1. Propagation of uncertainties

For propagation of errors (uncertainties) you should use the maximum propagated error. For a function \( F \) of \( x, y, z \), this is equal to:

\[
\frac{dF}{dx} \left| dx \right| + \frac{dF}{dy} \left| dy \right| + \frac{dF}{dz} \left| dz \right|
\]

In equation (1) the uncertainty in \( F \) is \( dF \), the uncertainty in \( x \) is \( dx \), etc. Frequently, the equations that we will be using in class use common mathematical operations such as addition, multiplication, and raising to a power, and for most of these cases equations for determining the maximum propagated errors have been tabulated. A useful tabulation of these errors (listed under \( du \) in the table) is found in R. J. Sime, *Physical Chemistry: Methods, Techniques, Experiments*, Saunders College Publishing, 1988, p. 153. This is Table 7-11 in Sime.

2. Statistical analysis of results

The uncertainties that you use in your propagation of error will often be the result of some form of statistical analysis of your results. For example, in an experiment with multiple trials you can calculate an average, standard deviation, standard error, and a confidence limit for your results. You may also use a \( Q \)-test to eliminate outlying data points. A summary of these calculations is given in Chapter II of Shoemaker, Garland and Nibler. Especially see section II.B.

### A. Average (<\( x >\>)

is normally calculated with Excel using the formula \texttt{AVERAGE()}. The mathematical formula for the average (or \textit{mean}) is:

\[
\langle x \rangle = \bar{x} = \frac{1}{n} \sum_{i=1}^{n} x_i
\]

In equation (2) \( n \) is the number of data points and \( x_i \) is each individual data point. This equation just says to sum all of your data points and then divide by the number of points.

### B. Standard deviation (\( S \))

is normally calculated with Excel using the formula \texttt{STDEV()}. The mathematical formula for standard deviation is:

\[
S = \sqrt{\frac{\sum_{i=1}^{n} (x_i - \bar{x})^2}{n-1}}
\]

In equation (3), \( x_i \) is each individual data point, \( n \) is the number of data points, and \( \bar{x} \) is the average value of \( x \).
C. **Standard error** \((S_m)\) is equal to the standard deviation divided by the square root of the number of data points. This is also sometimes called the standard deviation of the mean. In Excel, you will also get a parameter called the standard error \((S_m)\) when you perform a regression calculation. This is a measure of how well your data fits the curve which you are calculating and it may be used in the same way as \(S_m\) to calculate a \(\Delta_{95}\) (see below) for your fit.

\[
S_m = S / (n^{1/2}) \quad (4)
\]

D. The **confidence limit** \((\Delta_{95})\) is equal to the standard error times \(t\), which is tabulated in SGN Table II.3, p. 49. To use the table, find the value of \(\nu\) equal to \(n - 1\), where \(n\) is your number of data points (\(\nu\) is the degrees of freedom). Then go across to the 95% confidence limit column \((P = 0.95)\) to find the value of \(t\). For example, if you need \(t\) for 10 data points \((n = 10)\), you would read across the row with \(\nu = 9\), and under the column for \(P = 0.95\) you find that \(t = 2.26\). The confidence limit gives the range within which there is a 95% chance of finding the true value of your parameter. For example, if your average is 96.8 g and the confidence limit is 0.4 g, then you could report the result as 96.8(4) g at the 95% confidence level.

\[
\Delta_{95} = S_m \times t \quad (5)
\]

E. **A \(Q\)-test** may be used to eliminate data points that appear to be outliers compared to the rest of the data. To use a \(Q\)-test, you must calculate a value of \(Q_{\text{calc}}\) (the rejection quotient) and compare it with a tabulated value \((Q_c, the critical value of Q)\). A table of \(Q_c\) values is given in SGN Table II.1, p. 41, where \(N\) is the number of data points (including the suspect point). If the calculated \(Q_{\text{calc}} \geq Q_c\) the data point should be dropped. \(Q_{\text{calc}}\) is calculated by:

\[
Q_{\text{calc}} = \left| \frac{\text{suspect value} - \text{closest data point}}{\text{highest value} - \text{lowest value}} \right| \quad (6)
\]