Introduction to Measurement Data Analysis

rev. 2.2

Outline

Measurement and Measurement Uncertainties

Because of limitations of measurement devices, imperfect measurement procedures and randomness of environmental conditions, as well as human factors related to the experimenter himself, no measurement can ever be perfect. Its result may therefore only be treated as an estimate of what we call the "exact value" of a physical quantity. The experiment may both overestimate and underestimate the value of the physical quantity, and it is crucial to provide a measure of the *error*, or better *uncertainty*, that a result of the experiment carries. The two common measures are

$$\text{absolute measurement error} \quad = \quad \text{measurement result} - \text{exact value}$$
$$\text{relative error} \quad = \quad \frac{\text{absolute measurement error}}{\text{exact value}}$$

With respect to their origin, measurement uncertainties/errors may be classified as *systematic* or *random*.

Random errors refer to the situation, when under the same conditions, multiple measurements of a physical quantity produce different results. Both the magnitude and the sign of these errors are not possible to be predicted and have random nature. Their origin is related to statistical fluctuations in the conditions of the experiment, including the measurement devices used and the experimenter himself. All these factors influence the outcome of the experiment each time it is performed and contribute to the overall random measurement error (random uncertainty).

Although it is not possible to predict random errors for a single experiment, multiple realizations of the experiment allow us to comment on some features that may be effectively analyzed using the theory of probability and statistics.

Systematic Errors

Systematic errors may be caused by a number of factors

1. Approximations implied by theoretical models and formulas. For example, the formula for the period of oscillations of a simple pendulum $T = 2\pi\sqrt{l/g}$ is approximate.

2. Imperfections of measurement devices. For example, inaccuracy of the scale of a thermometer.

3. Environmental conditions, such as temperature and humidity, may also affect the precision of measurement devices. All devices are usually designed to work efficiently in a certain range of environmental conditions.

4. Human and psychological factors that may bias results of measurements based on human action (*e.g.* manual operation of a stopwatch).

A characteristic feature of systematic errors is their permanence. Their impact on measurements cannot be reduced by increasing the number of measurements. **Therefore it is extremely important to identify and eliminate any systematic errors**. They are often the main contribution to uncertainty of measurements.

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Estimation of Measurement Uncertainties

Result of any experiment should not only give an estimate of the "exact value" of the physical quantity that it is designed to find, but also provide information about the uncertainty of the result. Giving the result only, without any information about the uncertainty, cannot be considered as a scientifically acceptable outcome of any experiment.

Measurement uncertainties are commonly classified into one of two categories: A and B with the corresponding uncertainty magnitudes denoted as Δ_A and Δ_B, respectively.

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Type-A (Random) Uncertainties

Normal (Gauss) Distribution

Unpredictability is characteristic to random uncertainties. However, with a large number of realizations of a measurement, some of their statistical properties may be identified. In experiments in physics, the distribution of measured values x of a physical quantity X usually follows the Gauss (or normal) probability distribution described by the probability density function

$$f(x) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$$

where μ is the average (in this case also the most probable) value of X, and σ is the so-called standard deviation quantifying to what extent are the results of the measurement scattered around μ (see figure 1).
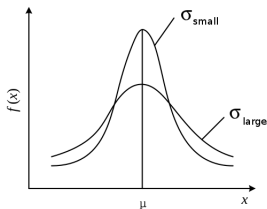

Figure: Probability density function for the normal distribution. Note the difference in the shape of the two curves.

Normal (Gauss) Distribution

The interpretation of the probability density function follows from the formula

$$\Pr\left(x_1 < X < x_2\right) \overset{\text{def}}{=} \int_{x_1}^{x_2} f(x)\,dx$$

giving the probability that the result x of a single measurement of the physical quantity X lies somewhere in the interval (x_1, x_2). In particular, for the normal probability distribution,

$$\Pr\left(\mu - \sigma < X < \mu + \sigma\right) = 0.683,$$

that is a single measurement X, yields a value from the interval $(\mu - \sigma, \mu + \sigma)$ with probability 0.683. The interval is often referred to as the 0.683–confidence interval.

Of course the probability that the measurement yields a value from a wider interval centred around the average value μ is greater. In particular,

$$\Pr\left(\mu - 2\sigma < X < \mu + 2\sigma\right) = 0.954, \qquad \Pr\left(\mu - 3\sigma < X < \mu + 3\sigma\right) = 0.997.$$

Standard Deviation of the Average Value

Although the exact value μ_X of a physical quantity X objectively exists, because of the randomness of measurement outcomes, it is impossible to measure it directly and its value can only be estimated. If a large number of independent measurements is performed, it may be shown that the probability density curve assumes the shape of a Gaussian with the *arithmetic mean* $\bar{X}$ (often simply called the average value) being the <u>best estimate</u> of the exact value μ_X.

If we perform n independent measurements of a physical quantity X, obtaining a set of results $x_1, x_2, \ldots, x_n$, the average value $\bar{X}$ is defined as

$$\bar{X} = \frac{1}{n} \sum_{i=1}^{n} x_i,$$

and the standard deviation σ_X may be estimated using the expression

$$s_X = \sqrt{\frac{1}{n-1} \sum_{i=1}^{n} \left(x_i - \bar{X}\right)^2},$$

quantifying dispersion of measurement results around the average value. Again, if the number of measurements is large, the interval $(\bar{X} - s_X, \bar{X} + s_X)$ estimates the 0.683–confidence interval.

Because the arithmetic mean provides us with the best estimate of the exact value of a physical quantity, for obvious reasons we are also interested in the dispersion of $\bar{X}$ (i.e. in the precision of the average value). Within the probability theory it may be shown that the standard deviation of $\bar{X}$ may be estimated as

$$s_{\bar{X}} = \frac{s_X}{\sqrt{n}} = \sqrt{\frac{1}{n(n-1)} \sum_{i=1}^{n} \left(x_i - \bar{X}\right)^2} \tag{1}$$

The above discussion clearly indicates that the standard deviation of the arithmetic mean (calculated based on n measurements) is estimated at $1/\sqrt{n}$ of the value corresponding to a single measurement, which means that the "exact value" of the physical quantity lies in the interval $(\bar{X} - s_{\bar{X}}, \bar{X} + s_{\bar{X}})$, which is narrower than $(\bar{X} - s_X, \bar{X} + s_X)$.

In the case when the number of measurements used to calculate $\bar{X}$ is relatively small, the statistical distribution of the average value is better described by the so-called Student's t–distribution (or simply t–distribution) than the normal (Gauss) distribution. Then the probability that the interval $(\bar{X} - s_{\bar{X}}, \bar{X} + s_{\bar{X}})$ covers the exact value is not 0.683. In this case a ξ–confidence interval is defined as $(\bar{X} - t_\xi s_{\bar{X}}, \bar{X} + t_\xi s_{\bar{X}})$. Usually the confidence level $\xi = 0.95$ is used. The values of $t_{0.95}$ and $t_{0.95}/\sqrt{n}$ are given in Table 1.

n	3	4	5	6	7	8	9	10	15	20	≥ 100
$t_{0.95}$	4.30	3.18	2.78	2.57	2.45	2.36	2.31	2.26	2.14	2.09	≤ 1.97
$\frac{t_{0.95}}{\sqrt{n}}$	2.48	1.59	1.204	1.05	0.926	0.834	0.770	0.715	0.553	0.467	≤ 0.139

Table: The values of $t_{0.95}$ and $t_{0.95}/\sqrt{n}$.

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Type B-Uncertainties

Type B-Uncertainties

Measurement uncertainties of type B, denoted as Δ_B, do not have a statistical nature, but rather result from the design of a measurement instrument itself. These uncertainties may be estimated in a simple way by the maximum uncertainty Δ_{dev} inherent to the instrument working in a given measurement range.

Device	Range	Graduation	Maximum Error
	150 mm	1 mm	± 0.10 mm
steel ruler	500 mm	1 mm	± 0.15 mm
	1000 mm	1 mm	± 0.20 mm
steel tape meter	1 m	1 mm	± 0.8 mm
	2 m	1 mm	± 1.2 mm
calliper	125 mm	0.02 mm	± 0.02 mm
		0.05 mm	± 0.05 mm
micrometer screw gauge	$0 \sim 25$ mm	0.01 mm	± 0.004 mm

Table: Some measurement devices and their measurement uncertainties (see the handbook for more examples).

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Presentation of Measurement Results

Presentation of Measurement Results

The value of a physical quantity that is found from an experiment, should always be accompanied by the information about its uncertainty, and presented in the following form

$$x = \bar{X} \pm u, \qquad u_r = \frac{u}{\bar{X}} \times 100\% \qquad (2)$$

where $\bar{X}$ is the average value of a multiple measurement, $u = \sqrt{\Delta_A^2 + \Delta_B^2}$ is the measurement uncertainty and u_r denotes the relative uncertainty. On graphs, the uncertainty of the data is indicated by error bars.
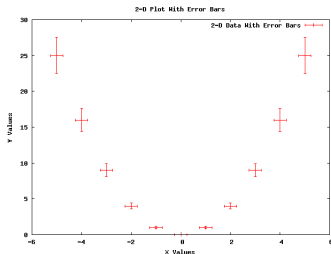

Figure: Experimental data with uncertainties indicated by error bars (Source: nsnam.org).

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Uncertainty of Directly Measurable Quantities

A single measurement is performed in the following situations:

1. Resolution of the measurement device used in the experiment is relatively low, so that multiple measurements would yield the same result.

2. Very high precision of the measurement is not required.

3. Because of environmental limitations (e.g. high temperature, high concentration of poisonous gases), it is possible to complete only a single measurement.

In case of a single measurement, its result is also presented in the form (2) with u usually taken equal to Δ_{dev}.

Multiple Measurements

In the case of multiple measurements of a physical quantity, yielding the results $x_1, x_2, \ldots, x_n$, the uncertainty of that physical quantity is calculated using the following procedure:

1. Calculate the average value (arithmetic mean) of measurement results $\bar{X} = \frac{1}{n} \sum\limits_{i=1}^{n} x_i$

2. Calculate $s_X = \sqrt{\frac{1}{n-1} \sum\limits_{i=1}^{n} \left(x_i - \bar{X}\right)^2}$

3. Find $\Delta_A = s_X \ t_{0.95}/\sqrt{n}$. For example, if the number of measurements $n = 6$, then $t_{0.95}/\sqrt{n} = 1$ and $\Delta_A = s_X$

4. According to the resolution of the measurement device, determine the maximum error Δ_{dev} and assume $\Delta_B = \Delta_{\mathrm{dev}}$

5. Calculate the total uncertainty $u = \sqrt{\Delta_A^2 + \Delta_B^2}$ and relative uncertainty $u_r = \frac{u}{\bar{X}} \times 100\%$.

6. Write down the result as $x = \bar{X} \pm u$ and $u_r = \frac{u}{\bar{X}} \times 100\%$.

Example

At the room temperature, using the resonance interference method, the length λ of an ultrasonic wave propagating in air has been measured (see Table 3). What is the result of this measurement and its uncertainty?

i	1	2	3	4	5	6
λ [cm]	0.6872	0.6854	0.6840	0.6880	0.6820	0.6880

Table: Measurement data.

The result, *i.e.* the average value of the wavelength measured in this experiment

$$\bar{\lambda} = \frac{1}{6} \sum_{i=1}^{6} \lambda_i = 0.6858 \text{ cm},$$

and the standard deviation of the result can be estimated as

$$s_\lambda = \sqrt{\frac{1}{6-1} \sum_{i=1}^{6} \left(\lambda_i - \bar{\lambda} \right)^2} = \sqrt{\frac{1}{5} \times 2.9 \times 10^3 \times 10^{-8}} \text{ m} \approx 0.0024 \text{ cm}.$$

The instrument used to measure the wavelength has the maximum error $\Delta_{\mathrm{dev}} = 0.002 \mathrm{~cm}$. Hence, the A–type uncertainty of the wavelength found by this experimental method is $\Delta_A = s_\lambda t_{0.95}/\sqrt{6} = 0.0024 \mathrm{~cm}$ (here $n = 6$ and $t_{0.95}/\sqrt{n} = 1$, so that $\Delta_A = s_\lambda$). The B–type uncertainty is $\Delta_B = \Delta_{\mathrm{dev}} = 0.002 \mathrm{~cm}$.

Hence, the combined uncertainty is

$$u_\lambda = \sqrt{\Delta_A^2 + \Delta_B^2} = \sqrt{(0.0024)^2 + (0.0020)^2} \mathrm{~cm} \approx 0.003 \mathrm{~cm}$$

and the corresponding relative uncertainty

$$u_{r\lambda} = \frac{u_\lambda}{\bar{\lambda}} \times 100\% = 0.5\%.$$

The experimentally found wavelength is

$$\lambda = 0.686 \pm 0.003 \mathrm{~cm}, \qquad u_{r\lambda} = 0.5\%.$$

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Indirect Measurements. Uncertainty Propagation

Usually, we are not able to measure the physical quantity in question directly. Instead, we measure other physical quantities and then find that quantity by applying a formula (a law of physics or a definition)

$$F = F(X, Y, Z, \dots). \tag{3}$$

If $X, Y, Z, \dots$ are measured, some values $x, y, z, \dots$, are obtained with the corresponding measurement uncertainties $u_x, u_y, u_z, \dots$. Of course, these uncertainties contribute to the uncertainty u_F of the value f of the physical quantity F that is to be determined from the experiment. Treating the uncertainties as small increments and recalling the formula for the total differential of a function of many variables, the propagated uncertainty is usually estimated using the formula

$$u_F = \sqrt{\left(\frac{\partial F}{\partial X}\right)^2 (u_X)^2 + \left(\frac{\partial F}{\partial Y}\right)^2 (u_Y)^2 + \left(\frac{\partial F}{\partial Z}\right)^2 (u_Z)^2 + \dots} \tag{4}$$

with the relative uncertainty

$$u_{rF} = \frac{u_F}{\bar{F}} = \sqrt{\left(\frac{\partial \ln F}{\partial X}\right)^2 (u_X)^2 + \left(\frac{\partial \ln F}{\partial Y}\right)^2 (u_Y)^2 + \left(\frac{\partial \ln F}{\partial Z}\right)^2 (u_Z)^2 + \dots} \tag{5}$$

The procedure of determining uncertainties of indirectly measurable quantities consists of the following steps

1. Find individual measurement uncertainties $u_x, u_y, u_z, \ldots$ corresponding to the results $x, y, z, \ldots$ of measurements of the physical quantities $X, Y, Z, \ldots$.

2. Use the relation $F = F(X, Y, Z, \ldots)$ to calculate the corresponding partial derivatives $\partial F/\partial X, \partial F/\partial Y, \partial F/\partial Z, \ldots$ or $\partial \ln F/\partial X, \partial \ln F/\partial Y, \partial \ln F/\partial Z, \ldots$.

3. Use the formulas (4) and (5) to find u_F and u_{rF}, respectively. (Formulas for the uncertainty of indirectly measured quantities for some common relations are listed in the handbook.)

4. Write down the result as $F = \bar{F} \pm u_F$ and $u_{rF} = \frac{u_F}{\bar{F}} \times 100\%$, where $\bar{F} = F(\bar{X}, \bar{Y}, \bar{Z}, \ldots)$.

Example

The inner diameter of a hollow metallic cylinder was measured at $D_1 = 2.880 \pm 0.004$ cm and the outer diameter $D_2 = 3.600 \pm 0.004$ cm. The cylinder's height is $H = 2.575 \pm 0.004$ cm. Find the volume of the cylinder and the uncertainty of the result.

Given the data, the volume of the cylinder is

$$V = \frac{\pi}{4} \left(D_2^2 - D_1^2 \right) H = \frac{\pi}{4} \times \left(3.600^2 - 2.880^2 \right) \times 2.575 \ \mathrm{cm}^3 = 9.436 \ \mathrm{cm}^3.$$

In order to find the relative uncertainty, first find the partial derivatives

$$\frac{\partial \ln V}{\partial D_2} = \frac{2D_2}{D_2^2 - D_1^2}, \qquad \frac{\partial \ln V}{\partial D_1} = -\frac{2D_1}{D_2^2 - D_1^2}, \qquad \frac{\partial \ln V}{\partial H} = \frac{1}{H}.$$

Then, according to formula (5), the relative uncertainty

$$u_{rV} = \frac{u_V}{V} = \sqrt{\left(\frac{2D_2}{D_2^2 - D_1^2} \right)^2 (u_{D_2})^2 + \left(-\frac{2D_1}{D_2^2 - D_1^2} \right)^2 (u_{D_1})^2 + \left(\frac{1}{H} \right)^2 (u_H)^2}$$

Substituting the numbers we obtain $u_{rV} = 0.008 = 0.8\%$. The absolute uncertainty $u_V = V u_{rV} = 9.436 \times 0.008 \approx 0.08 \ \mathrm{cm}^3$. Hence the result

$$V = 9.44 \pm 0.08 \ \mathrm{cm}^3, \qquad u_{rV} = 0.8\%.$$

Significant Digits

See your Vg100/Vc210 notes or the relevant section in the handbook.

Useful handout

http://graylab.jhu.edu/courses/540.202/docs/Significant_Figures.pdf

When determining the mean and standard deviation based on repeated measurements

- The mean cannot be more accurate than the original measurements. For example, the maximum number of significant figures in the mean when averaging measurements with 4 significant figures is 4.
- The standard deviation provides a measurement of experimental uncertainty.
- Experimental uncertainty should almost always be rounded to one significant figure. The only exception is when the uncertainty (if written in scientific notation) has a leading digit of 1 when a second digit should be kept.

For example if the average of 4 masses is 1.2345 g and the standard deviation is 0.323 g, the uncertainty in the tenths place makes the following digits meaningless so the uncertainty should be written as ± 0.3 g. The number of significant figures in the value of the mean is determined using the rules of addition and subtraction. The value should be written as (1.2 ± 0.3) g.

The exception is when the uncertainty (if written in scientific notation) has a leading digit of 1 when a second digit should be kept. For example (1.234 ± 0.172) g should be written as (1.23 ± 0.17) g.

Presentation of Experimental Data

Measurement data should be arranged in tables when recorded, as it is convenient to check for potential errors. Data tables should be brief and clear. Symbols representing physical quantities and their units should be placed in the first row of the table and not put in each row repeatedly. The data in the table should include the correct number of significant digits. If the final results are presented in the table they should be accompanied by their uncertainty.

Graphs

Graphs are often used to illustrate and discuss results of experiments. They are intended to reveal relations between physical quantities. For example, for a linear relation $Y = mX + b$ between two physical quantities X and Y, it is possible to determine the value of m from the slope and the value of b from the intercept. In general, a value y, not measured in the experiment, corresponding to the value x can be also found from the line $Y = Y(X)$ (interpolation). Under certain conditions it is possible to read a value beyond the range of the measurement data (extrapolation).

When the functional relation to be tested in the experiment is nonlinear, a change of variables can be performed in order to transform it to a linear one. For example, to illustrate the relation $PV = C$, the graph P vs. V can be replaced by the graph P vs. $1/V$.
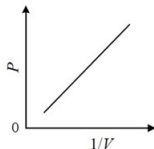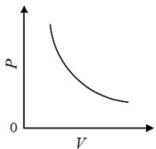
Plotting Rules

1. Choose an appropriate scale: linear, logarithmic, or double logarithmic.

2. Generally, the horizontal axis represents the independent variable and the vertical axis represents the dependent variable. Place the symbols representing the physical quantities and their units next to the axes. Adjust the scale of the horizontal and vertical axes and the position of the origin properly, in order to have the curve plotted in the center of the graph covering $70\% - 80\%$ of the graph sheet. Notes for the scale:

   1. The number of significant digits for experimentally measured data read from the graph should not be less than that obtained in the experiment. For example, for physical variables measured directly, the scale of the smallest axis grid should not be greater than the graduation of the measuring instrument.

   2. The scales of the horizontal and the vertical axis can be different in order to accommodate the graph.

   3. If numbers are particularly large (or small), a multiplication factor, such as $\times 10^3$ or $\times 10^{-6}$ can be written in front of the units.

1. The position of the measured data points should be marked on the graph with a small character "$+$" and uncertainties should be indicated by error bars. When several curves are to be drawn in a single graph, each series of data should be marked with different symbols like $\times$, $\odot$, $\triangle$, $\square$, *etc.* Depending on circumstances draw a curve. Remember that the curve does not have to (and usually will not) pass all points (see the next section).

2. To plot graphs with the experimental data, use data processing and plotting software (*e.g.* R, Origin).
   Remember to use only software you hold a valid license for.

The Least-Squares Method

The Least-Squares Method

In general, there are situations when given the experimental data, one looks for a curve that fits the data in the "best" possible way. One case is when the form of the functional relation between two physical quantities is known, *i.e.* it is known that $y = f(x; \text{parameters})$, and the "best" values of these parameters should be found. For example, we know that the relation is linear, but do not know the slope nor intercept of the line. In the other case, the functional dependence should be first determined and then the "best" values of parameters should be found. In experimental physics most fitting problems belong to the first class, thus only this method will be introduced.

Let us assume, as in the comment above, that the functional relation between two physical quantities is linear

$$y = b_0 + b_1 x \tag{6}$$

i.e. there is only one independent variable x. In this case the method is known as simple linear regression.

The experimental data is given as two sets of numbers

$$x_1, x_2, ..., x_k$$
$$y_1, y_2, ..., y_k.$$

The Least-Squares Method

If the experimental data did not carry any uncertainty, both sides of Eq. (6) should be equal when the pairs $(x_1, y_1), (x_2, y_2), \ldots, (x_k, y_k)$ are substituted for (x, y). However, in a real situation, some uncertainty is always present and it is represented by the residuals $\varepsilon_1, \varepsilon_2, \ldots, \varepsilon_k$. Then

$$
\begin{aligned}
y_1 - b_0 - b_1 x_1 &= \varepsilon_1, \\
y_2 - b_0 - b_1 x_2 &= \varepsilon_2, \\
&\vdots \\
y_k - b_0 - b_1 x_k &= \varepsilon_k.
\end{aligned}
$$

The idea of the method is to determine the uncertain parameters b_0 and b_1, and by requiring that the sum of squares of the residuals $\sum_{i=1}^{k} \varepsilon_i{}^2$ is minimum. Rewriting the sum as

$$
\sum_{i=1}^{k} \varepsilon_i{}^2 = \sum_{i=1}^{k} \left(y_i - b_0 - b_1 x_i \right)^2, \tag{7}
$$

the problem simplifies to finding a minimum of a function of two variables b_0 and b_1 defined by the right hand side of Eq. (7).

The Least-Squares Method

The outlined procedure allows one to find

1. The optimal (in the least-squares sense) estimate of the slope and the intercept of the regression line

$$
\begin{aligned}
b_1 &= \frac{\overline{xy} - \overline{x} \cdot \overline{y}}{\overline{x^2} - \overline{x}^2}, \\
b_0 &= \overline{y} - b_1 \overline{x},
\end{aligned}
$$

where the bar denotes the arithmetic average.

2. The standard deviation of all quantities: the standard deviation of the dependent variable $\sigma_y = \sqrt{\frac{1}{k-n}\sum\limits_{i=1}^{k} \varepsilon_i{}^2}$ where k is the number of measurements, and n is the number of unknown quantity; the standard deviation of the slope estimator $\sigma_{b_1} = \frac{\sigma_y}{\sqrt{\overline{x^2} - \overline{x}^2}}$ and the standard deviation of the intercept estimator $\sigma_{b_0} = \sqrt{\overline{x^2}}\sigma_{b_1}$.

Various fitting procedures (including the least-squares method) are implemented in data processing software (*e.g.* R, Origin).