

# ERROR ANALYSIS

"To err is human; to evaluate and analyze the error is scientific".

## I Introduction

Every measured physical quantity has an **uncertainty or error** associated with it. An experiment, in general, involves

- (i) **Direct measurement** of various quantities (primary measurements) and
- (ii) **Calculation** of the physical quantity of interest which is a function of the measured quantities. An uncertainty or error in the final result arises because of the errors in the primary measurements (assuming that there is no approximation involved in the calculation). For example, the result of a recent experiment to determine the velocity of light (Phys. Rev. Lett. **29**, 1346 (1972)) was given as

$$C = (299, 792, 456.2 \pm 1.1) \text{ m/s.}$$

The error in the value of C arises from the errors in primary measurements, viz., frequency and wavelength. [g,  $\sigma$ ]

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$$C = 299, 792, 458 \text{ m/sec.}$$

<u>Physical Quantity</u>	<u>Relative standard uncertainty</u>	
	2006	2002
<i>Electronic charge</i>	$2.5 \times 10^{-8}$	$8.5 \times 10^{-8}$
<i>Planck's constant</i>	$5 \times 10^{-8}$	$17 \times 10^{-8}$
<i>Avogadro number</i>	$5 \times 10^{-8}$	$17 \times 10^{-8}$
<i>Fine structure constant (<math>e^2/\hbar c</math>)</i>	$6.8 \times 10^{-10}$	$33 \times 10^{-10}$
<i>Compton wavelength (<math>\hbar/m_0 c</math>)</i>	$1.4 \times 10^{-9}$	$6.7 \times 10^{-9}$
“G”	$1.0 \times 10^{-4}$	$1.5 \times 10^{-4}$
“C”	$< 3.3 \times 10^{-9}$	---

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Error analysis, therefore, consists of

- (i) **Estimating** the errors in all primary measurements, and
- (ii) **Propagating** the error at each step of the calculation. This analysis serves two purposes. First, the error in the final result ( $\pm 1.1 \text{ m/sec}$  in the above example) is an indication of the precision of the measurement and, therefore, an important part of the result. Second, the analysis also tells us which primary measurement is causing

more error than others and thus indicates the direction for further improvement of the experiment.

For example, in measuring 'g' with a simple pendulum, if the error analysis reveals that the errors in 'g' caused by measurements of l (length of the pendulum) and T (time period) are  $0.5 \text{ cm/sec}^2$  and  $3.5 \text{ cm/sec}^2$  respectively, then we know that there is no point in trying to devise a more accurate measurement of l. Rather, we should try to reduce the uncertainty in T by counting a larger number of periods or using a better device to measure time. Thus, error analysis **prior to the experiment** is an important aspect of planning the experiment.

## Nomenclature

- (i) '**Discrepancy**' denotes the difference between two measured values of the same quantity.
- (ii) '**Systematic errors**' are errors which occur in every measurement in the same way-often in the same direction and of the same magnitude - for example, length measurement with a faulty scale. These errors can, in principle, be eliminated or corrected for.
- (iii) '**Random errors**' are errors which can cause the result of a measurement to deviate in either direction from its true value. We shall confine our attention to these errors, and discuss them under two heads: estimated and statistical errors.

## II Estimated Errors

### Estimating a primary error

An estimated error is an estimate of the maximum extent to which a measured quantity might deviate from its true value. For a primary measurement, the estimated error is often taken to be the least count of the measuring instrument. For example, if the length of a string is to be measured with a meter stick, the limiting factor is the accuracy in the least count, i.e.  $0.1 \text{ cm}$ . [1/2 LC] A note of caution is needed here.

What matters really is the **effective least count** and **not** the nominal least count. For example, in measuring electric current with an ammeter, if the smallest division corresponds to  $0.1 \text{ amp}$ , but the marks are far enough apart so that you can easily make out a quarter of a division, then the effective least count will be  $0.025 \text{ amp}$ . On the other hand, if you are reading a vernier scale where five successive marks on the vernier scale (say,  $27^{\text{th}}$  to  $31^{\text{st}}$ ) look equally well in coincidence with the main scale, the effective least count is 3 times the nominal one. Therefore, **make a judicious estimate of the least count**. The estimated error is, in general, related to the **limiting factor** in the accuracy. This limiting factor need not always be the **least count**. Another example, in a null-point electrical measurement, suppose the deflection in the galvanometer remains zero for all values of resistance R from  $351 \Omega$  to  $360 \Omega$ . In that case, the uncertainty in R is  $10 \Omega$  (rather  $5 \Omega$ ), even though the least count of the resistance box may be  $1 \Omega$ . [Stop-watch]

### Propagation of estimated errors

How to calculate the error associated with f, which is a function of the measured quantities a, b, and c ?

Let  $f = f(a, b, c).$  (1)

From differential calculus (Taylor's series in the 1st order)

$$df = \frac{\partial f}{\partial a} da + \frac{\partial f}{\partial b} db + \frac{\partial f}{\partial c} dc . \quad (2)$$

Eq. (2) relates the differential increment in  $f$  resulting from differential increments in  $a$ ,  $b$ ,  $c$ . Thus, if our errors in  $a$ ,  $b$ ,  $c$  (denoted as  $\delta a$ ,  $\delta b$ ,  $\delta c$ ) are small compared to  $a$ ,  $b$ ,  $c$ , respectively, then we may say

$$\delta f = \left| \frac{\partial f}{\partial a} \right| \delta a + \left| \frac{\partial f}{\partial b} \right| \delta b + \left| \frac{\partial f}{\partial c} \right| \delta c . \quad (3)$$

where the modulus signs have been put because errors in  $a$ ,  $b$ , and  $c$  are **independent** of each other and may be in the **positive or negative** direction. Therefore, the maximum possible error will be obtained only by adding absolute values of all the independent contributions. (All the  $\delta$ 's are considered positive by definition). Special care has to be taken when all errors are not independent of each other. This will become clear in special case (V) below.

### Some simple cases

(i) For **addition or subtraction**, the absolute errors are added, e.g.,

$$\begin{aligned} \text{if } f &= a + b - c , \text{ then} \\ \delta f &= \delta a + \delta b + \delta c . \end{aligned} \quad (4)$$

(ii) For **multiplication and division**, the fractional (or percent) errors are added, e.g.,

$$\begin{aligned} \text{if } f &= \frac{ab}{c} , \text{ then} \\ \left| \frac{1}{f} \right| \delta f &= \left| \frac{1}{a} \right| \delta a + \left| \frac{1}{b} \right| \delta b + \left| \frac{1}{c} \right| \delta c . \end{aligned} \quad (5)$$

(iii) For raising to constant **powers**, including fractional powers, the fractional error is multiplied by the power, e.g.,

$$\begin{aligned} \text{if } f &= a^{3.6} , \text{ then} \\ \left| \frac{1}{f} \right| \delta f &= \left| 3.6 \times \frac{1}{a} \right| \delta a . \end{aligned} \quad (6)$$

(iv) In **mixed calculations**, break up the calculation into simple parts, e.g.,

if  $f = \frac{a}{b} - c^{\frac{3}{2}}$ , then

$$\delta f = \delta\left(\frac{a}{b}\right) + \delta\left(c^{\frac{3}{2}}\right).$$

$$\text{As } \left|\frac{b}{a}\right| \delta\left(\frac{a}{b}\right) = \left|\frac{1}{a}\right| \delta a + \left|\frac{1}{b}\right| \delta b$$

$$\text{and } \left|\frac{1}{c^{\frac{3}{2}}}\right| \delta\left(c^{\frac{3}{2}}\right) = \left|\frac{3}{2c}\right| \delta c$$

$$\text{So, } \delta f = \left|\frac{1}{b}\right| \delta a + \left|\frac{a}{b^2}\right| \delta b + \left|\frac{3}{2} c^{\frac{1}{2}}\right| \delta c. \quad (7)$$

Note that the same result could have been derived directly by differentiation.

(v) Consider  $f = \frac{ab}{c} - a^2$ .

The relation for error, **before** putting the modulus signs, is

$$\delta f = \left(\frac{b}{c}\right) \delta a + \left(\frac{a}{c}\right) \delta b - \left(\frac{ab}{c^2}\right) \delta c - 2a \delta a.$$

Note that the  $\delta a$  factors in the first and fourth terms are **not** independent errors. Therefore, we must **not** add the absolute values of these two terms indiscriminately. The correct way to handle it is to collect the coefficients of each independent errors **before** putting modulus signs, i.e.,

$$\delta f = \left|\frac{b}{c} - 2a\right| \delta a + \left|\frac{a}{c}\right| \delta b + \left|\frac{ab}{c^2}\right| \delta c. \quad (8)$$

### III Statistical Errors

#### Statistical distribution and standard deviation

Statistical errors arise when making measurements on **random processes**, e.g., counting particles emitted by a radioactive source. Suppose we have a source giving off 10 particles/sec. on the average. In order to evaluate this count rate experimentally, we count the number of particles for 20 seconds. Shall we get 200 counts? Not necessarily. In fact, we may get any number between zero and infinity. Therefore, in a measurement on a random process, **one cannot specify a maximum possible error**. A good measure of uncertainty in such a case is the standard deviation (s.d.) which specifies the range within which the result of any measurement is "**most likely**" to be.

The exact definition of "most likely" depends on the distribution governing the random events. For all random processes whose probability of occurrence is small and constant, **Poisson distribution** is applicable, i.e.,

$$P_n = \frac{m^n}{n!} e^{-m}, \quad (9)$$

where  $P_n$  is the probability that you will observe a particular count  $n$ , when the expectation value is  $m$ .

It can be shown that if an infinite number of measurements are made, (i) their average would be  $m$  and (ii) their standard deviation (s.d.) would be  $\sqrt{m}$ , for this distribution. Also, if  $m$  is not too small, then **68%** or nearly two-thirds of the measurements would yield numbers within one s.d. in the range  $m \pm \sqrt{m}$ .

In radioactive decay and other nuclear processes, the Poisson distribution is generally valid. This means that we have a way of making certain conclusions without making an infinite number of measurements. Thus, if we measure the number of counts only once, for 100 sec, and the number is, say 1608, then (i) our result for average count rate is 16.08/sec, and (ii) the standard deviation is  $\sqrt{1608} = 40.1$  counts which corresponds to 0.401/sec. So our result for the count rate is  **$(16.1 \pm 0.4) \text{ sec}^{-1}$** . The meaning of this statement must be remembered. **The actual count rate need not necessarily lie within this range, but there is 68% probability that it lies in that range.**

The experimental definition of s.d. for  $k$  measurements of a quantity  $x$  is

$$\sigma_x = \sqrt{\sum_{n=1}^k \left( \frac{\delta x_n^2}{k-1} \right)}, \quad (10)$$

where  $\delta x_n$  is the deviation of measurement  $x_n$  from the mean. However, since we know the distribution, we can ascribe the s.d. even to a single measurement.

### Propagation of statistical errors

For a function  $f$  of independent measurements  $a, b, c$ , the statistical error  $\sigma_f$  is

$$\sigma_f = \sqrt{\left( \frac{\partial f}{\partial a} \sigma_a \right)^2 + \left( \frac{\partial f}{\partial b} \sigma_b \right)^2 + \left( \frac{\partial f}{\partial c} \sigma_c \right)^2}. \quad (11)$$

A few simple cases are discussed below.

(i) For **addition or subtraction**, the **squares of errors** are added, e.g.

$$\begin{aligned} \text{if } f &= a + b - c \\ \text{then, } \sigma_f^2 &= \sigma_a^2 + \sigma_b^2 + \sigma_c^2. \end{aligned} \quad (12)$$

(ii) For **multiplication or division**, the **squares of fractional errors** are added, e.g.

$$\text{if } f = \frac{ab}{c},$$

$$\text{then } \left( \frac{\sigma_f}{f} \right)^2 = \left( \frac{\sigma_a}{a} \right)^2 + \left( \frac{\sigma_b}{b} \right)^2 + \left( \frac{\sigma_c}{c} \right)^2 \quad (13)$$

(iii) If a measurement is repeated  $n$  times, the error in the mean is a factor  $\sqrt{n}$  less than the error in a single measurement, i.e.,

$$\sigma_{\bar{f}} = \frac{\sigma_f}{\sqrt{n}} \quad (14)$$

Note that Eqs. (11-14) apply to any statistical quantities  $a$ ,  $b$ , etc, i.e., primary measurements as well as computed quantities whereas

$$\sigma_m = \sqrt{m} \quad (15)$$

**applies only to a directly measured number**, say, number of  $\alpha$ -particle counts **but not to computed quantities like** count rate.

## IV Miscellaneous

### Repeated measurements

Suppose a quantity  $f$ , whether statistical in nature or **otherwise**, is measured  $n$  times. The best estimate for the actual value of  $f$  is the  $\bar{f}$  average of all measurements. It can be shown that this is the value with respect to which the sum of squares of all deviations is a minimum. Further, **if** errors are assumed to be randomly distributed, the error in **the mean value** is given by

$$\delta_{\bar{f}} = \frac{\delta_f}{\sqrt{n}} \quad (16)$$

where  $\delta_f$  is the error in one measurement. Hence one way of **minimising random errors** is to **repeat the measurement** many times.

### Combination of statistical and estimated errors

In cases where some of the primary measurements have statistical errors and others have estimated errors, the error in the final result is indicated as a s.d. and is calculated by treating all errors as statistical.

### Errors in graphical analysis

The usual way of indicating errors in quantities plotted on graph paper is to draw error bars. The curve should then be drawn so as to pass through all or most of the bars.

Here is a simple method of obtaining the best fit for a straight line on a graph. Having plotted all the points  $(x_1, y_1) \dots (x_n, y_n)$ , plot also the centroid  $(\bar{x}, \bar{y})$ . Then consider all straight lines through the centroid (use a transparent ruler) and visually judge which one will represent the best mean.

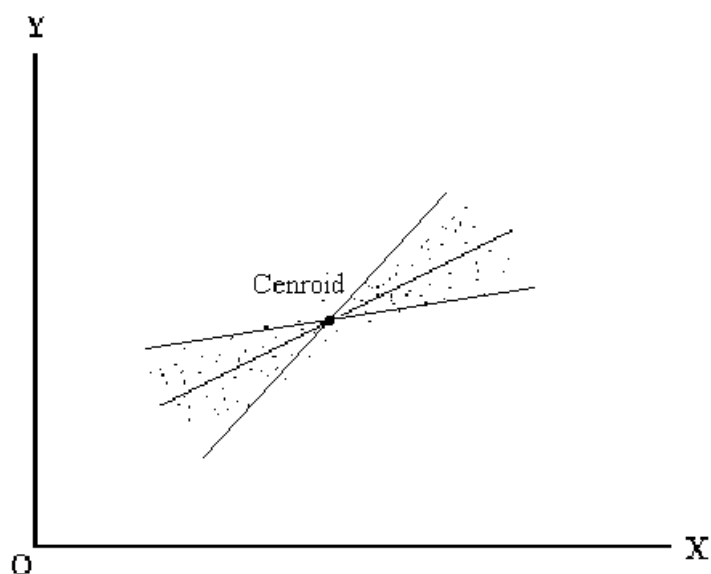


Fig. 1

Having drawn the best line, estimate the error in slope as follows. Rotate the ruler about the centroid until its edge passes through the cluster of points at the 'top right' and the 'bottom left'. This new line gives one extreme possibility; let the difference between the slopes of this and the best line be  $\Delta m_1$ . Similarly determine  $\Delta m_2$  corresponding to the other extreme. The error in the slope may be taken as

$$\Delta m = \frac{\Delta m_1 + \Delta m_2}{2} \cdot \frac{1}{\sqrt{n}}, \quad (17)$$

where  $n$  is the number of points. The factor  $\frac{1}{\sqrt{n}}$  comes because evaluating the slope from the graph is essentially an **averaging process**.

It should be noted that if the scale of the graph is not large enough, the least count of the graph may itself become a limiting factor in the accuracy of the result. Therefore, it is desirable to select the scale so that the least count of the graph paper is much smaller than the experimental error.

### Significant figures (Hide)

A result statement such as  $f = 123.4678 \pm 1.2331 \text{ cm}$  contains many superfluous digits. Firstly, the digits 678 in quantity  $f$  do not mean anything because they represent something much smaller than the uncertainty  $\delta f$ . Secondly  $\delta f$  is an approximate estimate for error and should not need more than two significant figures. The correct expression would be  $f = 123.5 \pm 1.2 \text{ cm}$ .

## V Instructions

1. Calculate the **estimated/statistical error** for the final result. In any graph you plot, show **error bars**. (If the errors are too small to show up on the graph, then write them somewhere on the graph).
2. If the same quantity has been measured/calculated many times, you need not determine the errors each time. Similarly, **one typical error bar** on the graph will be enough.
3. In propagating errors, the **contributions to the final error** from various independent measurements must be shown. For example

$$\begin{aligned} \text{if } f &= ab; \quad \frac{\delta f}{|f|} = \frac{\delta a}{|a|} + \frac{\delta b}{|b|}, \\ a &= 10.0 \pm 0.1, \quad b = 5.1 \pm 0.2 \\ \text{then, } \delta f &= 51.0 \left[ \frac{0.1}{10.0} + \frac{0.2}{5.1} \right] \\ &= 0.51 + 2.0 \\ &\approx 2.5 \\ \text{Therefore, } f &= 51.0 \pm 2.5. \end{aligned}$$

Here the penultimate step must **not be skipped because** it shows that the contribution to the error from  $\delta b$  is large.

4. Where the final result is a known quantity (for example,  $e/m$ ), show the **discrepancy** of your result from the **standard value**. If this is much greater or even less than the estimated error, this is abnormal and **requires explanation**. ( $g = 9.3 \pm 0.1$  or  $10.0 \pm 0.5$ ) OR ( $g = 9.8 \pm 0.5$  or  $9.8 \pm 0.1$ ).

5. Where a quantity is determined many times, the standard deviation should be calculated from Eq.(10). Normally, **the s.d. should not be more than the estimated error**. Also the individual measurements should be distributed only on both sides of the standard value.

**EXERCISE:  $L = (1.1 \pm 0.1)$  cm. What is  $A \pm \Delta A$  ???**

## VI Mean and Standard Deviation

If we make a measurement  $x_1$  of a quantity  $x$ , we expect our observation to be close to the quantity but not exact. If we make another measurement we expect a difference in the observed value due to random errors. As we make more and more measurements we expect them to be distributed around the correct value, assuming that we can neglect or **correct for systematic errors and avoid blunders**. If we make a very large number of measurements we can determine how the data points are distributed in the so-called **parent distribution**. In any practical case, one makes a finite number of measurements and one tries to describe the parent distribution as best as possible.



Consider N measurements of quantity x, yielding values  $x_1, x_2, \dots, x_N$ . One defines

$$\text{Mean} : \bar{x} = \lim_{N \rightarrow \infty} \left[ \left( \frac{1}{N} \sum_{i=1}^N x_i \right) \right], \quad (18)$$

which is equivalent to the centroid or average value of the quantity x.

**Deviations:** The deviation  $d_i$  of any measurement  $x_i$  from the mean  $\bar{x}$  of the parent distribution is defined as

$$d_i = x_i - \bar{x}. \quad (19)$$

Note that if the  $\bar{x}$  is the true value of the quantity being measured,  $d_i$  is also the true error in  $x_i$ .

The arithmetic average of the deviations for an infinite number of observations must vanish, by definition of (Eq.(18))

$$\lim_{N \rightarrow \infty} \left[ \left( \frac{1}{N} \sum_{i=1}^N (x_i - \bar{x}) \right) \right] = \lim_{N \rightarrow \infty} \left[ \left( \frac{1}{N} \sum_{i=1}^N x_i \right) \right] - \bar{x} = 0. \quad (20)$$

There are several indices one can use to indicate the spread (dispersion) of the measurements about the central value, i.e., the mean value. The dispersion is a measure of precision. One can define average deviation  $d$  as the average of the **magnitudes** of the deviations (absolute values of the deviations)

$$d = \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{i=1}^N (|x_i - \bar{x}|).$$

This can be used as a measure of the dispersion of the expected observation about the mean. However, a more appropriate measure of the dispersion is found in the parameter called standard deviation  $\sigma$ , defined as

$$\sigma^2 = \lim_{N \rightarrow \infty} \left[ \frac{1}{N} \sum_{i=1}^N (x_i - \bar{x})^2 \right] = \lim_{N \rightarrow \infty} \left( \frac{1}{N} \sum_{i=1}^N x_i^2 \right) - (\bar{x})^2. \quad (21)$$

$\sigma^2$  is known as **VARIANCE and the STANDARD DEVIATION**  $\sigma$  is the square root of the variance. In other words it is the root mean square (rms) of the deviations. That is

$$\sigma = \sqrt{\frac{\sum_{i=1}^N d_i^2}{N}}. \quad (22)$$

The expression derived from a statistical analysis is

$$\sigma = \sqrt{\frac{\sum_{i=1}^N d_i^2}{(N-1)}} \quad (23)$$

where the denominator is N-1 instead of N. In practice, the distinction between these formulae is unimportant. According to the general theory of statistics the reliability of a result depends upon the number of measurements and, in general, improves with the square root of the number.

**Significance:**  $\bar{x}$ , the mean, is a parameter which characterizes the information we are seeking when we perform an experiment. The mean is, of course, not the most probable value if the parent distribution is not symmetrical but nevertheless it is a reasonable parameter to characterize the distribution. In place of mean, one can characterize the distribution in terms of **median** or **most probable value (mode)**. It can be proved that if we use the average (**mean**) of the measured values for calculating the deviations, the sum of **the square of the deviations is a minimum**. The standard deviation is simply related to this minimum value of the square of the deviations and is used for specifying error quantitatively.

The standard deviation characterizes the uncertainties associated with our experimental attempts to determine the "**true**" value, namely the mean value (defined by Eq.(18)) for all practical purposes.  $\sigma$ , for a given finite number of observations, is the uncertainty in determining the mean of the parent distribution. Thus it is an appropriate measure of the uncertainty in the observations.

## VII Method of Least Squares

Our data consist of pairs of measurements  $(x_i, y_i)$  of an independent variable  $x$  and a dependent variable  $y$ . We wish to fit the data to an equation of the form

$$y = a + bx \quad (24)$$

by determining the values of the coefficients  $a$  and  $b$  such that the discrepancy is minimized between the values of our measurements  $y_i$  and the corresponding values  $y = f(x_i)$  given by Eq. (24). We **cannot determine the coefficients exactly** with only a **finite number of observations**, but we do want to extract from these data the most probable estimates for the coefficients.

The problem is to establish **criteria for minimizing the discrepancy** and optimizing the estimates of the coefficients. For any arbitrary values of  $a$  and  $b$ , we can calculate the deviations  $\delta y_i$  between each of the observed values  $y_i$  and the corresponding calculated values

$$\delta y_i = y_i - a - bx_i \quad (25)$$

If the coefficients are well chosen, these deviations should be relatively small. The sum of these deviations is **not a good measure** of how well we have approximated the data with our calculated straight line because large positive deviations can be balanced by large negative ones to yield a small sum even when the fit is bad. We might however consider **summing up the absolute values** of the deviations, but this leads to difficulties in obtaining an analytical solution. We consider instead the sum of the squares of deviations.

There is no unique correct method for optimizing the coefficients which is valid for all cases. There exists, however, a method which can be **fairly well justified**, which is **simple and straightforward**, which is **well established experimentally (???)** as being appropriate, and which is **accepted by convention**. This is *the* method of least squares which we will explain using the method of maximum likelihood.

## Method of maximum likelihood

Our data consist of a “**sample of observations**” extracted from a parent distribution which determines the probability of making any particular observation. Let us define **parent coefficients  $a_0$  and  $b_0$**  such that the actual relationship between  $y$  and  $x$  is given by

$$y(x) = a_0 + b_0 x \quad . \quad (26)$$

For any given value of  $x = x_i$ , we can calculate the probability  $P_i$  for making the observed measurement  $y_i$ , assuming a Gaussian distribution with a standard deviation  $\sigma_i$  for the observations about the actual value  $y(x_i)$ . It is given by

$$P_i = \frac{1}{\sigma_i \sqrt{2\pi}} \exp \left[ -\frac{1}{2} \left\{ \frac{y_i - y(x_i)}{\sigma_i} \right\}^2 \right] \quad . \quad (27)$$

The probability for making the observed set of measurements of the  $N$  values of  $y_i$  is the **product of these probabilities**

$$P(a_0, b_0) = \Pi P_i = \Pi \left[ \frac{1}{\sigma_i \sqrt{2\pi}} \exp \left\{ -\frac{1}{2} \left( \frac{y_i - y(x_i)}{\sigma_i} \right)^2 \right\} \right] \quad , \quad (28)$$

where the product  $\Pi$  is taken for  $i$  ranging from 1 to  $N$ .

Similarly, for any estimated values of the coefficients  **$a$  and  $b$** , we can calculate the probability that we should make the observed set of measurements

$$P(a, b) = \Pi \left( \frac{1}{\sigma_i \sqrt{2\pi}} \right) \exp \left[ -\frac{1}{2} \left( \frac{\delta y_i}{\sigma_i} \right)^2 \right] \quad . \quad (29)$$

The **method of maximum likelihood** consists of making the assumption that the observed set of measurements is more likely to have come from the actual parent distribution of Eq. (26) than from any other similar distribution with different coefficients and, therefore, the probability in **Eq. (28) is the maximum probability attainable with Eq. (29)**. The best estimates for  $a$  and  $b$  are therefore those values which **maximise the probability in Eq. (29)**. The first term of Eq. (29) is a constant, independent of the values of  $a$  or  $b$ . Thus, **maximizing the probability  $P(a, b)$  is equivalent to minimizing the sum in the exponential**. We define the quantity  $\chi^2$  to be this sum

$$\chi^2 = \sum \left( \frac{\delta y_i}{\sigma_i} \right)^2 = \sum \left[ \frac{1}{\sigma_i^2} (y_i - a - b x_i)^2 \right] \quad , \quad (30)$$

where  $\Sigma$  always implies  $\sum_{i=1}^N$  and consider this to be the **appropriate measure of the goodness of fit**.

Our method for finding the optimum fit to the data will be to minimize this weighted sum of squares of deviations and, hence, to find the fit which produces the smallest sum of squares or the least-squares fit.

**Minimizing  $\chi^2$ :** In order to find the values of the coefficients  $a$  and  $b$  which yield the minimum value for  $\chi^2$ , we use the method of differential calculus for minimizing the function with respect to more than one coefficient. The minimum value of the function  $\chi^2$  of Eq. (30) is one which yields a value of zero for both of the partial derivatives with respect to each of the coefficients.

$$\begin{aligned}\frac{\partial}{\partial a} \chi^2 &= \frac{\partial}{\partial a} \left[ \sum \frac{1}{\sigma_i^2} (y_i - a - bx_i)^2 \right] \\ &= -\frac{2}{\sigma^2} \sum (y_i - a - bx_i) = 0 \\ \frac{\partial}{\partial b} \chi^2 &= -\frac{2}{\sigma^2} \sum [x_i (y_i - a - bx_i)] = 0 ,\end{aligned}\quad (31)$$

where we have for the present **assumed** all of the standard deviations equal,  $\sigma_i = \sigma$ . In other words, errors in  $y$ 's are assumed to be the same for all values of  $x$ . These equations can be rearranged to yield a pair of simultaneous equations

$$\sum y_i = aN + b \sum x_i \quad (32)$$

$$\text{and} \quad \sum x_i y_i = a \sum x_i + b \sum x_i^2 ,$$

where we have substituted  $N$  for  $\sum_{i=1}^N a$  since the sum runs from  $i = 1$  to  $N$ .

We wish to solve Eqs. (32) for the coefficients  $a$  and  $b$ . This will give us the values of the coefficients for which  $\chi^2$ , the sum of squares of the deviations of the data points from the calculated fit, is a minimum. The solutions are:

$$\begin{aligned}a &= \frac{1}{\Delta} \left( \sum x_i^2 \sum y_i - \sum x_i \sum x_i y_i \right) \\ b &= \frac{1}{\Delta} \left( N \sum x_i y_i - \sum x_i \sum y_i \right) \\ \Delta &= N \sum x_i^2 - \left( \sum x_i \right)^2 .\end{aligned}\quad (33)$$

**Errors in the coefficients  $a$  and  $b$ :** Now we enquire what errors should be assigned to  $a$  and  $b$ . In general, the errors in  $y$ 's corresponding to different values of  $x$  will be different. To find standard deviation in ' $a$ ', say  $S_a$ , we approach in the following way. The deviations in ' $a$ ' will get contributions from variations in individual  $y_i$ 's. The contribution of the deviation,  $\delta y_n$  of a typical measured value,  $y_n$  to the standard deviation  $S_a$  is found using the first equation of Eq.(33) reproduced below as

$$a = \frac{\sum x_n^2 \sum y_n - \sum x_n \sum (x_n y_n)}{N \sum x_n^2 - \left( \sum x_n \right)^2} . \quad (34)$$

By differentiating it partially with respect to  $y_i$  we get

$$\frac{\partial a}{\partial y_i} \delta y_i = \frac{\sum x_n^2 - (\sum x_n)x_i}{N \sum x_n^2 - (\sum x_n)^2} \delta y_i . \quad (35)$$

Since  $\delta y_i$  is assumed statistically independent of  $x_i$  we may replace  $\delta y_i$  by its average value

$$\overline{\delta y_i} = \sigma_y = \sqrt{\sum \frac{(\delta y_i)^2}{N}} . \quad (36)$$

Thus this contribution becomes

$$\frac{\partial a}{\partial y_i} \delta y_i = \sigma_y \left[ \frac{\sum x_n^2 - (\sum x_n)x_i}{N \sum x_n^2 - (\sum x_n)^2} \right] . \quad (37)$$

The standard deviation  $S_a$  of the slope 'a' is found by squaring this expression, summing over all measured values of  $y$  (that is, summing the index  $i$  from 1 to  $N$ ), and taking the square root of this sum. Also, it should be realized that  $\sum x_i = \sum x_n$ , and  $\sum x_i^2 = \sum x_n^2$ . The result of this calculation is

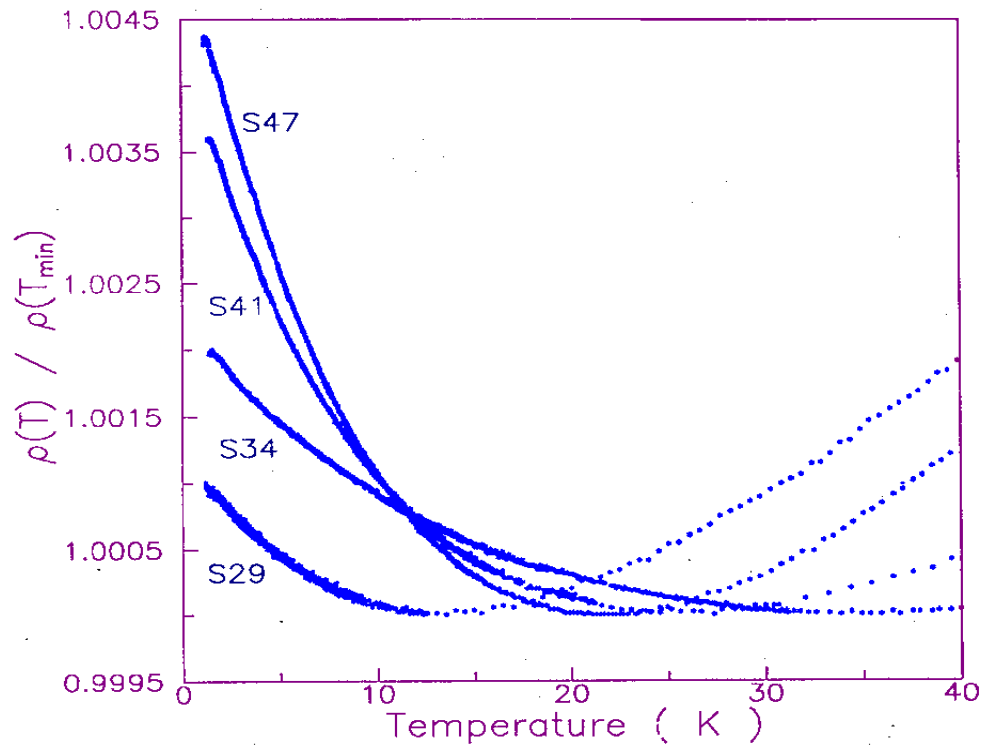
$$S_a = \sigma_y \sqrt{\frac{\sum x_n^2}{[N \sum x_n^2 - (\sum x_n)^2]}} . \quad (38)$$

In a similar manner, the standard deviation  $S_b$  of the intercept 'b' can be found as

$$S_b = \sigma_y \sqrt{\frac{N}{[N \sum x_n^2 - (\sum x_n)^2]}} . \quad (39)$$

### EXAMPLE I

$\rho(T)$  for some Ni-rich Ni-Fe-Cr permalloys



$\rho(T)/\rho_{\min}$  vs.  $T$  taken with a *home-made apparatus*.

- All show minima at  $T_{\min}$ .
- Data every 50 mK below  $T_{\min}$ .

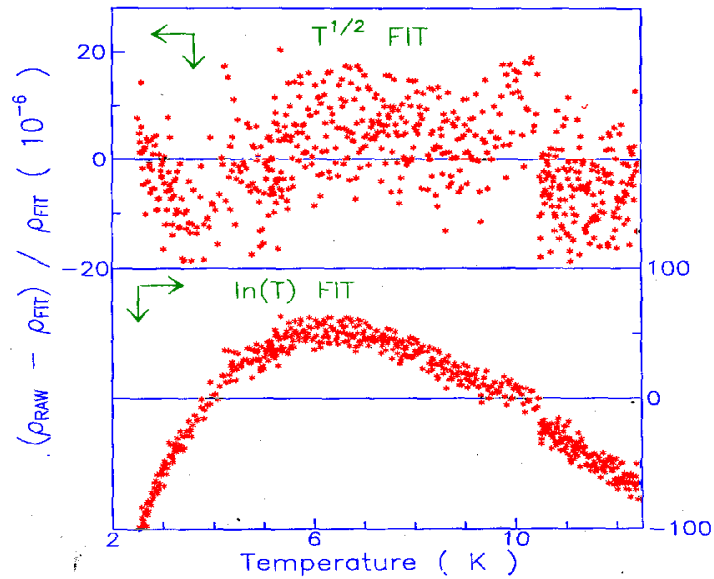
For  $2\text{ K} < T < T_{\min}/2$

Very dilute alloys show Kondo minima where  $\rho(T)$  is given by

$$\rho(T) = \rho_0 - m \ln T. \quad \text{Eq. (1)}$$

e - e interaction in the presence of weak localization gives

$$\rho(T) = \rho_0 - m' \sqrt{T}. \quad \text{Eq. (2)}$$



Random residuals, order of magnitude smaller values of normalized  $\chi^2$  ( $\sim 10^{-10}$ ) for the  $\sqrt{T}$  fit as against systematic residuals &  $\chi^2 \sim 10^{-9}$  for the  $\ln T$  fit.

Exptal. accuracy of ours is  $\sim 5$  ppm (how ???, repeated mmts., fluctuations of nanovoltmeter, crimp connections).

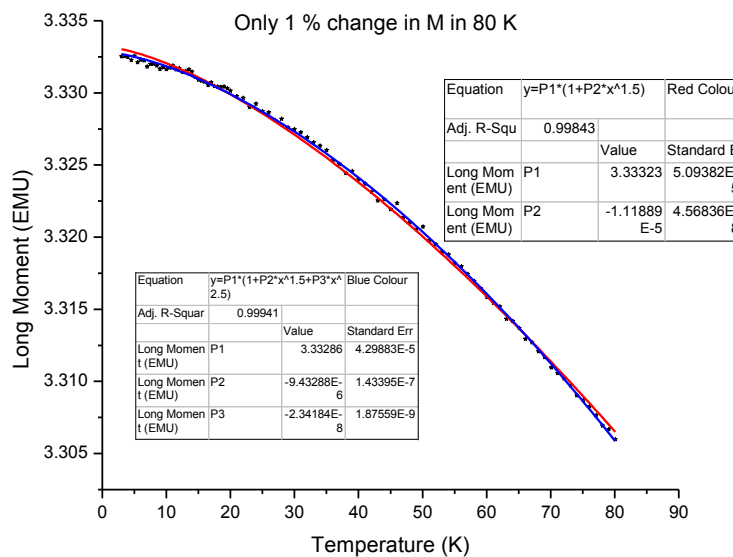
Goodness of fit  $\sim 10$  ppm [ $\chi^2$  ( $\sim 10^{-10}$ )]  $\Rightarrow$  Good fit to that extent!!!

If our accuracy was better than 1 ppm, the fit would have been considered *poor*.

## EXAMPLE II

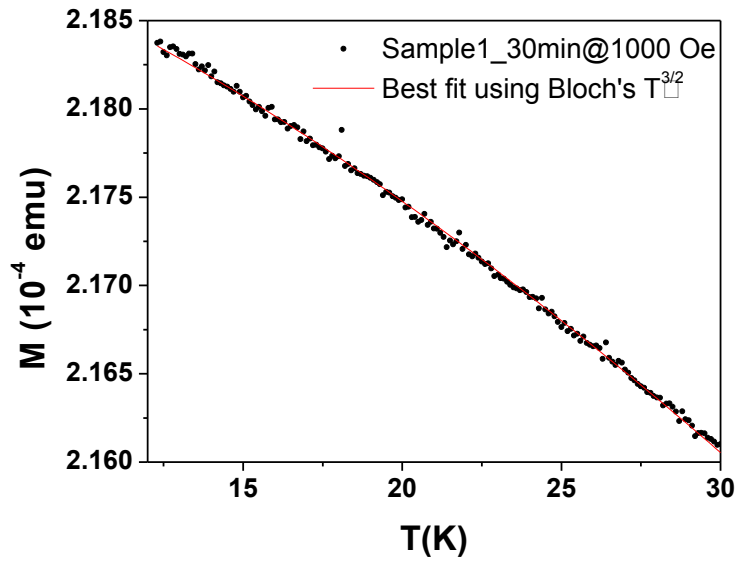
### Spin waves in bulk permalloys

$M(T) = M(0) \cdot (1 + \alpha T^{3/2} + \beta T^{5/2})$ , Fit from 2 K till  $T_C/10$  or 10.



Sample Composition (Sample ID)	M(0) (emu)	$\alpha$ ( $10^{-4} \text{ K}^{-3/2}$ )	$\beta$ ( $10^{-6} \text{ K}^{-5/2}$ )	$T_c$ (K)	Norm $\chi^2$ ( $10^{-7}$ )	$R^2$	D $\text{meV}\text{\AA}^2$
Ni <sub>81.0</sub> Fe <sub>16.7</sub> Mo <sub>2.3</sub> (Mo2)	3.33323± 0.00005	-0.1189± 0.0004	-	<b>720</b>	0.099	0.99843	219
	3.33286± 0.00004	-0.094± 0.001	-0.023 ±0.001		0.036	0.99941	

### *Spin waves in permalloy thin films*



M (T) between 10 and 30 K ( $\ll T_c$ ) fit quite well to Bloch's  $T^{3/2}$  law giving spin-wave stiffness constant  $D = 157$  and  $195 \text{ meV}\text{\AA}^2$  for the thickest films of Mo  $\sim 13.5\%$  and  $10.9\%$ .

Change is still 1 % but the absolute change is only  $2 \times 10^{-6}$  emu as against  $2 \times 10^{-2}$  emu for the bulk. The sample is just push-fitted into the straw with no packing whatsoever.

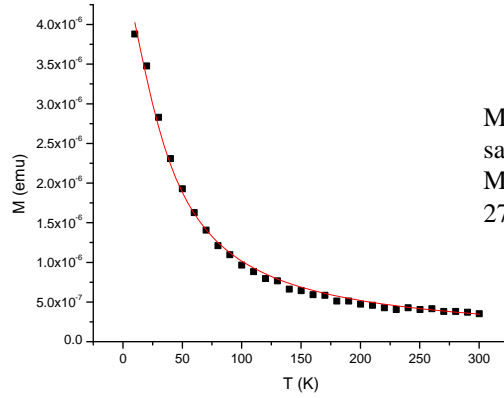


## Superparamagnetism

Samples are single layers of Ni nanoparticles with non-conducting  $\text{Al}_2\text{O}_3$  on both sides deposited on both Si and Sapphire substrates using PLD technique.

$M(H, T)$  measured using Quantum Design MPMS (SQUID magnetometer).

Diamagnetic contribution of substrate subtracted (typically  $\chi = -2 \times 10^{-4}$  emu/tesla).



$M(T)$  at  $H = 200$  Oe for 6 nm Ni sample. Langevin/Brillouin function  $M = (\coth x - 1/x)$  fits well with  $\mu = 2700 \mu_B$  where  $x = \mu H / k_B T$ .

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