Analysis of experimental errors

1.1. Introduction to the theory of errors

Goal: Correct determination of physical quantities using results of experimental observations.

A *measured* value of some physical quantity cannot be expected to be the exactly equal to the *true* value. Therefore, it is necessary not only to give the best possible estimate for the true value but, also, to indicate how close this result is likely to be to the true value we are looking for. The latter would require some numerical evaluation indicative of precision or reliability of the measured result.

1.1.1. How large can we expect to be the difference between the true value and the result of a measurement?

The answer to this question must always be reported together with the measured value. This is referred to as the indication of *the measurement error*.

Example: The result of measurement of the focal distance of a lens can be given as follows:

$$f = (301 \pm 5) \text{ mm}.$$

This expression means that we expect (with large probability) that the true focal length will be between 296 en 306 mm. However, we can never be 100% sure that f lies between these limits. In some cases the expected probability indicating that the result lies in the quoted interval of values is directly reported (for instance: 90% confidence interval).

Why the correct estimate of the measurement error is so important?

Without estimate of the measurement accuracy, i.e., the value of the measurement error, one cannot say whether or not the measured difference between physical quantities is significant, i.e., bears additional physical information.

Examples: Discoveries which happen thanks to correct evaluation of the experimental error.

Discovery of Ar (Raleigh and Ramsay, 1895):

The density of the gas remaining after removing O_2, H_2O, and CO_2 from air is found to be 0.5% higher than the density of N_2 obtained from chemical source (NH_3).

What this difference tells us?

There is 1% of a heavier gas in the earth atmosphere: ^{40}Ar.

Discovery of deuterium isotope of hydrogen (^{2}H) (Birge and Menzel, 1931)

Mass ratio between H and ^{16}O atoms can be determined in two ways:

-Mass-spectrometry (Aston, 1927): Mass(H)/Mass(^{16}O)= (1.00778 ± 0.00005)/16.

-Chemical balance: Mass(H)/Mass(^{16}O)= (1.00799 ± 0.00002)/16.

These precise measurements indicate that there is difference between H masses by far exceeding the measurement error.

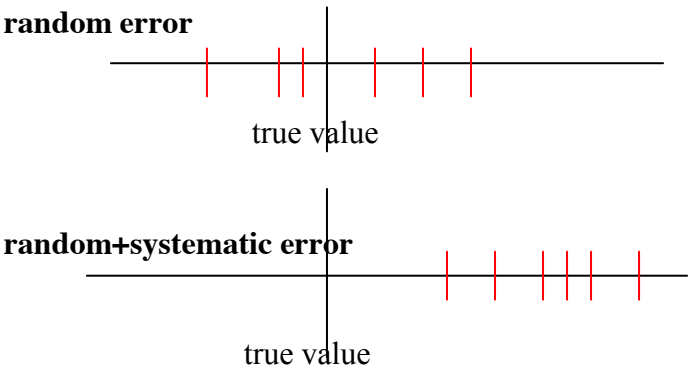
Explanation consists in the presence of a small (1 part in 5000) fraction of heavier hydrogen isotope with mass 2 in the natural hydrogen gas (as measured in chemical experiment)

1.1.2. Systematic and random errors

When considering measurement errors, two kinds of them can be pointed out:

-The ***random error*** changes during the measurement sequence with equal probability to provide positive or negative contribution to the reading.

-The ***systematic error*** remains constant throughout set of measurements. This kind of error causes a systematic shift of readings with respect to the true value of the quantity to be determined.



Examples of systematic errors:

- Time interval measurements using manual timer (prone to delay).
- Parallax error in visual readout from a flat measurement scale.
- Deviation of the measurement device performance from the expected (nominal) one.

The systematic error can be evaluated on the basis of known accuracy of the measurement instruments (e.g., the class of the meter) and using analysis and evaluation of potential contributions of additional physical effects to the measured value, for instance, thermal expansion in the mechanical part of an instrument.

Examples of physical effects which may result in a systematic error:

-Thermovoltage generated at the contacts of conductors of different type;

-Effect of thermal expansion on the accurate length and distance measurements.

General sources of the systematic errors:

-not-ideal measurement set-up (calibration can help);

-"invisible" or unknown contribution to the result of the measurements (thorough analysis of all concomitant physical effects is required);

-inaccurate physical model of the observed phenomenon (more realistic description must be developed).

If one can bring the *systematic* error to a minimum, i.e., the result becomes relatively free from the errors of this kind, one speaks about *accurate measurements*.

Examples of random errors:

Noise = random fluctuations in the signal we want to measure.

Another random factor: Deviation of the physical value of the component(s) we use (resistance, capacitance, inductance…) from the nominal value caused by instability (irreproducibility) of the fabrication process.

Random errors contribute to the result of every experiment. This contribution can be evaluated using statistical methods. In many cases repetitive measurements allow one to make the contribution of the random factors small (average them out). In this case of small influence of the *random* errors one speaks about *precise measurements*.

Therefore, *accuracy* and *precision* have different meaning in the experimental physics.

1.2. Error calculation for one variable

In most of the cases the upper limits of systematic error are either known *a priori*, e.g., given as accuracy of the measurement device by its producent, or may be evaluated from the preliminary measurement system calibration or the readout accuracy estimate, e.g., as the value of the least significant digit. On the basis of these errors one may calculate the *expected* accuracy limits as determined by the known factors. If results of several independent measurements are used to obtain the result, their contribution can be taken into account using the error combination expressions (see section 1.3).

Evaluation of random error represents the most complicated part of the task because it commonly stems from unknown fluctuating influences. Let us suppose that we performed a set of *n* measurements of the same physical quantity X: (x_1, x_2, …x_n) which is **free from systematic error, i.e., these measurements are accurate**.

The results of individual measurements x_i (i=1,…*n*) may vary due to contribution of random errors. The mean value $\bar{x}$ (the arithmetic average of x_i) we can take as the best value of the measured quantity. However, there is no guarantee that this mean will be exactly equal to the true value of the measured physical quantity X.

Key question: How close can we expect $\bar{x}$ to be to X?

This difference we cannot determine exactly as X remains unknown. The best we can do is to establish that there is a definite probability that X will be inside a certain interval around $\bar{x}$.

1.2.1. Definition of statistical distribution

The probability that the value obtained in an arbitrary measurement will be in the interval between x and x+Δx is equal to $f(x)\Delta x$, where $f(x)$ is called the *distribution function*. From this definition of the distribution function as a probability follows the normalization rule: The integral of the distribution function $f(x)$ over the whole range of possible x values is equal to 1. In the limit of very large number of measurements *N* we can assume that mean of the distribution function will be equal to the true value X of the measured quantity:

$$< x >= \int x f(x) dx = X \,. \qquad (1.1)$$

Important ! There is a difference between $\bar{x}$, the mean taken over a certain set of measurements, and <x>, the mean of very large number of measurements which might be done.

1.2.2. Standard error in a single observation and the mean value

In one measurement with value x the real error is equal to

$$e \equiv x - X \ . \tag{1.2}$$

The root mean square of this error for all measurements in the statistical distribution is denoted as σ and is called *the standard deviation*:

$$\sigma^2 \equiv < e^2 > = \int (x - X)^2 f(x) dx \, . \tag{1.3}$$

The value σ^2 is known as the *variance* of the distribution *f*(x).

These values are the properties of the distribution function indicating the spread of the distribution, i.e., the scatter of the measured values. The value of σ can be taken as the measure of error in a single observation and, therefore, σ is also referred to as *the standard error in a single observation*.

As the next step, let us consider a set of the measurements $x_1, x_2, \ldots, x_n$. The mean of these measurements is equal to

$$\bar{x} \equiv \frac{1}{n} \sum_{i=1}^{n} x_i \ , \tag{1.4}$$

with the error in *i*-s measurement equal to $e_i = x_i - X$.

*How large will be the error in the average of **n** measurements E= $\bar{x}$-X?*

Should we continue to perform measurements in series of *n* readouts in each, we could calculate the mean in each of the taken sets of the data. The standard deviation in the mean (not in a single measurement!) over a single set of n measurements can be used as the *standard error in the mean*, σ_m (m means *mean*):

$$\sigma_m^2 \equiv < E^2 > . \tag{1.5}$$

The relationship between σ and σ_m can easily be found:

$$E = \bar{x} - X = \frac{1}{n}\sum_{i=1}^{n}(x_i - X) = \frac{1}{n}\sum_{i=1}^{n} e_i \,. \qquad (1.6)$$

Thus, for a single set of measurements,

$$E^2 = \frac{1}{n^2}\sum_{i=1}^{n}(e_i)^2 + \frac{1}{n^2}\sum_{i=1}^{n}\sum_{i\neq j\, j=1}^{n} e_i e_j \,. \qquad (1.7)$$

This relationship will be true for each set of n measurements we have done. Now we can sum the equations of type (1.7) for all the measurement sets and then divide the result by the number of sets in order to calculate the global mean value: The average of Σe_i^2 is $n\langle e^2\rangle$; the average of each term in the double sum is zero (the errors e_i and e_j are independent, and the average of each of them is zero because of their random character). Therefore,

$$\langle E^2 \rangle = \frac{1}{n}\langle e^2 \rangle \quad , \qquad (1.8a)$$

and, according to the definitions,

$$\sigma_m = \frac{\sigma}{\sqrt{n}} \,. \qquad (1.8b)$$

The standard error in the mean of n measurements is √n times smaller than the standard error in a single observation.

Important note: Insufficient accuracy of the measurement instrument may result in a **systematic** deviation of the measured results from the true value. This deviation cannot be reduced by statistical methods using the repetitive measurements. One needs a *better instrument*.

Example: Visual readout of the values may lead to a parallax error. Better statistics will not help.

1.2.3. How to calculate the error?

Problem: We still not ready to calculate σ_m from experimentally measured values because we do not know the value of σ.

To determine this error we need to know the true value X, which remains unknown. How we can solve this problem? We can use instead of real errors e_i so-called *residuals* d_i calculated with respect to the mean value:

$$d_i = x_i - \bar{x}. \tag{1.9}$$

In Eq. (1.9) all the values are known. Therefore, they can be used to determine the *standard deviation s in the sample*:

$$s^2 \equiv \frac{1}{n}\sum_{i=1}^{n} d_i^2 = \frac{1}{n}\sum_{i=1}^{n}(x_i - \bar{x})^2 . \tag{1.10}$$

Further, we can express residuals through the error and the standard error in the mean:

$$d_i = x_i - \bar{x} = \left[x_i - X\right] - \left[\bar{x} - X\right] = e_i - E. \tag{1.11}$$

Therefore,

$$s^2 \equiv \frac{1}{n}\sum_{i=1}^{n} d_i^2 = \frac{1}{n}\sum_{i=1}^{n}(x_i - \bar{x})^2 = \frac{1}{n}\sum_{i=1}^{n}(e_i - E)^2 = \frac{1}{n}\sum_{i=1}^{n} e_i^2 - \frac{2}{n}E\sum_{i=1}^{n} e_i + E^2 \tag{1.12}$$

This is calculated, again, for one set of *n* measurements. If we will take, as before, the average of this equation over a large number of measurement sets in the distribution, then

$$< s >^2 = \sigma^2 - \sigma_m^2 = \sigma^2 - \frac{\sigma^2}{n} \quad . \tag{1.13}$$

From this equation and from Eq. (1.8b) we obtain, respectively:

$$\sigma^2 = \frac{n}{n-1} < s^2 >; \sigma_m^2 = \frac{1}{n-1} < s^2 > . \tag{1.14}$$

As the quantity $<s^2>$ is not known (we have only one set of the measurement results), instead we can use our best estimate s^2 obtained using Eq. (1.10). This allows us to express the standard error in the mean value as

$$\sigma_m \approx \frac{s}{\sqrt{n-1}} \quad . \tag{1.15}$$

This expression contains only the values known from experiment and, therefore, can directly be used to analyse the data.

1.2.4. The Gaussian distribution

So far we have not specified the shape of the distribution function *f*(x), so all the results derived above will be insensitive to the particular probability distribution. To proceed further it will be useful to consider the particular case of Gaussian distribution which represents the best choice when *the measurements are influenced by a large number of independent (small) errors, all of the same order of magnitude and having the same chance to take positive or negative value*.

This assumption of the Gaussian probability distribution has direct relationship with the use of the mean value as the best value for the measured physical quantity. The meaning of the "best" in this context can be defined as follows: Let us assume the distribution function in the form *f*(x-X) where X is the true value.

Further, we can take ε as the smallest signal variation that can be seen by our measurement device (the resolution) and assume that this variation is small. The probability that during n measurements the results will be $x_1, x_2, \ldots x_n$ can be written as

$$f(x_1 - X)\varepsilon \times f(x_2 - X)\varepsilon \times \ldots f(x_n - X)\varepsilon = f(x_1 - X) \times f(x_2 - X) \times \ldots f(x_n - X)\varepsilon^n \quad (1.16)$$

We can define the "best" value of X as the value corresponding to the maximum of the function given by Eq. (1.16). It is then possible to give an analytical proof that if *f*(x-X) represents the Gaussian distribution function, the best value of X will be equal to the mean of the measured values $x_1, \ldots x_n$.

Though the only Gaussian probability distribution will be analysed further, other types of distributions can be encountered in physical experiments. For instance, phenomena in which the random process gives rise to discrete measured values (particle count, nuclear fusion, etc.) are described by the Poisson distribution. What distribution function (statistical hypothesis) is relevant to the particular experiment can be found using the χ^2*-test*.

1.2.5. Error calculation in the case of Gaussian distribution

When using the Gaussian function of normal distribution analytical solutions become possible:

$$f(x)=\frac{1}{\sigma\sqrt{2\pi}}e^{-\frac{(x-X)^2}{2\sigma^2}} \tag{1.17}$$

$$(st.deviation)^2=\int_{-\infty}^{\infty}(x-X)^2 f(x)dx=\sigma^2 \tag{1.18}$$

The formula of Peeters *for a simple numerical error calculations:*

The average of absolute values of the residuals

$$r\equiv\frac{1}{n}\sum_{i=1}^{n}|d_i| \tag{1.19}$$

can be used to calculate (approximately) the standard error in the mean of *n* measurements:

$$\sigma_m=\frac{5}{4}\frac{r}{\sqrt{n-1}}, \tag{1.20}$$

and the standard error in a single observation:

$$\sigma=\frac{5}{4}r\sqrt{\frac{n}{n-1}}. \tag{1.21}$$

These expressions are valid if the number of measurements taken in one set is *n*≥5!

If the number of measurements is smaller, the error must be calculated using Eq. (1.15).

1.2.6. Error in the error

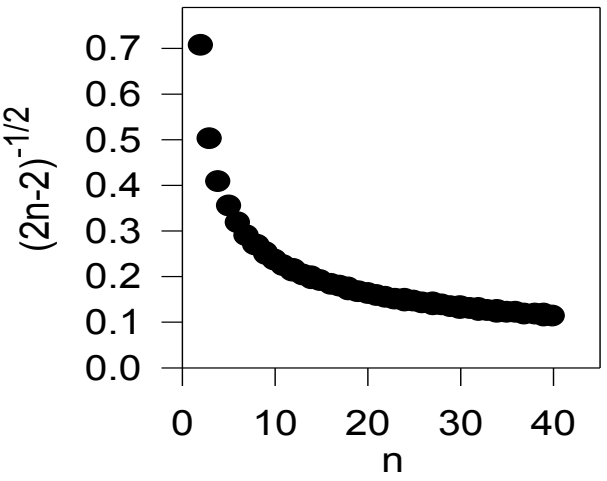
Using the hypothesis of the Gaussian distribution function we can provide an answer to the question how large is the difference between the true error $<s^2>$ and the value $s^2 = (1/n)\Sigma d_i^2$ we used as the best estimate we can get from a set of measurements. The "error in the error" can be written in the form of variation

$$u = s^2 - < s^2 > . \qquad (1.22)$$

It is possible to prove mathematically (Appendix C in the book of Squires) that over the Gaussian distribution the mean value of u^2 taken over large number of measurements n is $[2/(n\text{-}1)]<s^2>^2$. Therefore, the fractional standard deviation of s^2, i.e., $u/<s^2>$, will be $[2/(n\text{-}1)]^{1/2}$. If n is fairly large, the fractional standard deviation of s is approximately one half of this value:

$$\frac{\sigma(s)}{s} \approx (2n-2)^{-\frac{1}{2}} \qquad (1.23)$$

This function is shown in the figure from which one can see that for n= 9 the relative error in the error is about ≈25%!



In other words, even for substantial number of measurements the error estimate has significant uncertainty by itself.

Practical conclusion: *In most cases the error can be given with accuracy of only one significant digit. Reporting more digits is of no use taking into account the above estimate of the error determination accuracy. The result (the mean value) must also be reported with accuracy corresponding to that of the error.*

1.2.7. Quoting the error

Let us consider measurement of the width of piece of A4 paper, **x**, which can be determined using the standard ruler with accuracy of about 1/3 mm. Thus, we may conclude regarding the result of our measurement: $x = (210.2 \pm 0.3)$ mm. The 210.2 mm we call the measured value; 0.3 mm is the measurement accuracy or, else, the absolute measurement error, Δx. It is also possible to quote the relative accuracy, (or the relative error) $\delta x = \Delta x/x$, which is in this example 0.3/210.2 or 0.0014, or the percent accuracy (the percent error) $100\Delta x/x = 0.14\%$.
It is generally accepted convention in physics that the final error is always quoted as the absolute error.

The final error can be quoted with maximal precision of two significant digits. Usually, two-digit error value might be given only if the first meaningful digit has value of 1 or 2. The reported final result must be given with the same last significant digit as the quoted absolute error.

Excessively reported significant digits suggest insufficient insight into the real accuracy of the experiment.

1.2.8. Estimate of the measurement error: practical guide

The accuracy of the measurement and, therefore, the estimate how accurate the obtained result is must be evaluated by an experimentalist on the basis of known parameters of the experimental devices/procedures and of the dataset obtained in the course of repetitive measurements. These two factors determine two ways of the measurement error evaluation, both to be preferably applied, and the results of both to be compared: The *instrumental accuracy* and the *spread of the data*.

The instrumental error indicates the uncertainty of the result expected on the basis of the *known inaccuracy* of the measurement device or in the measurement procedure. It includes the errors associated with the calibration accuracy, the tolerance limits of the used components (e.g., electrical or optical), the readout error (if it is done by an observer), etc. Very often the instrumental accuracy is given in the measurement device manual by a manufacturer as absolute

or percent error indicating the expected limits of the possible deviation of the measured value from the true one. If we have a measurement instrument with accuracy of 1%, we must take this as the relative error in the measurement result. Moreover, if we have a visual readout from a scale, we have to add to this uncertainty the absolute error of 1/3 or 1/2 of the smallest division visible on the scale. In the case of a digital indicator, 1 in the least significant digit must be taken as the readout error.

The evaluated in this way *instrumental error* includes only the *a priori* known contributions to the uncertainty, indicating the accuracy limits expected for the given experiment. Thus, **the instrumental error is its origin a known systematic error.** This approach neglects entirely the unknown (invisible) sources of uncertainty or even of a systematic error.

Is this expected instrumental error realistic or do we miss some factors in estimating it?

Additional **systematic errors** in the measurement can be traced with the help of the measurement of a known signal. This is referred to as *the calibration procedure*.

Examples:

-1 kHz meander signal in the oscilloscope.

-Potential difference on the normal element in voltage measurements.

-Known atomic optical or electron spectrum.

If the measured result differs from the known value of calibration signal, one may use the difference to correct the readout (add *the offset value*). The error in the offset value must be taken equal to the error in the calibration signal (if any) plus the readout error.

How to handle random errors?

Their influence can be evaluated on the basis of data spread using above discussed statistical approximation. The random errors originating from known and unknown sources are handled together to obtain estimate of the standard error in a single measurement σ or the standard error in the mean σ_m.

For a set of the measured values $x_1, x_2, \ldots, x_n$ of an unknown physical quantity X the best experimental value of X is taken as the mean value:

$$\overline{x} = (1/n)\sum_k x_k \ . \tag{1.24}$$

Next, using the residuals defined as deviation of the individual measurement from the mean,

$$d_k = x_k - \bar{x}, \tag{1.25}$$

the *standard error* (or standard deviation) is defined as

$$s = \left[\frac{1}{n-1} \sum_k (d_k)^2 \right]^{1/2}, \tag{1.26}$$

and the *standard error in the mean* is calculated

$$\sigma_m = s/\sqrt{n}. \tag{1.27}$$

This error can be used to quote the statistical error on the measured value of the quantity X

$$X = \bar{x} \pm \sigma_m \quad , \tag{1.28}$$

indicating the measure of the spread of data points around the mean value. Obviously, the spread of the individual measurement points will not change substantially with the number *n* of the readouts taken. However, the standard error in the mean will decrease with increasing *n* thus making the statistical error smaller.

Now we end up with two error estimates: The instrumental error and the statistical error in the mean.

Difficult choice is to be made: What error must be quoted when reporting the final result?

One may answer this question using the experimental logic: If the error of the measurement system given by the fabricant, supplemented by the readout error or other known factors appears to be larger than the error found on the basis of the statistical analysis of data spread, the instrumental error must be quoted as the final one because within the limits it indicates a systematic deviation of the measured value from the true value may exist.

If the standard deviation in the mean σ_m exceeds the instrumental error, it must be quoted because it includes the contributions of both known and unknown error sources. Perhaps we have missed some of them when calculating the instrumental error.

Therefore, we can formulate the universal rule:

Larger error = Real error

Important reminder:

Estimates of the measurement accuracy on the basis of the instrumental error and using the statistical approximation deal with physically different methods of error evaluation. If considering measurements done using one instrument, these must be calculated separately and can never be mixed.

Instrumental error indicates the expected uncertainty caused by known factors in the measurement procedure of in the readout.
All a priori unknown factors are neglected.

The standard error in the mean calculated using statistical methods gives a measure of influence of only random factors of different origin on the final result.
All systematic errors and deviations are neglected.

Practical hints for the Practicum

If not stated otherwise:

- all measurement devices are correctly calibrated, i.e., no systematic errors are expected to appear;
- the accuracy of the measurement devices is either directly indicated or can be taken as equal to 1% of the measured value;
- the accuracy of visual readout using a visible scale (ruler, the screen of oscilloscope, the scale in the optical ocular, the calibration plate, the goniometer circle, …) is ½ of the smallest visible scale division;
- the accuracy of readout using a digital indicator (including PC) is 1 in the least significant digit.
- the human reaction time is about 0.25-0.3 s. Do not forget this error when using the stopwatch!

1.3. Applications of the statistics

1.3.1. Combining the errors

Experimental determination of some physical quantity F almost always requires combination of measurements of other quantities (A±ΔA, B±ΔB, C±ΔC,…) followed by calculation of the desired value using some functional relationship F = F(A, B, C, …). Then, the uncertainty in F can be calculated from the errors encountered in the measurements of the primary physical quantities as

$$\Delta F = \left[\left(\frac{\partial F}{\partial A} \Delta A \right)^2 + \left(\frac{\partial F}{\partial B} \Delta B \right)^2 + \left(\frac{\partial F}{\partial C} \Delta C \right)^2 + \cdots \right]^{1/2}, \qquad (1.29)$$

provided that the variables A, B, C, … may be considered as independent (uncorrelated) values. **This kind of calculations delivers the most probable error in the value of F and can be used to determine both the expected (instrumental) error and the statistical one.**
The error calculated in this way does not show the largest possible deviation of the measurement from the true value but the most probable one. This difference can easily be illustrated:

Let us consider two (dimensionless) quantities A = 3 ± 1 and B = 5 ± 2, and the final function in a form of simple sum S = A + B. In Eq. (1.29) we will have

$$\partial S/\partial A = \partial S/\partial B = 1 ,$$

and $$\Delta S = [(1)^2 + (2)^2]^{1/2} = \sqrt{5} = 2.2 ,$$

resulting in: $S = 8.0 \pm 2.2$ (and $\delta S = 0.28$).

The ‘direct’ summation of the quantities and errors (3 ± 1) + (5 ± 2) would result in (8 ± 3) with δS = 0.38, which would represent all possible results including even those (S = 5) when A and B appear at their lowest limit at the same time. The last situation is very improbable, and for this reason not reflected in the value of the standard error. Would all the values from the intervals (3 ± 1) and (5 ± 2) come out with the same probability, then (8.0 ± 2.2) covers the interval 92,5% of all possible sums. Moreover, would we consider ‘normal’ cases when the

values close to the true value have larger probability to be obtained than in the wings of the Gaussian distribution, than the result (8,0 ± 2,2) covers more than 99% of all possible results.

Conclusion: Eq. (1.29) delivers a realistic description of the uncertainty in a function, and will be used as valid error calculation procedure in the Practicum.

Note that errors originating from independent sources are always summated providing an increasing contribution to the final error as the number of independent measurements needed to reach the final result increases (*the error propagation*). As a consequence, measurement techniques requiring long calculations are intrinsically less accurate than the experimental meathods based on direct measurement of the desired physical value.

1.3.2. Practical error combining

Though the Eq. (1.29) always delivers good estimate of the error in a function, for a number of functions more simple relationships can be obtained which helps to simplify the calculations.

Sum and product relations

The above discussed case of a simple sum can be extended to an arbitrary combination of summation and subtraction terms $F = A - B + C + \ldots$ leading to

$$\Delta F = \left[(\Delta A)^2 + (\Delta B)^2 + (\Delta C)^2 + \cdots\right]^{1/2} \quad , \qquad (1.30)$$

because both $\partial F/\partial A = 1$ and $\partial F/\partial B = -1$ give +1 in a square.

Eq. (1.30) is called *the sum rule*. From this rule it becomes clear that the absolute error in a sum of in a difference can never become smaller than the uncertainty in any of its terms.

In the same spirit one can obtain a rule to calculate the error in the function including the product and division of the primary quantities:

$$F = \frac{A\,B\,G\cdots}{C\,D} \quad . \qquad (1.31)$$

According to Eq. (1.29)

$$\Delta F = \left[\left(\frac{BG\cdots}{CD} \Delta A \right)^2 + \left(\frac{AG\cdots}{CD} \Delta B \right)^2 + \left(\frac{-ABG\cdots}{C^2 D} \Delta C \right)^2 + \cdots \right]^{1/2}, \qquad (1.32)$$

and dividing Eq. (1.32) by Eq. (1.31) results in

$$\frac{\Delta F}{F} = \left[\left(\frac{\Delta A}{A} \right)^2 + \left(\frac{\Delta B}{B} \right)^2 + \left(\frac{-\Delta C}{C} \right)^2 + \cdots \right]^{1/2}, \qquad (1.33a)$$

or, using definition of the relative error,

$$\delta F = \left[(\delta A)^2 + (\delta B)^2 + (\delta C)^2 + \cdots \right]^{1/2}. \qquad (1.33b)$$

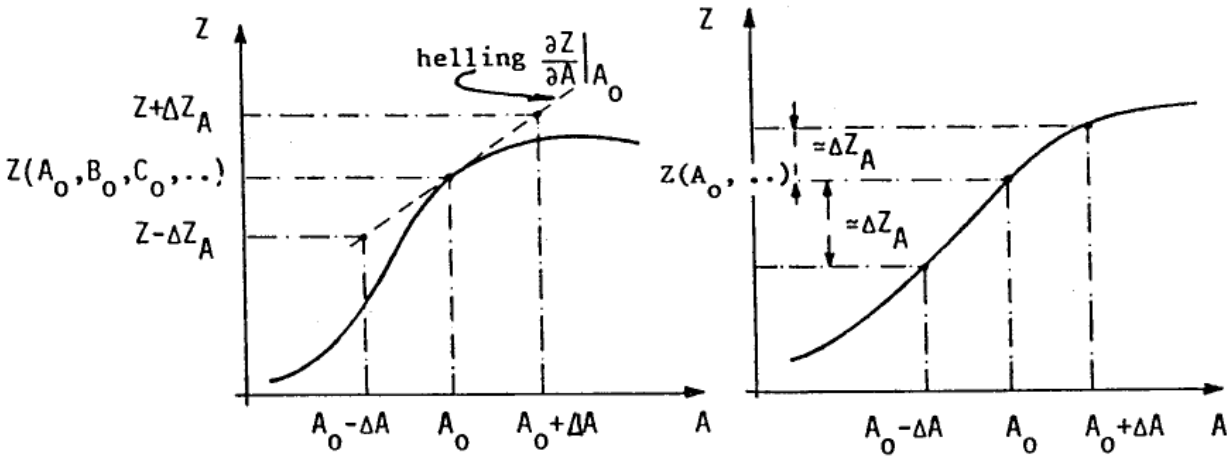
Eq. (1.33b) is usually referred to as *the product rule*. It importantly indicated that the relative (or percent) error in the product function is at least as large as the largest relative error in the primary factors it combines.

1.3.3. Method of partial derivatives

If the function F cannot be represented in a form of sum and product combination we have to apply Eq. (1.29) directly. In this case every $(\partial F/\partial x)\Delta x$ term will contribute to the final error in F, which is sometimes quoted as *the partial error in F due to error in x*. If taking the first derivative appears to be too complicated, this error can also be evaluated from the variance of the function F:

$$\Delta F_A \cong F(A + \Delta A, B, C, \ldots) - F(A, B, C, \ldots),$$
$$\Delta F_B \cong F(A, B + \Delta B, C, \ldots) - F(A, B, C, \ldots), \quad \text{etc}\ldots \qquad (1.34)$$

In other words, the difference between the values of the function calculated in points x and x + Δx with all other parameters remaining constant can be used to evaluate the partial error. This conclusion results actually from the definition of the partial derivative and delivers sufficient accuracy as long as Δx remains small. This is evident from the figure shown below which illustrates the difference between two methods of calculating the partial error in function Z(A, B, C) caused by the error in factor A.



Reference table for error calculations in the case of simple functional relationships

In the table below are given the results relevant to the error calculations in the case of often encountered functional relationships between the function F and the primary quantities A, B, and C treated as independent variables. The parameters *k*, *m*, and *n* are exact constants, which bear no uncertainty by themselves.

Relationship between F and A, B, C	**Relationship between ΔF or δF and ΔA, ΔB, ΔC, δA, δB, δC**
$F = kA$	$\Delta F = k\Delta A$
$F = A + B$ *of* $F = A - B$	$\Delta F = [(\Delta A)^2 + (\Delta B)^2]^{1/2}$
$F = kA - mB$	$\Delta F = [(k\Delta A)^2 + (m\Delta B)^2]^{1/2}$
$F = A + B - C$	$\Delta F = [(\Delta A)^2 + (\Delta B)^2 + [(\Delta C)^2]^{1/2}$
$F = n + A + mB$	$\Delta F = [(\Delta A)^2 + (m\Delta B)^2]^{1/2}$
$F = A.B$ *of* $F = A/B$ *of* $F = kA/B$	$\delta F = [(\delta A)^2 + (\delta B)^2]^{1/2}$
$F = A.B/C$	$\delta F = [(\delta A)^2 + (\delta B)^2 + (\delta C)^2]^{1/2}$
$F = A^n$	$\delta F = n\delta A$
$F = A^2 - B^2$	$\delta F = (2/F)\,[(A\Delta A)^2 + (B\Delta B)^2]^{1/2}$
$F = ln\ A$	$\Delta F = \delta A$
$F = e^A$	$\delta F = \Delta A$
$F = \sin A$	$\Delta F = (\cos A).\Delta A$

1.4. The method of least squares and the linear regression

Experiment: A physical quantity *y* is measured as a function of one or more physical parameters.

Examples

- Current as a function of voltage;
- Voltage as a function of frequency;
- The fall time as a function of height.

How this functional relationship can be analysed and with what accuracy?

Two issues are to be addressed:

- What function corresponds best to the available set of the experimental data (the best fit)? This question is often related to the choice of correct physical model.

- How one can find the numerical parameters of the chosen functional relationship?

1.4.1. Functional analysis of experimental results

Goal: To clarify the functional relationship between the measured quantities.

An experimental curve may be fit using one or several response (model) functions. If y_i is the measured value and y_i^* is calculated from the value of the argument x_i in the *i*-measurement point using a chosen response function, the quality of the fit may be evaluated using **the mean square error** value:

$$m.s.e. \equiv \sum_{i=1}^{n} \left(y_i - y_i^* \right)^2 , \tag{1.35}$$

where *n* is the number of the experimentally measured points. The criterion for "the best fit" can be formulated as the minimal m.s.e. This condition may further be used to find the best model function and/or the best parameters of this function.

Problems:

- In the case of non-linear fitting it becomes difficult to determine error in the fit parameters;
- A larger number of parameters will definitely result in a better fit. Do they have a physical meaning or do they represent the numerical artefact?
- The parameters may become sensitive to each other (the cross-correlation);

One must be very careful with a multi-parameter non-linear fitting.

Solution to be recommended: Try to find a way to linearization of the functional relationship.

Example: The frequency-dependent harmonic signal transfer in RC circuit:

$$\frac{V_C}{V_0} = \frac{1}{\sqrt{1+\omega^2\tau^2}} \Rightarrow y \equiv \left(\frac{V_0}{V_C}\right)^2 - 1 = \omega^2\tau^2$$

where y becomes a linear function of the measured ω^2, while τ^2 can be found from the slope of the straight line.

1.4.2. Linear regression

The best method of curve fitting is *the method of least squares* based on the minimization of the m.s.e. given by Eq. (1.35). In the particular case of linear response function this method is also known as *the linear regression* technique.

The response function in this case is taken in the form

$$y = a + bx \quad , \tag{1.36}$$

in which a corresponds to the portion of the quantity y independent on x, and b shows the rate of variation of y as a function of x.

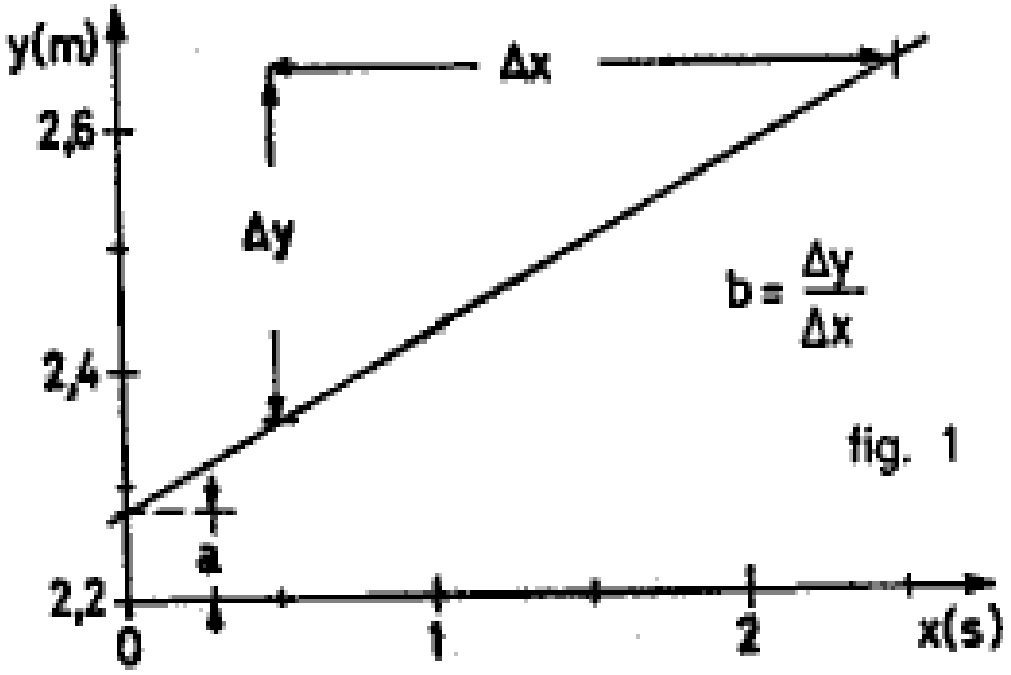


fig. 1

The linear regression can also be used to fit functions which through a mathematical transformation can be re-written in a simple linear form given by Eq. (1.36):

$$z = a\exp\left(-\frac{E}{kT}\right) \quad \rightarrow \quad \text{y = a' + bx} \quad \text{where y = } ln(\text{z}) \text{ en a' = } ln(\text{a})$$

This expression corresponds to the Arrhenius plot used for extraction of the activation energy E from the temperature-dependent transition rate.

$$\text{y} = \text{a} + \text{bz}^2 \qquad \rightarrow \qquad \text{y = a + bx} \qquad \text{given that} \quad \text{x = z}^2 .$$

This equation describes the results of free fall experiment aimed at determination of the gravity acceleration *g*.

1.4.3. Simplified methods for linear function (not requiring a calculator)

Data analysis through pairwise grouping

From expressions

$$y_1 = a + bx_1 \quad \text{and} \quad y_2 = a + bx_2 \quad , \tag{1.37}$$

it follows immediately that

$$b = \frac{y_1 - y_2}{x_1 - x_2} \quad \text{and} \quad a = \frac{y_2 x_1 - y_1 x_2}{x_1 - x_2} \quad . \tag{1.38}$$

From the 2n data pairs (y_1,x_1), (y_2,x_2), … (y_n,x_n), (y_{n+1},x_{n+1}), … (y_{2n},x_{2n}) it is possible to obtain n independent sets of (*a*,*b*)-values. Then the mean value of *a* and *b* can be calculated as the best measured value of these parameters with the standard error determined using Eq. (1.15) or the formula of Peeters Eq. (1.20).

As the accuracy of each individual (*a*,*b*) pair will depend on the difference terms like $x_1 - x_2$ or $y_1 - y_2$, the most effective way of choosing data pairs would be to couple one point out of the first half of the measurement set to the point from the second half of the set:

$$b_1 = \frac{y_{n+1} - y_1}{x_{n+1} - x_1} \; , \quad b_2 = \frac{y_{n+2} - y_2}{x_{n+2} - x_2} \; , \; \ldots \quad b_n = \frac{y_{2n} - y_n}{x_{2n} - x_n} \tag{1.39}$$

leading to the mean b-value

$$\bar{b} = \frac{1}{n}\left(b_1 + b_2 + \cdots + b_n\right) \; . \tag{1.40}$$

Graphical analysis

A simple graphical method can be used to estimate the best *a* and *b* values for the response function $y = a + bx$ from a plot of the measurements set of (y_i,x_i) pairs. One draws a straight line, which – visually – corresponds best to the measured data (the filled line in Fig. 2). For instance, the data points must be distributed in a reasonably symmetric way above and below the line. The slope of the line *b* can be found from the ratio in variations of Δy and Δx, the approximate error can be estimated from the possible range of line slopes that also look "not so bad" (the dashed line in Fig. 2) when compared to the "best line". The value of *a* can be directly read on the y-axis.

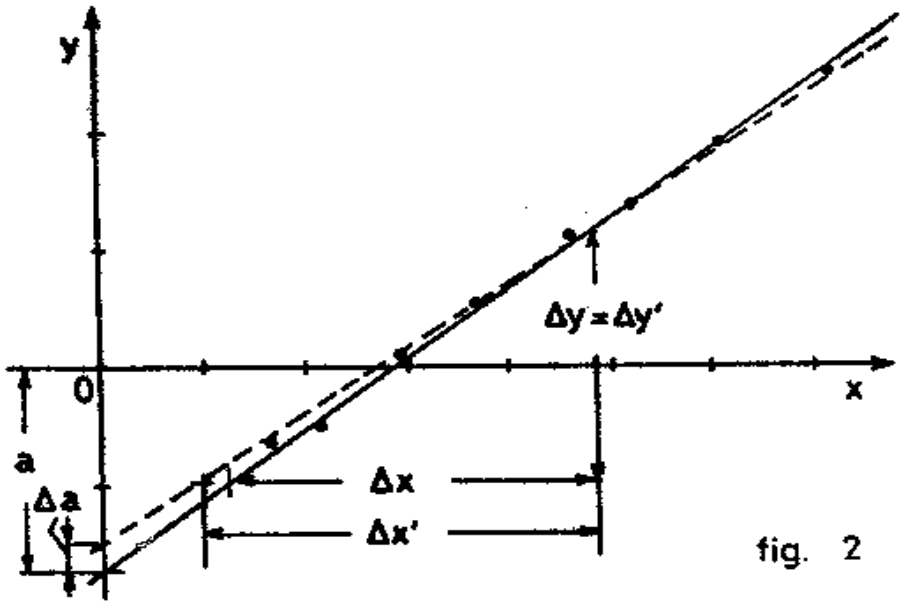


fig. 2

Note: Δx and Δy are taken from the points on the drawn the "best curve", not as the measured (x_i,y_i) values.

Problem: subjective technique, large influence of the observer.

1.4.4. Method of least squares

A bit of theory …

To find a line which describes the available measurements in a best way we have to set a criterion corresponding to the requirement that the deviation of the experimental points from the fitted curve must be as small as possible.

Minimal m.s.e. requirement:

The sum of the squared deviations of the measured **y** values from those obtained by linear fit must be minimal $\sum_i (y_i - a - bx_i)^2$. The values of the parameters *a* and *b* corresponding to the minimum of the m.s.e. function can be found from the equations corresponding to zero derivative of the m.s.e.:

$$\frac{\partial}{\partial a}\sum_i (y_i - a - bx_i)^2 = 0 \,, \tag{1.41}$$

$$\frac{\partial}{\partial b}\sum_i (y_i - a - bx_i)^2 = 0 \,. \tag{1.42}$$

From Eq.(1.41) it follows that

$$\sum_i 2(y_i - a - bx_i)(-1) = 0,$$

or, else,

$$\sum_i y_i = \sum_i a + \sum_i bx_i \quad .$$

In the case of *n* measurement points $\sum_i a = na$, and, consequently,

$$\bar{y} = a + b\bar{x} \,, \tag{1.43}$$

where $\bar{y} = (\sum_i y_i)/n$ and $\bar{x} = (\sum_i x_i)/n$ are the mean values of the measured y- and x-values, respectively. From this relationship it becomes obvious that the best fit line y = *a* + *b*x line will always go through the point $(\bar{x}, \bar{y})$.

In its turn, from Eq. (1.42) it follows that

$$\sum_i 2(y_i - a - bx_i)(-x_i) = 0,$$

or

$$\sum_i (y_i x_i) - a \sum_i x_i - b \sum_i (x_i^2) = 0. \qquad (1.44)$$

By substituting in Eq.(1.44) the value $a = \bar{y} - b\bar{x}$ from Eq.(1.43) one can resolve the equation to find parameter *b*:

$$b = \frac{n\sum_i (x_i y_i) - (\sum_i x_i)(\sum_i y_i)}{n\sum_i (x_i^2) - (\sum_i x_i)^2} \quad . \qquad (1.45)$$

By inserting this result back to Eq.(1.43) we obtain the best value for *a*.

...and the practice

Along with the calculated values of *a* and *b* the PC often provides also value of the *correlation coefficient R* which shows how good the measured points are represented by the linear fit. This coefficient may take values from 0 (the measured points are randomly distributed in all directions, "the star sky") and 1 (all points are perfectly on the fitted line). The usefulness of the correlation coefficient consists in possibility of using it to calculate uncertainties in the factors *a* and *b* obtained through the linear regression analysis. Once R is known, then

$$\Delta b = b\left[\frac{1}{n-2}\left(\frac{1}{R^2} - 1\right)\right]^{1/2}, \qquad (1.46)$$

and

$$\Delta a = \Delta b\left[\frac{1}{n}\sum_i (x_i^2)\right]^{1/2} \quad . \qquad (1.47)$$

If using a calculator, the values of *n* (the number of measured points) and $\sum_i (x_i^2)$ in Eqs. (1.46) and (1.47) one may store in the memory along with $\sum_i x_i$, $\sum_i y_i$, $\sum_i (y_i^2)$ and $\sum_i (x_i y_i)$ from which R is eventually calculated

$$R = \frac{n\sum_i (x_i y_i) - (\sum_i x_i)(\sum_i y_i)}{\left[n\sum_i (x_i{}^2) - (\sum_i x_i)^2\right]^{\frac{1}{2}} \left[n\sum_i (y_i{}^2) - (\sum_i y_i)^2\right]^{\frac{1}{2}}}. \qquad (1.48)$$

1.4.5. Some useful expressions

Obviously, the calculations used in the linear regression can be programmed. As the intermediate results one can calculate values of $\bar{x} = (\sum_i x_i)/n$, $\bar{y} = (\sum_i y_i)/n$ and the residuals $d_i = x_i - \bar{x}$ which would allow to re-write Eq.(1.45) as

$$b = \sum_i (d_i y_i) \Big/ \sum_i (d_i{}^2), \qquad (1.49)$$

and then to calculate *a* using Eq. (1.43).

Further, using calculations of other residuals $D_i = y_i - a - bx_i$ one can estimate uncertainties in b- and a-values

$$\Delta b = \left[\sum_i (D_i{}^2) \Big/ (n-2)\sum_i (d_i{}^2)\right]^{\frac{1}{2}} \quad , \qquad (1.50)$$

and

$$\Delta a = \Delta b \left[\frac{1}{n}\sum_i (d_i{}^2) + \bar{x}^2\right]^{\frac{1}{2}}. \qquad (1.51)$$

This complete regressive analysis must always be preferred over simplified methods.

Some more useful expressions:

The case a=0: The line through the origin y = bx

In *the data pairing method* every measurement point can be considered together with the point (0,0) to obtain the set of values $b_i = y_i / x_i$.

In *the graphic method* one can always use the point (0,0) to draw the line.

In the least square analysis for $a = 0$ we have immediately:

$$b = \sum_i (x_i y_i) \Big/ \sum_i (x_i^2), \tag{1.52}$$

with the corresponding error estimate

$$\Delta b = \frac{\left[\sum_i (y_i^2) \sum_i (x_i^2) - (\sum_i x_i y_i)^2\right]^{\frac{1}{2}}}{\sqrt{n-1}\left(\sum_i x_i^2\right)}. \tag{1.53}$$

1.4.6. Curves and surfaces

The approach of the m.s.e. minimalization described above for the simple case of a linear function may also be extended to more complicated functions describing curves and surfaces. As an example, one may consider the application of the least square method to the response function in the form $y = a + bx + cx^2$. This would require minimalization of the m.s.e. function in the form of

$$S = \sum_i (y_i - a - bx_i - cx_i^2)^2, \tag{1.54}$$

leading to three minima conditions

$$\frac{\partial S}{\partial a} = \frac{\partial S}{\partial b} = \frac{\partial S}{\partial c} = 0. \tag{1.55}$$

These three conditions yield a system of three linear equations which can easily be solved providing the values of a, b, and c. There are many other functions which can be used to fit the data using conditions like those given by Eq. (1.55). These functions may also include more than one argument describing the surfaces: application of the least square method to the response function in the form of a plane $z = a + bx + cy$ or a second order surface $z = a + bx + cx^2 + dy^2$ is not fundamentally different from the above described cases. What may become different when considering more complicated response functions – and, therefore, not discussed here – are the cases when partial derivatives in Eq.(1.55) result in a system of non-linear equations with respect to the fitting parameters which may have no analytical solution.

1.5. Statistical weight of the results and the weighted mean

1.5.1. Definition of the statistical weight

Suppose that a quantity z is measured 10 times, but the measurements are done in 2 series: 7 measurements with one adjustment of the measurement device and another 3 with other adjustment. From each set of the measurements one can calculate separate mean value:

$$z_1 = (x_1 + x_2 + \ldots x_7)/7; z_2 = (x_8 + x_9 + x_{10})/3.$$

Taking now the best value for z out of the complete set of the measurements, we obtain

$$z_{10} = (x_1 + x_2 + \ldots x_{10})/10 = (7z_1 + 3z_2)/10.$$

The factors 7 and 3 are called the *weights* or the *relative weights* of values z_1 and z_2, respectively. In general case the best value of the quantity z is given by

$$\overline{z} = \frac{\sum_{i=1}^{n} w_i z_i}{\sum_{i=1}^{n} w_i}, \qquad (1.56)$$

which represents definition to *the weighted mean* (or *the weighted average*).

Important note: Only the relative weights are important, not their absolute values. We can multiply all the weights by the same factor but this will not influence the calculated mean value.

1.5.2. Error in the weighted mean

What influence has the introduction of the weighted mean on the standard error?

If we consider a set of measurements series ($z_i \pm \Delta z_i$) i=1 …N, we can suppose (like in the example above) that w_i must be proportional to the number of measurement points in the original measurement series n_i.

Important assumption:

All the measurements are coming from the same statistical distribution characterized by the standard error in a single measurement σ.

Thus: $$\Delta z_i = \frac{\sigma}{\sqrt{n_i}}; w_i = n_i = \frac{\sigma^2}{(\Delta z_l)^2} \quad . \qquad (1.57)$$

Then the standard error in the mean value will be $\Delta\,\bar{z} = \sigma/(\Sigma n_i)^{1/2}$.

From Eqs. (1.56) and (1.57) it follows that the best value for **z** and its standard error are given by the expression

$$\bar{z} = \frac{\sum z_i (\Delta z_i)^{-2}}{\sum (\Delta z_i)^{-2}} \pm \frac{1}{\left[\sum (\Delta z_i)^{-2}\right]^{\frac{1}{2}}} . \qquad (1.58)$$

This expression can be used only in the case of *statistical weights*, determined through the number of measurement points in each sub-series of the measurements.

Combination of results with different *instrumental error*.

What to do if z_i values are obtained using different instruments characterized by different intrinsic accuracy?

Example: Astronomic observations from different telescopes or satellites.

Logical hypothesis:

The most accurate result gives the largest contribution to the mean value.

Therefore, the weight might be taken in proportion with $(\Delta z_i)^{-p}$. Using p=2 from Eq. (1.57) we obtain the same expression for the mean as in the case of statistical weights:

$$\bar{z} = \frac{\sum z_i (\Delta z_i)^{-2}}{\sum (\Delta z_i)^{-2}} \quad . \qquad (1.59)$$

What is the difference between two cases?

The instrumental error does not depend on the number of measurements in the set!

Thus, instead of $\Delta z_i = \sigma/\sqrt{n_i}$ we must use Δz_i= const which would lead to different expression for the standard error in the weighted mean value:

$$\Delta\bar{z} = \left[\frac{N}{\sum w_i^2}\right]^{\frac{1}{2}} = \left[\frac{N}{\sum (\Delta z_i)^{-2}}\right]^{\frac{1}{2}}. \qquad (1.60)$$

The difference factor between the errors given by Eq. (1.58) and Eq. (1.60) is equal to $(N)^{1/2}$ and can become large if measurements are repeated many times.

It is important to understand the kind of the error when using the weighted mean calculation.

General recommendation: The weighted mean method is worth to apply when the results are significantly different in the error value (by factor of at least 2).

1.5.3. Linear regression in the case of measurements with different statistical weight

Also when fitting the data using the least square method one may give the most accurate measurements a larger influence on the fit parameters. A simple multiple introduction of the same (good) measurement point according to its statistical weight is the most primitive way to reach the goal. More scientifically sound would be to replace the sum in the expression for m.s.e. [Eq.(1.35)] by the weighted sum

$$m.s.e. = \sum_i w_i \left(y_i - a - bx_i \right)^2 . \tag{1.61}$$

Accordingly, the weights will enter in the expressions for derivatives given by Eqs. (1.41) and (1.42). The resulting system of linear equations

$$b \sum_i w_i {x_i}^2 + a \sum_i w_i x_i = \sum_i w_i x_i y_i , \tag{1.62}$$

$$b \sum_i w_i x_i + a \sum_i w_i = \sum_i w_i y_i , \tag{1.63}$$

can be resolved to obtain the weighted values for a and b in the general line function $y = a + bx$:

$$b = \frac{\sum_{i=1}^{n} w_i (x_i - \bar{x}) y_i}{D_w} \pm \left[\frac{\sum_{i=1}^{n} w_i d_i^2}{(n-2) D_w} \right]^{\frac{1}{2}} , \tag{1.64}$$

$$a = \left[\bar{y} - b\bar{x} \right] \pm \left[\frac{1}{n-2} \left(\frac{D_w}{\sum_{i=1}^{n} w_i} + \bar{x}^2 \right) \frac{\sum_{i=1}^{n} d_i}{D_w} \right]^{\frac{1}{2}} , \tag{1.65}$$

where $\bar{x} = \frac{\sum_{i=1}^{n} w_i x_i}{\sum_{i=1}^{n} w_i}$; $\bar{y} = \frac{\sum_{i=1}^{n} w_i y_i}{\sum_{i=1}^{n} w_i}$;

$$D_w = \sum_{i=1}^{n} w_i x_i \left(x_i - \bar{x}\right),$$

and $d_i = y_i - a - bx_i$.

Line through origin (0,0) $y = bx$:

$$b = \frac{\sum_{i=1}^{n} w_i x_i y_i}{\sum_{i=1}^{n} w_i x_i^2} \pm \left[\frac{\sum_{i=1}^{n} w_i x_i^2 \sum_{i=1}^{n} w_i y_i^2 - \left(\sum_{i=1}^{n} w_i x_i y_i \right)^2}{(n-1)\left(\sum_{i=1}^{n} w_i x_i^2 \right)^2} \right]^{\frac{1}{2}}$$

with (1.66)

$$d_i = y_i - bx_i .$$