Error Analysis

1 Introduction and some useful terminology

Every measurement in experimental science has an error or uncertainty associated with it. This uncertainty is the difference between the true value and a calculated value. Sometimes we do not know what the true value is and therefore quantitative results must include the uncertainty associated with the result. Other times, we know what the true value is, but repeated measurements by different observers and techniques can give varying results leading to a spread or discrepancy in the result. Therefore, the error must be reported to determine the reliability of the experimental measurement.

• There are usually two types of uncertainties:

1. Non-random or systematic error: this type of error is reproducible and results from faulty equipment, incorrect calibration, bias from the observer, etc.

2. Random error: the error arising due to random fluctuations in the apparatus, observations or both give rise to irreproducible errors.

• Reporting uncertainty in measurement:

1. Absolute precision (or uncertainty): when the result of N measurements of quantity R is reported as $\langle R \rangle \pm \delta R$, where $\langle R \rangle$ is the average value and $\delta R$ is the uncertainty, then one claims absolute uncertainty.

2. Relative precision (or uncertainty) If the above result were expressed as $\langle R \rangle \pm \frac{\delta R}{\langle R \rangle} \times 100$ then one claims relative precision on the measurement.

• What uncertainty $\delta R$ should one use?

1. Case 1: Consider one set of N measurements of quantity R. If we assume that the only source of error is random error then the deviation of the independent measurements from the mean value is a good indicator of the uncertainty. The various quantities are:

   (a) Mean, $\langle R \rangle = \frac{1}{N} \times \Sigma_i R_i$

   (b) Variance, $\sigma^2 = \frac{1}{N} \times \Sigma_i (R_i - \langle R \rangle)^2$
(c) Sample standard deviation,

\[ \sigma = \sqrt{\frac{1}{(N - 1)} \times \sum_i (R_i - \langle R \rangle)^2} \]

In this situation, a good estimate of the error \( \delta R \) is \( \sigma \), i.e. \( R = \langle R \rangle \pm \sigma \).

2. Case 2: Consider \( m \) sets of \( N \) measurements of quantity \( R \). Now we have \( m \) different values of \( R \) and \( \sigma \). How do we report the final result and error? For a situation where each measurement has the same uncertainty \( \sigma \), a new term called the Standard Deviation of the Mean (SDM), \( \sigma_{N_m} \), for each set of \( N \) measurements, can be used to estimate the true error in the mean of the total \( N \times m \) measurements, \( \sigma_{N_m} \). (Bevington, Chap 4) These are given by:

(a) SDM for each set of \( N \) measurements, \( \sigma_{N \times \sigma} / \sqrt{N} \). The error for each set of \( N \) measurements is reported as \( R = \langle R \rangle_N = \sigma_N \).

(b) SDM for \( m \) sets of \( N \) measurements, \( \sigma_{N \times m} = \sigma_N / \sqrt{m} = \sigma / \sqrt{Nm} \). This is the same result as part (a) for a total of \( N \times m \) measurements.

(c) Most probable value, \( \langle R \rangle_{N \times m} = \sum_i \frac{\langle R \rangle_m}{m} \), where \( \langle R \rangle_{N \times m} \) is now the average from the \( m \) sets of \( \langle R \rangle_m \) values.

In this case, the error is reported as \( R = \langle R \rangle_{N \times m} \pm \sigma_{N \times m} \).

3. Case 3: In the above example, if the SDM \( \sigma_N \) in each set is not equal, then the corresponding estimation of \( \sigma_{N \times m} \) must be modified accordingly. For the case of random error, the new SDM can be written as:

(a) SDM, \( \sigma_{N \times m} = \sqrt{\frac{1}{\sum_i (1/\sigma_i^2)} \times \sum_i (1/\sigma_i^2)} \).

• How many significant digits should be used in reporting data?

The # of significant digits is calculated as

1. Leftmost non-zero digit is most significant digit.

2. If there is no decimal point, the rightmost nonzero digit is the least significant. For example, 1,234 and 1.234 \( \times 10^3 \) both have 4 significant digits.

3. If there is a decimal point, the right most digit is least significant, even if it is 0 (e.g \( 10.10 \) has 4 significant digits)

The # of significant figures should be at least one more than the uncertainty. For example, if \( \langle R \rangle = 10.88 \) cm and \( \sigma = 3.4 \) cm, then the answer should be reported as 10.9 \( \pm \) 3.4 cm.

2 Error Propagation

In the above example, the quantity \( R \) was measured \( N \) times. Consider now the situation where the quantity \( R \) depends on two independent variables \( x \) and \( y \), i.e. \( R = R(x, y) \). Now let us make \( N \) measurements of \( (x, y) \). If the errors in \( x \) and \( y \) are independent of each other and random, then how do we determine the final error in \( R \)? To estimate this we make use of error propagation, whose mathematical formulation is given below.
Consider a box having length \( L \), width \( W \) and height \( H \). How is the change of volume \( V \) of the box related to the changes in length, height and width? Since \( V = LWH \), if only the length varies the change in volume is \( \Delta V = \Delta LWH \), and \( L\Delta HW \) if only the height changes and \( LH\Delta W \) if only the width changes. If all three dimensions change, then the change in volume is simply the sum of these individual changes:

\[
\Delta V = \Delta LWH + L\Delta HW + LH\Delta W
\]  

(2)

The variation of a function of several variables due to the change in only one of the variables is how we define partial derivatives. The first term in the equation above is simply the partial derivative of \( V \) with respect to \( L \) times the change in length \( L \). We can write the total differential change in volume in terms of partial derivatives as:

\[
dV = \frac{\delta V}{\delta L} dL + \frac{\delta V}{\delta H} dH + \frac{\delta V}{\delta W} dV
\]

(3)

Now suppose \( g(x,y,z) \) is a quantity that is a function of the measured variables \( x, y, z \). Then \( g \) itself is uncertain due to the uncertainties of each of these measured values. A measure of the scatter of the individual measured values of each variable about their mean is provided by the average square deviation of \( g \) and is given by the sum of the square deviations divided by \( N \). In fact, this becomes the commonly accepted definition of the square of the standard deviation, \( \sigma \), when \( N \) is replaced by \( N-1 \).

\[
\sigma^2_g = \frac{1}{N-1} \sum_i (g_i - \bar{g})^2
\]

(4)

(\text{where } g_i \text{ is an individual value and } \bar{g} \text{ is the average value})

This definition keeps \( \sigma \) meaningful for small populations (when \( N = 1 \), or a small number). Statistically, 68\% of the measurements will fall within \( 1\sigma \) and 95\% within \( 2\sigma \). The variation (deviation from the mean) of the \( i^{th} \) value of \( g \) is related to the variations of the measured variables by:

\[
(g_i - \bar{g}) = (x_i - \bar{x}) \frac{\delta g}{\delta x} + (y_i - \bar{y}) \frac{\delta g}{\delta y} + (z_i - \bar{z}) \frac{\delta g}{\delta z}
\]

(5)

Therefore, the square of the standard deviation is given by:

\[
\sigma^2_g = \left( \frac{1}{N-1} \right) \sum_i [(x_i - \bar{x}) \frac{\delta g}{\delta x} + (y_i - \bar{y}) \frac{\delta g}{\delta y} + (z_i - \bar{z}) \frac{\delta g}{\delta z}]^2
\]

(6)

or after expansion by:

\[
\sigma^2_g = \left( \frac{1}{N-1} \right) \left[ \sum_i (x_i - \bar{x})^2 \left( \frac{\delta g}{\delta x} \right)^2 + \sum_i (y_i - \bar{y})^2 \left( \frac{\delta g}{\delta y} \right)^2 + \sum_i (z_i - \bar{z})^2 \left( \frac{\delta g}{\delta z} \right)^2 \right]
\]

(7)
The cross terms (second line in Eq. 7) vanish in the summation if the variables are linearly independent. That is, if the variation in \( x \), for instance, is independent of the variations in \( y \) and \( z \). Note also that:

\[
\sigma_x^2 = \frac{1}{N-1} \sum_i (x_i - \bar{x})^2 ; \quad \sigma_y^2 = \frac{1}{N-1} \sum_i (y_i - \bar{y})^2 ; \quad \sigma_z^2 = \frac{1}{N-1} \sum_i (z_i - \bar{z})^2
\]

Substituting the expressions from Eq. 8 into Eq. 7 yields:

\[
\sigma_y^2 = \sigma_x^2 \left( \frac{\delta g}{\delta x} \right)^2 + \sigma_y^2 \left( \frac{\delta g}{\delta y} \right)^2 + \sigma_z^2 \left( \frac{\delta g}{\delta z} \right)^2
\]

which relates the standard deviation of the computed function \( \sigma_y \) to the standard deviations of the measured quantities. Since the standard deviation \( \sigma \) is related to the standard deviation of the mean (or standard error) \( \sigma_m \) by the relationship \( \sigma_m = \sigma / \sqrt{N} \), we can find the expected uncertainty of the computed quantity \( g \) from the uncertainties of the measured quantities \( x,y,z \). This quantity is also known as the standard deviation of the mean or the standard error of the mean. Now let's see how this works for the different functional forms.

2.1 Addition and Subtraction

First we consider a quantity \( g(x,y,z) \) that is a function of three independent parameters consisting of sums and differences:

\[
g(x, y, z) = ax + by + cz \quad \text{or} \quad g(x, y, z) = ax - by - cz
\]

The partial derivatives are

\[
\frac{\delta g}{\delta x} = a, \quad \frac{\delta g}{\delta y} = \pm b, \quad \frac{\delta g}{\delta z} = \pm c
\]

The sign depends upon whether the terms are added or subtracted. We can use the expression derived above (Eq. 9) to find \( \sigma_y \) as a function of \( \sigma_x \), \( \sigma_y \) and \( \sigma_z \)

\[
\sigma_y^2 = \sigma_x^2 \left( \frac{\delta g}{\delta x} \right)^2 + \sigma_y^2 \left( \frac{\delta g}{\delta y} \right)^2 + \sigma_z^2 \left( \frac{\delta g}{\delta z} \right)^2 = a^2 \sigma_x^2 + b^2 \sigma_y^2 + c^2 \sigma_z^2
\]

Note here that the minus signs vanish because of the squares. The square of the standard error is

\[
\sigma_m^2 = \frac{\sigma_y^2}{N} = \frac{a^2 \sigma_x^2 + b^2 \sigma_y^2 + c^2 \sigma_z^2}{N} = a^2 \sigma_{mx}^2 + b^2 \sigma_{my}^2 + c^2 \sigma_{mz}^2
\]

Thus, the uncertainty for measurements that have a functional dependence that involves sums and differences is

\[
\sigma_m = \sqrt{a^2 \sigma_{mx}^2 + b^2 \sigma_{my}^2 + c^2 \sigma_{mz}^2} = \sqrt{\frac{1}{N}(a^2 \sigma_x^2 + b^2 \sigma_y^2 + c^2 \sigma_z^2)}
\]

Rule for Addition and Subtraction

The overall uncertainty is equal to the square root of the sum of the squares of the uncertainties of each of the individual terms.
2.2 Multiplication and Division

Next we consider a quantity \( g(x,y) \) that is a function of two independent parameters consisting of a single multiplication or division

\[
g(x,y) = \pm axy \quad \text{or} \quad g(x,y) = \pm ax/y
\]

(15)

For the case of multiplication we have

\[
\frac{\delta g}{\delta x} = \pm ay \quad \text{and} \quad \frac{\delta g}{\delta y} = \pm ax
\]

and

\[
\sigma_g^2 = \sigma_x^2 \left( \frac{\delta g}{\delta x} \right)^2 + \sigma_y^2 \left( \frac{\delta g}{\delta y} \right)^2 = a^2 y^2 \sigma_x^2 + a^2 x^2 \sigma_y^2
\]

and for division

\[
\frac{\delta g}{\delta x} = \pm \frac{a}{y} \quad \text{and} \quad \frac{\delta g}{\delta y} = \pm \frac{ax}{y^2}
\]

and

\[
\sigma_g^2 = \sigma_x^2 \left( \frac{\delta g}{\delta x} \right)^2 + \sigma_y^2 \left( \frac{\delta g}{\delta y} \right)^2 = \frac{a^2}{y^2} \sigma_x^2 + \frac{a^2 x^2}{y^4} \sigma_y^2
\]

Dividing by \( g^2 \) (in each case) results in the following expression

\[
\frac{\sigma_g^2}{g^2} = \frac{\sigma_x^2}{x^2} + \frac{\sigma_y^2}{y^2}
\]

for both multiplication and division. Now, recalling that the standard error is \( \sigma_m = \sigma / \sqrt{N} \), and that \( \sigma_m / g \) is the fractional error of \( g \), we have

\[
\frac{\sigma_m}{g} = \sqrt{\left( \frac{\sigma_{mx}}{x} \right)^2 + \left( \frac{\sigma_{my}}{y} \right)^2}
\]

for both multiplication and division.

**Rule for Multiplication and Division**

The Fractional Error of the quantity (fractional overall uncertainty) is equal to the square root of the sum of the squares of the individual fractional errors (note that \( \sigma_{mx} / x \) is the fractional error of \( x \), etc.).
2.3 Powers

At first glance one may think that powers are just products and we proceed as described above for multiplication. For instance, the function, \( g(x,y) = Cx^2 = Cxy \) is a constant \( C \) times the product of three variables \( x, y \) and \( y \), but the last two are obviously not independent variables. Therefore, the treatment above is no longer valid and we must develop the proper expression for variables raised to some power.

Consider a function of a single variable given by

\[
g(x) = ax^{b}
\]

which has the following partial derivative

\[
\frac{\delta g}{\delta x} = \pm abx^{b-1}
\]

Since

\[
\sigma_g^2 = \sigma_x^2 \left( \frac{\delta g}{\delta x} \right)^2 \quad \text{or} \quad \sigma_g = \sigma_x \frac{\delta g}{\delta x} = \sigma_x abx^{b-1}
\]

we can obtain the fractional uncertainty by dividing Eq. 16 by \( g = ax^{b} \)

\[
\frac{\sigma_g}{g} = b \frac{\sigma_x}{x}
\]

Recalling that the standard error is defined as

\[
\sigma_m = \frac{\sigma}{N}
\]

we obtain the fractional uncertainty in terms of the standard error

\[
\frac{\sigma_m}{g} = b \frac{\sigma_{mx}}{x}
\]

Rule for Powers

For measurements that have the functional form, the fractional error on \( g(x,y,z) = Cx^n y^a z^r \), the fractional error on \( g \) is given by

\[
\frac{\sigma_m}{g} = \sqrt{\left( p \frac{\sigma_{mx}}{x} \right)^2 + \left( q \frac{\sigma_{my}}{y} \right)^2 + \left( r \frac{\sigma_{mz}}{z} \right)^2}
\]

3 Least Squares Fitting

In many cases the measurement of the function \( f(x), f(x,y), \) etc. is performed by varying one of the independent variables over a large range. For example, consider the function \( y = A + Bx \). Instead of making numerous measurements of \( y \) for one particular value of \( x \), we can make a series of \( N \) measurements of \( y_i \), one for each of several values of the quantity \( x = x_i \), where \( i \) runs from 1 to \( N \). Therefore we have \( N \) sets of data points represented as \( (x_i, y_i) \). Given this situation, what will be the best estimate for the values \( A \) and \( B \) and the error in the various quantities \( y, A \) and \( B \)? One powerful approach to determine these quantities is that of least-squares fitting and is discussed below.
3.1 The true or most probable value for random or Gaussian error

It can be shown that when a quantity \( y_i \) consists of random uncertainty such that the probability \( P(y_i) \) of obtaining the value \( y_i \) belongs to a Gaussian distribution, then

\[
P(y_i) = \frac{1}{\sqrt{2\pi}\sigma_i} e^{\frac{-(y_i - \bar{y})^2}{2\sigma_i^2}} \tag{17}
\]

where \( \sigma_i \) and \( \bar{y} \) are the standard deviation and mean of the the quantity \( y \).

Under these circumstances, the most probably value of \( y \) is when the probability \( P(y_i) \) is at a maximum. This is called the method maximum likelihood. Now, \( P(y_i) \) is at its maximum when the term in the exponential, i.e. \( (y_i - \bar{y})^2 \) is a minimum, or in other words, when \( y_i = \bar{y} \). There it is clear that for a random Gaussian situation, the most probably value of \( y \) is its mean value. This is the approach which is utilized in the method of least squares, i.e. obtaining the minima the the squared term of the exponential.

3.2 Applying the least-squares

Returning back to the situation of \( y = A + Bx \), assuming that the experimental measurements suffer from a random or Gaussian error, the probability of measuring a value \( y_i \) can now be expressed as:

\[
P(y_i) = \frac{1}{\sqrt{2\pi}\sigma_i} e^{\frac{-(y_i - (A + Bx_i))^2}{2\sigma_i^2}} \tag{18}
\]

where the true value of \( y \) is given as \( \bar{y} = A + Bx_i \).

Remember, our goal is to determine \( A \) and \( B \) and the associated errors. Now let us make \( N \) measurements of \( y_i \). The probability of all these measurements can be expressed as:

\[
P(y_1, y_2, ..., y_N) \propto \frac{1}{\sigma_y^2} e^{-\frac{1}{2\sigma_y^2} \sum_{i=1}^{N} (y_i - A - Bx_i)^2} \propto \frac{1}{\sigma_y^2} e^{-\frac{\chi^2}{2}} \tag{19}
\]

Now the best set of measurement of \( y \) will occur when \( P(y_1, y_2, ..., y_N) \) is a maximum or:

\[
\frac{\chi^2}{2} = \text{minimum} \tag{20}
\]

This is the concept of Least-squares, i.e. the sum of the squares should be “least” and is done as follows:

\[
\frac{\delta \chi^2}{\delta A} = \frac{-2}{\sigma_y^2} \sum_{i=1}^{N} (y_i - A - Bx_i) = 0; \quad \text{and} \quad \frac{\delta \chi^2}{\delta B} = \frac{-2}{\sigma_y^2} \sum_{i=1}^{N} (y_i - A - Bx_i)x_i = 0 \tag{21}
\]

These two can be simplified to:

\[
AN + B \sum x_i = \sum y_i \quad \text{and} \quad A \sum x_i + B \sum x_i^2 = \sum x_i y_i
\]

These two equation can be solved for \( A \) and \( B \), giving:

\[
A = \frac{\left(\sum x_i^2\right) \left(\sum y_i\right) - \left(\sum x_i\right) \left(\sum x_i y_i\right)}{N \left(\sum x_i^2\right) - (\sum x_i)^2} = \Delta; \quad \text{and} \quad B = \frac{N \left(\sum x_i y_i\right) - \left(\sum x_i\right) \left(\sum y_i\right)}{\Delta} \tag{22}
\]

Equation 22 can be solved by tabulating the various quantities as shown in table 1:
### 3.3 Uncertainties in A, B and y

The standard deviation for the various quantities can be evaluated as under:

$$\sigma_y^2 = \frac{1}{N - 2} \sum_{i=1}^{N} (y_i - A - Bx_i)^2$$  \hspace{1cm} (23)

The denominator of N-2 comes from the fact that there are only N -2 independent variable in the N measurements, as we have determined A and B.

$$\sigma_A^2 = \sigma_y^2 \frac{\sum x_i^2}{\Delta} \quad \text{and} \quad \sigma_B^2 = \frac{N \sigma_y^2}{\Delta}$$  \hspace{1cm} (24)

where $\Delta$ is the denominator of equation 22.

### 4 Data Rejection

Sometimes when we make a series of measurements of a specific quantity one of the measured values disagrees strikingly with all the other measured values. When this happens the experimenter is presented with the situation where he/she must decide whether the anomalous measurement resulted from some mistake (glitch in the measurement system) and should be rejected or was a bona fide measurement that should be kept. If careful records were kept sometimes we can establish a definite cause for the anomalous measurement and therefore justifiably reject the measurement.

If an external cause can not be found for the anomalous result, then the truly honest course of action is to repeat the measurement many times. If the anomaly shows up again then hopefully the cause may be found. Either as a glitch in the measurement system or as a real physical effect. If the anomaly does not recur, then due to the increased number of measurements made there will be no significant difference in our final answer whether we include the anomaly or not.

If it is impossible to re take the measurements then the experimenter must decide whether or not to reject the anomaly by examining the measured data and the properties of a Gaussian distribution. The rejection of data is a subjective controversial question, on which experts disagree. The experimenter who rejects data may reasonably be accused of fixing his/her data. The situation is made worse by the possibility that the anomalous result may reflect some important physical effect. One criterion for rejecting suspect data is Chauvenet’s criterion.

<table>
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<tr>
<th>$x_i$</th>
<th>$y_i$</th>
<th>$x_i^2$</th>
<th>$x_i y_i$</th>
<th>$y_i - A - Bx_i$</th>
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<td>$\sum x_i y_i$</td>
<td>$\sum (y_i - A - Bx_i)^2$</td>
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Table 1: Least-squares analysis for straight line fitting
4.1 Chauvenet’s Criterion for Data Rejection

Suppose we make $N$ measurements $x_1, x_2, \ldots, x_N$ of the same quantity $x$.

1. Using all the values of the $N$ measurements made calculate the mean ($\bar{x}$) and standard deviation ($\sigma_x$). If one of the measurements (call it $x_{\text{suspect}}$) greatly differs from $\bar{x}$ and looks suspicious, then calculate

   $$t_{\text{suspect}} = \frac{x_{\text{suspect}} - \bar{x}}{\sigma_x}$$

   the number of standard deviations by which $x_{\text{suspect}}$ differs from $\bar{x}$.

2. We next find the probability $P(\text{outside } t_{\text{suspect}} \sigma_x)$ that a legitimate measurement will differ from $\bar{x}$ by or $t_{\text{suspect}}$ or more standard deviations.

   $$P(\text{outside } t_{\text{suspect}} \sigma_x) = 1 - P(\text{within } t_{\text{suspect}} \sigma_x)$$

3. Finally, we multiply by $N$, the total number of measurements, to arrive at

   $$n(\text{worse than } x_{\text{suspect}}) = N P(\text{outside } t_{\text{suspect}} \sigma_x)$$

   This $n$ is the number of measurements expected to be at least as bad as $x_{\text{suspect}}$.

   If $n$ is less than $\frac{1}{2}$, then $x_{\text{suspect}}$ fails Chauvenet’s criterion and is rejected.
Table A. The percentage probability,  
\[ P(\text{within } t\alpha) = \frac{\int_{-\alpha}^{\alpha} \frac{1}{\sqrt{2\pi}} e^{-x^2/2} dx}{\int_{-\infty}^{\alpha} \frac{1}{\sqrt{2\pi}} e^{-x^2/2} dx} \] 
as a function of \( t \).

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