathematical form as the standard deviation (except that N is replaced by N-1), and has the symbol S_x.