

## 4. Statistics and the Treatment of Experimental Data

Statistics plays an essential part in all the sciences as it is the tool which allows the scientist to treat the uncertainties inherent in all measured data and to eventually draw conclusions from the results. For the experimentalist, it is also a design and planning tool. Indeed, before performing any measurement, one must consider the tolerances required of the apparatus, the measuring times involved, etc., as a function of the desired precision on the result. Such an analysis is essential in order to determine its feasibility in material, time and cost.

Statistics, of course, is a subject unto itself and it is neither fitting nor possible to cover all the principles and techniques in a book of this type. We have therefore limited ourselves to those topics most relevant for experimental nuclear and particle physics. Nevertheless, given the (often underestimated) importance of statistics we shall try to give some view of the general underlying principles along with examples, rather than simple “recipes” or “rules of thumb”. This hopefully will be more useful to the physicist in the long run, if only because it stimulates him to look further. We assume here an elementary knowledge of probability and combinatorial theory.

### 4.1 Characteristics of Probability Distributions

Statistics deals with random processes. The outcomes of such processes, for example, the throwing of a die or the number of disintegrations in a particular radioactive source in a period of time  $T$ , fluctuate from trial to trial such that it is impossible to predict with certainty what the result will be for any given trial. Random processes are described, instead, by a *probability density* function which gives the expected frequency of occurrence for each possible outcome. More formally, the outcome of a random process is represented by a *random variable*  $x$ , which ranges over all admissible values in the process. If the process is the throwing of a single die, for instance, then  $x$  may take on the integer values 1 to 6. Assuming the die is true, the probability of an outcome  $x$  is then given by the density function  $P(x) = 1/6$ , which in this case happens to be the same for all  $x$ . The random variable  $x$  is then said to be *distributed* as  $P(x)$ .

Depending on the process, a random variable may be continuous or discrete. In the first case, it may take on a continuous range of values, while in the second only a finite or denumerably infinite number of values is allowed. If  $x$  is discrete,  $P(x_i)$  then gives the frequency at each point  $x_i$ . If  $x$  is continuous, however, this interpretation is not possible and only probabilities of finding  $x$  in finite intervals have meaning. The distribution  $P(x')$  is then a continuous density such that the probability of finding  $x'$  in the interval  $x$  to  $x + dx$  is  $P(x)dx$ .

### 4.1.1 Cumulative Distributions

Very often it is desired to know the probability of finding  $x$  between certain limits, e.g.,  $P(x_1 \leq x \leq x_2)$ . This is given by the cumulative or integral distribution

$$P(x_1 \leq x \leq x_2) = \int_{x_1}^{x_2} P(x) dx, \quad (4.1)$$

where we have assumed  $P(x)$  to be continuous. If  $P(x)$  is discrete, the integral is replaced by a sum,

$$P(x_1 \leq x \leq x_2) = \sum_{i=1}^2 P(x_i). \quad (4.2)$$

By convention, also, the probability distribution is normalized to 1, i.e.,

$$\int P(x) dx = 1 \quad (4.3)$$

if  $x$  is continuous or

$$\sum_i P(x_i) = 1 \quad (4.4)$$

if  $x$  is discrete. This simply says that the probability of observing one of the possible outcomes in a given trial is defined as 1. It follows then that  $P(x_i)$  or  $\int P(x) dx$  cannot be greater than 1 or less than 0.

### 4.1.2 Expectation Values

An important definition which we will make use of later is the *expectation value* of a random variable or a random variable function. If  $x$  is a random variable distributed as  $P(x)$ , then

$$E[x] = \int x P(x) dx \quad (4.5)$$

is the *expected* value of  $x$ . The integration in (4.5) is over all admissible  $x$ . This, of course, is just the standard notion of an average value. For a discrete variable, (4.5) becomes a sum

$$E[x] = \sum_i x_i P(x_i). \quad (4.6)$$

Similarly, if  $f(x)$  is a function of  $x$ , then

$$E[f(x)] = \int f(x) P(x) dx \quad (4.7)$$

is the expected value of  $f(x)$ .

To simplify matters in the remainder of this section, we will present results assuming a continuous variable. Unless specified otherwise, the discrete case is found by replacing integrals with a summation.

### 4.1.3 Distribution Moments. The Mean and Variance

A probability distribution may be characterized by its *moments*. The  $r$ th moment of  $x$  about some fixed point  $x_0$  is defined as the expectation value of  $(x - x_0)^r$  where  $r$  is an

integer. An analogy may be drawn here with the moments of a mass distribution in mechanics. In such a case,  $P(x)$  plays the role of the mass density.

In practice, only the first two moments are of importance. And, indeed, many problems are solved with only a knowledge of these two quantities. The most important is the first moment about zero,

$$\mu = E[x] = \int x P(x) dx . \quad (4.8)$$

This can be recognized as simply the *mean* or *average* of  $x$ . If the analogy with mass moments is made, the mean thus represents the “*center of mass*” of the probability distribution.

It is very important here to distinguish the mean as defined in (4.8) from the mean which one calculates from a set of repeated measurements. The first refers to the theoretical mean, as calculated from the theoretical distribution, while the latter is an *experimental* mean taken from a sample. As we shall see in Sect. 4.4.2, the sample mean is an estimate of the theoretical mean. Throughout the remainder of this chapter, we shall always use the Greek letter  $\mu$  to designate the theoretical mean.

The second characteristic quantity is the second moment about the mean (also known as the *second central moment*),

$$\sigma^2 = E[(x - \mu)^2] = \int (x - \mu)^2 P(x) dx . \quad (4.9)$$

This is commonly called the *variance* and is denoted as  $\sigma^2$ . The square root of the variance,  $\sigma$ , is known as the *standard deviation*. As can be seen from (4.9), the variance is the average squared deviation of  $x$  from the mean. The standard deviation,  $\sigma$ , thus measures the dispersion or width of the distribution and gives us an idea of how much the random variable  $x$  fluctuates about its mean. Like  $\mu$ , (4.9) is the theoretical variance and should be distinguished from the sample variance to be discussed in Sect. 4.4.

Further moments, of course, may also be calculated, such as the third moment about the mean. This is known as the *skewness* and it gives a measure of the distribution’s symmetry or asymmetry. It is employed on rare occasions, but very little information is generally gained from this moment or any of the following ones.

#### 4.1.4 The Covariance

Thus far we have only considered the simple case of single variable probability distributions. In the more general case, the outcomes of a process may be characterized by several random variables,  $x, y, z, \dots$ . The process is then described by a *multivariate* distribution  $P(x, y, z, \dots)$ . An example is a playing card which is described by two variables: its denomination and its suit.

For multivariate distributions, the mean and variance of each separate random variable  $x, y, \dots$ , are defined in the same way as before (except that the integration is over all variables). In addition a third important quantity must be defined:

$$\text{cov}(x, y) = E[(x - \mu_x)(y - \mu_y)] , \quad (4.10)$$

where  $\mu_x$  and  $\mu_y$  are the means of  $x$  and  $y$  respectively. Equation (4.10) is known as the *covariance* of  $x$  and  $y$  and it is defined for each pair of variables in the probability density. Thus, if we have a trivariate distribution  $P(x, y, z)$ , there are three covariances:  $\text{cov}(x, y)$ ,  $\text{cov}(x, z)$  and  $\text{cov}(y, z)$ .

The covariance is a measure of the linear correlation between the two variables. This is more often expressed as the *correlation coefficient* which is defined as

$$\rho = \frac{\text{cov}(x, y)}{\sigma_x \sigma_y}, \quad (4.11)$$

where  $\sigma_x$  and  $\sigma_y$  are the standard deviations of  $x$  and  $y$ . The correlation coefficient varies between  $-1$  and  $+1$  where the sign indicates the sense of the correlation. If the variables are perfectly correlated linearly, then  $|\rho| = 1$ . If the variables are independent<sup>1</sup> then  $\rho = 0$ . Care must be taken with the converse of this last statement, however. If  $\rho$  is found to be  $0$ , then  $x$  and  $y$  can only be said to be *linearly* independent. It can be shown, in fact, that if  $x$  and  $y$  are related parabolically, (e.g.,  $y = x^2$ ), then  $\rho = 0$ .

## 4.2 Some Common Probability Distributions

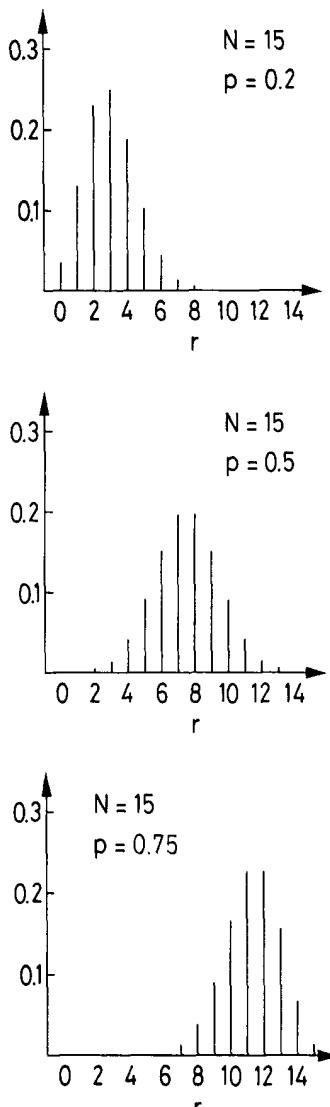


Fig. 4.1. Binomial distribution for various values of  $N$  and  $p$

While there are many different probability distributions, a large number of problems in physics are described or can be approximately described by a surprisingly small group of theoretical distributions. Three, in particular, the binomial, Poisson and Gaussian distributions find a remarkably large domain of application. Our aim in this section is to briefly survey these distributions and describe some of their mathematical properties.

### 4.2.1 The Binomial Distribution

Many problems involve repeated, independent trials of a process in which the outcome of a single trial is dichotomous, for example, *yes or no*, *heads or tails*, *hit or miss*, etc. Examples are the tossing of a coin  $N$  times, the number of boys born to a group of  $N$  expectant mothers, or the number of hits scored after randomly throwing  $N$  balls at a small, fixed target.

More generally, let us designate the two possible outcomes as *success* and *failure*. We would then like to know the probability of  $r$  successes (or failures) in  $N$  tries regardless of the order in which they occur. If we assume that the probability of success does not change from one trial to the next, then this probability is given by the *binomial distribution*,

$$P(r) = \frac{N!}{r!(N-r)!} p^r (1-p)^{N-r}, \quad (4.12)$$

where  $p$  is the probability of success in a single trial.

Equation (4.12) is a discrete distribution and Fig. 4.1 shows its form for various values of  $N$  and  $p$ . Using (4.8) and (4.9), the mean and variance may be calculated to yield

$$\mu = \sum_r r P(r) = Np \quad \text{and} \quad (4.13)$$

<sup>1</sup> The mathematical definition of independence is that the joint probability is a separable function, i.e.,  $P(x, y) = P_1(x)P_2(y)$ .

$$\sigma^2 = \sum_r (r - \mu)^2 P(r) = Np(1-p). \quad (4.14)$$

It can be shown that (4.12) is normalized by summing  $P(r)$  from  $r=0$  to  $r=N$ . Here it will be noticed that  $P(r)$  is nothing but the  $r$ th term of the binomial expansion (whence the name!), so that

$$\sum_r \frac{N!}{r!(N-r)!} p^r (1-p)^{N-r} = [(1-p) + p]^N = 1. \quad (4.15)$$

Finding the cumulative distribution between limits other than 0 and  $N$  is somewhat more complicated, however, as no analytic form for the sum of terms exist. If there are not too many, the individual terms may be calculated separately and then summed. Otherwise, tabulations of the cumulative binomial distribution may be used.

In the limit of large  $N$  and not too small  $p$ , the binomial distribution may be approximated by a Gaussian distribution with mean and variance given by (4.13) and (4.14). For practical calculations, using a Gaussian is usually a good approximation when  $N$  is greater than about 30 and  $p \geq 0.05$ . It is necessary, of course, to ignore the discrete character of the binomial distribution when using this approximation (although there are corrections for this). If  $p$  is small ( $\leq 0.05$ ), such that the product  $Np$  is finite, then the binomial distribution is approximated by the Poisson distribution discussed in the next section.

## 4.2.2 The Poisson Distribution

The *Poisson* distribution occurs as the limiting form of the binomial distribution when the probability  $p \rightarrow 0$  and the number of trials  $N \rightarrow \infty$ , such that the mean  $\mu = Np$ , remains finite. The probability of observing  $r$  events in this limit then reduces to

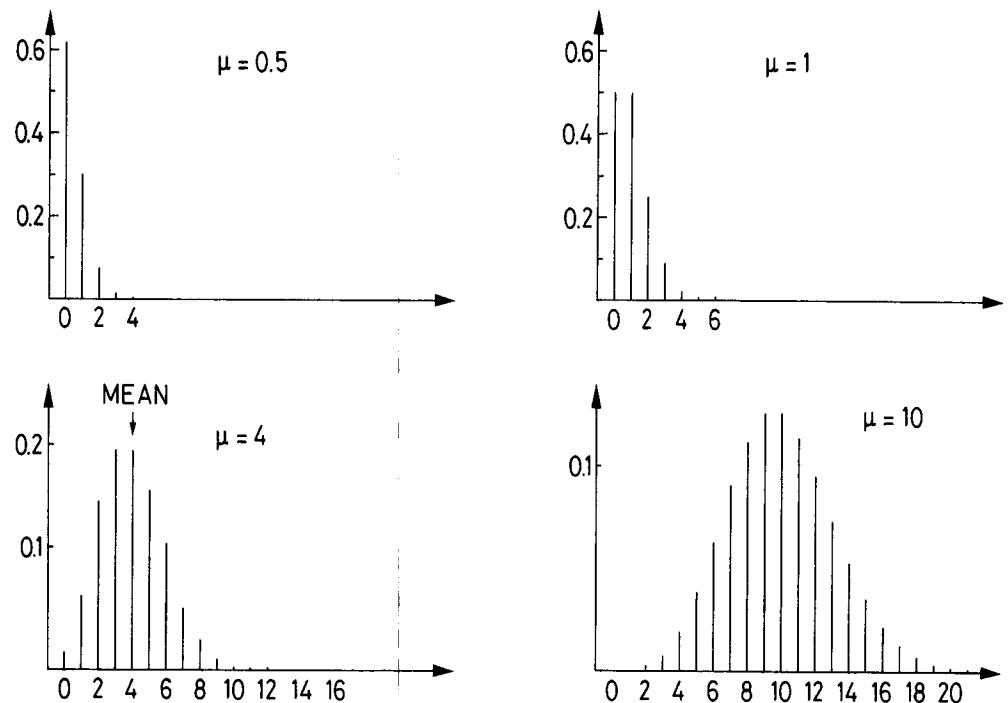
$$P(r) = \frac{\mu^r e^{-\mu}}{r!}. \quad (4.16)$$

Like (4.12), the Poisson distribution is discrete. It essentially describes processes for which the single trial probability of success is very small but in which the number of trials is so large that there is nevertheless a reasonable rate of events. Two important examples of such processes are radioactive decay and particle reactions.

To take a concrete example, consider a typical radioactive source such as  $^{137}\text{Cs}$  which has a half-life of 27 years. The probability per unit time for a single nucleus to decay is then  $\lambda = \ln 2/27 = 0.026/\text{year} = 8.2 \times 10^{-10} \text{s}^{-1}$ . A small probability indeed! However, even a 1  $\mu\text{g}$  sample of  $^{137}\text{Cs}$  will contain about  $10^{15}$  nuclei. Since each nucleus constitutes a *trial*, the mean number of decays from the sample will be  $\mu = Np = 8.2 \times 10^5$  decays/s. This satisfies the limiting conditions described above, so that the probability of observing  $r$  decays is given by (4.16). Similar arguments can also be made for particle scattering.

Note that in (4.16), only the mean appears so that knowledge of  $N$  and  $p$  is not always necessary. This is the usual case in experiments involving radioactive processes or particle reactions where the mean counting rate is known rather than the number of nuclei or particles in the beam. In many problems also, the mean per unit dimension  $\lambda$ , e.g. the number of reactions per second, is specified and it is desired to know the proba-

**Fig. 4.2.** Poisson distribution for various values of  $\mu$



bility of observing  $r$  events in  $t$  units, for example,  $t = 3$  s. An important point to note is that the mean in (4.16) refers to the mean number in  $t$  units. Thus,  $\mu = \lambda t$ . In these types of problems we can rewrite (4.16) as

$$P(r) = \frac{(\lambda t)^r e^{-\lambda t}}{r!} \quad (4.17)$$

An important feature of the Poisson distribution is that it depends on only one parameter:  $\mu$ . [That  $\mu$  is indeed the mean can be verified by using (4.8)]. From (4.9), we also find that

$$\sigma^2 = \mu, \quad (4.18)$$

that is the variance of the Poisson distribution is equal to the mean. The standard deviation is then  $\sigma = \sqrt{\mu}$ . This explains the use of the square roots in counting experiments (see Examples 1.1 and 1.2, on p. 11 and 12).

Figure 4.2 plots the Poisson distribution for various values of  $\mu$ . Note that the distribution is *not* symmetric. The peak or maximum of the distribution does not, therefore, correspond to the mean. However, as  $\mu$  becomes large, the distribution becomes more and more symmetric and approaches a Gaussian form. For  $\mu \geq 20$ , a Gaussian distribution with mean  $\mu$  and variance  $\sigma^2 = \mu$ , in fact, becomes a relatively good approximation and can be used in place of the Poisson for numerical calculations. Again, one must neglect the fact that we are replacing a discrete distribution by a continuous one.

#### 4.2.3 The Gaussian or Normal Distribution

The *Gaussian* or *normal* distribution plays a central role in all of statistics and is the most ubiquitous distribution in all the sciences. Measurement errors, and in particular,

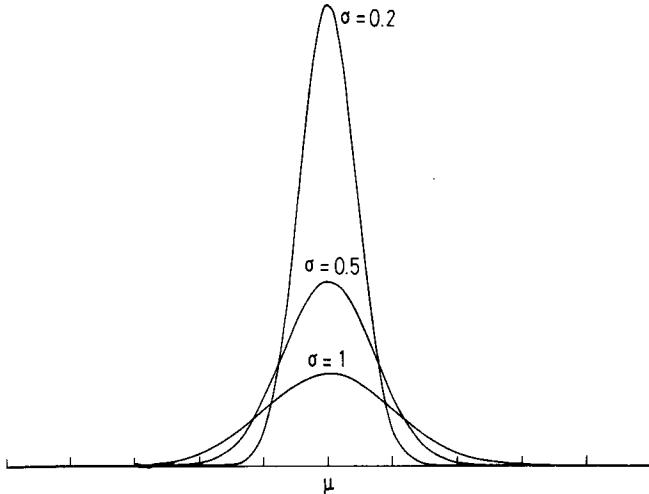


Fig. 4.3. The Gaussian distribution for various  $\sigma$ . The standard deviation determines the width of the distribution

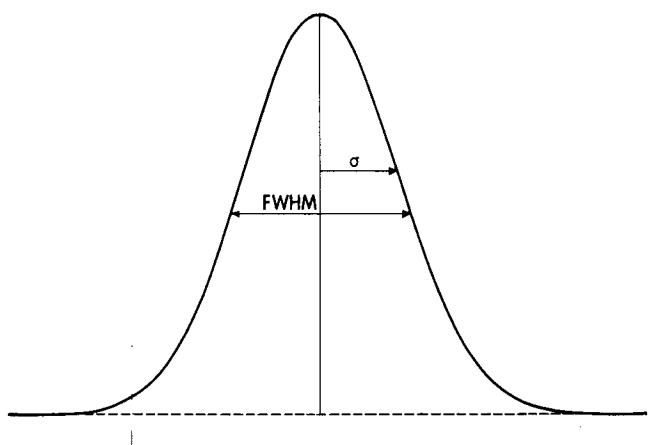


Fig. 4.4. Relation between the standard deviation  $\sigma$  and the full width at half-maximum (FWHM)

instrumental errors are generally described by this probability distribution. Moreover, even in cases where its application is not strictly correct, the Gaussian often provides a good approximation to the true governing distribution.

The Gaussian is a continuous, symmetric distribution whose density is given by

$$P(x) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right). \quad (4.19)$$

The two parameters  $\mu$  and  $\sigma^2$  can be shown to correspond to the mean and variance of the distribution by applying (4.8) and (4.9).

The shape of the Gaussian is shown in Fig. 4.3, which illustrates this distribution for various  $\sigma$ . The significance of  $\sigma$  as a measure of the distribution width is clearly seen. As can be calculated from (4.19), the standard deviation corresponds to the half width of the peak at about 60% of the full height. In some applications, however, the full width at half maximum (FWHM) is often used instead. This is somewhat larger than  $\sigma$  and can easily be shown to be

$$\text{FWHM} = 2\sigma\sqrt{2\ln 2} = 2.35\sigma. \quad (4.20)$$

This is illustrated in Fig. 4.4. In such cases, care should be taken to be clear about which parameter is being used. Another width parameter which is also seen in the literature is the full-width at one-tenth maximum (FWTM).

The integral distribution for the Gaussian density, unfortunately, cannot be calculated analytically so that one must resort to numerical integration. Tables of integral values are readily found as well. These are tabulated in terms of a *reduced Gaussian* distribution with  $\mu = 0$  and  $\sigma^2 = 1$ . All Gaussian distributions may be transformed to this reduced form by making the variable transformation

$$z = \frac{x-\mu}{\sigma}, \quad (4.21)$$

where  $\mu$  and  $\sigma$  are the mean and standard deviation of the original distribution. It is a trivial matter then to verify that  $z$  is distributed as a reduced Gaussian.

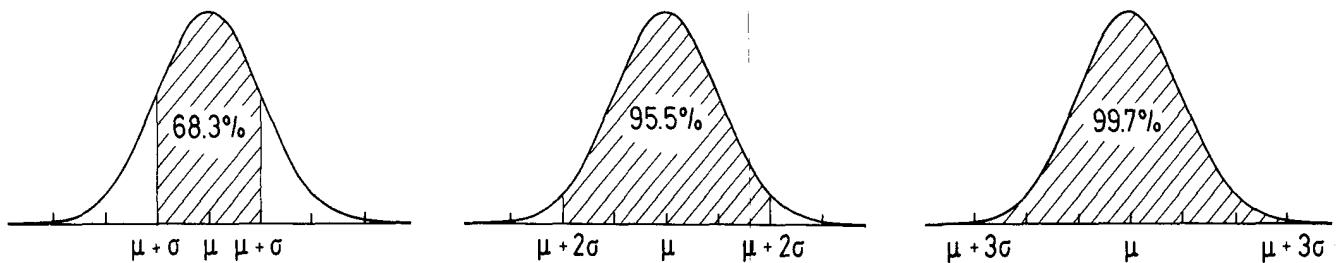


Fig. 4.5. The area contained between the limits  $\mu \pm 1\sigma$ ,  $\mu \pm 2\sigma$  and  $\mu \pm 3\sigma$  in a Gaussian distribution

An important practical note is the area under the Gaussian between integral intervals of  $\sigma$ . This is shown in Fig. 4.5. These values should be kept in mind when interpreting measurement errors. The presentation of a result as  $x \pm \sigma$  signifies, in fact, that the true value has  $\approx 68\%$  probability of lying between the limits  $x - \sigma$  and  $x + \sigma$  or a  $95\%$  probability of lying between  $x - 2\sigma$  and  $x + 2\sigma$ , etc. Note that for a  $1\sigma$  interval, there is almost a  $1/3$  probability that the true value is outside these limits! If two standard deviations are taken, then, the probability of being outside is only  $\approx 5\%$ , etc.

#### 4.2.4 The Chi-Square Distribution

As we will see in Sect. 4.7, the *chi-square* distribution is particularly useful for testing the *goodness-of-fit* of theoretical formulae to experimental data. Mathematically, the chi-square is defined in the following manner. Suppose we have a set of  $n$  independent random variables,  $x_i$ , distributed as Gaussian densities with theoretical means  $\mu_i$  and standard deviations  $\sigma_i$ , respectively. The sum

$$u = \sum_{i=1}^n \left( \frac{x_i - \mu_i}{\sigma_i} \right)^2 \quad (4.22)$$

is then known as the *chi-square*. This is more often designated by the Greek letter  $\chi^2$ ; however, to avoid confusion due to the exponent we will use  $u = \chi^2$  instead. Since  $x_i$  is a random variable,  $u$  is also a random variable and it can be shown to follow the distribution

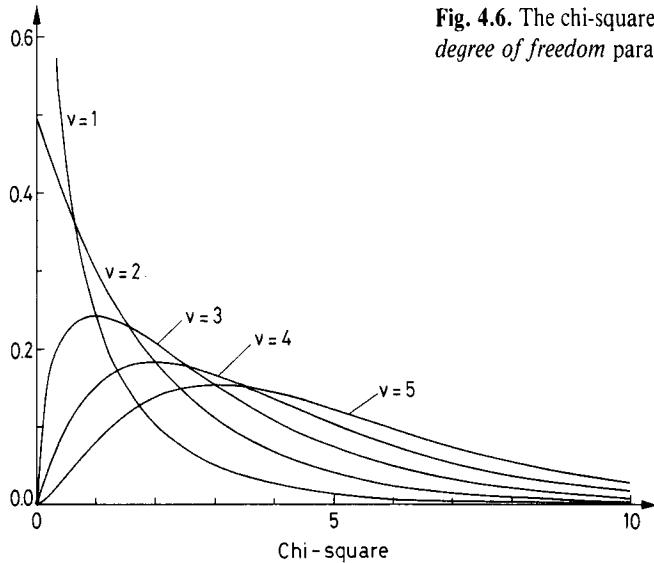
$$P(u) du = \frac{(u/2)^{(\nu/2)-1} \exp(-u/2)}{2\Gamma(\nu/2)} du, \quad (4.23)$$

where  $\nu$  is an integer and  $\Gamma(\nu/2)$  is the *gamma function*. The integer  $\nu$  is known as the *degrees of freedom* and is the sole parameter of the distribution. Its value thus determines the form of the distribution. The *degrees of freedom* can be interpreted as a parameter related to the number of independent variables in the sum (4.22).

Figure 4.6 plots the chi-square distribution for various values of  $\nu$ . The mean and variance of (4.23) can also be shown to be

$$\mu = \nu, \quad \sigma^2 = 2\nu. \quad (4.24)$$

To see what the chi-square represents, let us examine (4.22) more closely. Ignoring the exponent for a moment, each term in the sum is just the deviation of  $x_i$  from its theoretical mean divided by its expected dispersion. The chi-square thus characterizes



**Fig. 4.6.** The chi-square distribution for various values of the degree of freedom parameter  $v$

the fluctuations in the data  $x_i$ . If indeed the  $x_i$  are distributed as Gaussians with the parameters indicated, then on the average, each ratio should be about 1 and the chi-square,  $u = v$ . For any given set of  $x_i$ , of course, there will be a fluctuation of  $u$  from this mean with a probability given by (4.23). The utility of this distribution is that it can be used to test hypotheses. By forming the chi-square between measured data and an assumed theoretical mean, a measure of the *reasonableness* of the fluctuations in the measured data about this hypothetical mean can be obtained. If an improbable chi-square value is obtained, one must then begin questioning the theoretical parameters used.

## 4.3 Measurement Errors and the Measurement Process

Measurements of any kind, in any experiment, are always subject to uncertainties or *errors*, as they are more often called. We will argue in this section that the measurement process is, in fact, a random process described by an abstract probability distribution whose parameters contain the information desired. The results of a measurement are then samples from this distribution which allow an estimate of the theoretical parameters. In this view, measurement errors can be seen then as sampling errors.

Before going into this argument, however, it is first necessary to distinguish between two types of errors: *systematic* and *random*.

### 4.3.1 Systematic Errors

Systematic errors are uncertainties in the bias of the data. A simple example is the zeroing of an instrument such as a voltmeter. If the voltmeter is not correctly zeroed before use, then all values measured by the voltmeter will be biased, i.e., offset by some constant amount or factor. However, even if the utmost care is taken in setting the instrument to zero, one can only say that it has been zeroed to within some value. This value may be small, but it sets a limit on the degree of certainty in the measurements and thus to the conclusions that can be drawn.

An important point to be clear about is that a systematic error implies that all measurements in a set of data taken with the same instrument are shifted in the same direction by the same amount – in unison. This is in sharp contrast to random errors where each individual measurement fluctuates independently of the others. Systematic errors, therefore, are usually most important when groups of data points taken under the same conditions are being considered. Unfortunately, there is no consistent method by which systematic errors may be treated or analyzed. Each experiment must generally be considered individually and it is often very difficult just to identify the possible sources let alone estimate the magnitude of the error. Our discussion in the remainder of this chapter, therefore, will not be concerned with this topic.

#### 4.3.2 Random Errors

In contrast to systematic errors, random errors may be handled by the theory of statistics. These uncertainties may arise from instrumental imprecisions, and/or, from the inherent statistical nature of the phenomena being observed. Statistically, both are treated in the same manner as uncertainties arising from the finite sampling of an infinite population of events. The measurement process, as we have suggested, is a sampling process much like an opinion poll. The experimenter attempts to determine the parameters of a population or distribution too large to measure in its entirety by taking a random sample of finite size and using the sample parameters as an estimate of the true values.

This point of view is most easily seen in measurements of statistical processes, for example, radioactive decay, proton-proton scattering, etc. These processes are all governed by the probabilistic laws of quantum mechanics, so that the number of disintegrations or scatterings in a given time period is a random variable. What is usually of interest in these processes is the mean of the theoretical probability distribution. When a measurement of the number of decays or scatterings per unit time is made, a sample from this distribution is taken, i.e., the variable  $x$  takes on a value  $x_1$ . Repeated measurements can be made to obtain  $x_2$ ,  $x_3$ , etc. This, of course, is equivalent to tossing a coin or throwing a pair of dice and recording the result. From these data, the experimenter may estimate the value of the mean. Since the sample is finite, however, there is an uncertainty on the estimate and this represents our measurement error. Errors arising from the measurement of inherently random processes are called *statistical* errors.

Now consider the measurement of a quantity such as the length of a table or the voltage between two electrodes. Here the quantities of interest are well-defined numbers and not random variables. How then do these processes fit into the view of measurement as a sampling process? What distribution is being sampled?

To take an example, consider an experiment such as the measurement of the length of a table with say, a simple folding ruler. Let us make a set of repeated measurements reading the ruler as accurately as possible. (The reader can try this himself!). It will then be noticed that the values fluctuate about and indeed, if we plot the frequency of the results in the form of a histogram, we see the outlines of a definite distribution beginning to take form. The differing values are the result of many small factors which are not controlled by the experimenter and which may change from one measurement to the next, for example, play in the mechanical joints, contractions and expansions due to temperature changes, failure of the experimenter to place the zero at exactly the same point each time, etc. These are all sources of *instrumental error*, where the term

*instrument* also includes the observer! The more these factors are taken under control, of course, the smaller will be the magnitude of the fluctuations. The instrument is then said to be more *precise*. In the limit of an ideal, perfect instrument, the distribution then becomes a  $\delta$ -function centered at the true value of the measured quantity. In reality, of course, such is never the case.

The measurement of a fixed quantity, therefore, involves taking a sample from an abstract, theoretical distribution determined by the imprecisions of the instrument. In almost all cases of instrumental errors, it can be argued that the distribution is Gaussian. Assuming no systematic error, the mean of the Gaussian should then be equal to the true value of the quantity being measured and the standard deviation proportional to the precision of the instrument.

Let us now see how sampled data are used to estimate the true parameters.

## 4.4 Sampling and Parameter Estimation. The Maximum Likelihood Method

Sampling is the experimental method by which information can be obtained about the parameters of an unknown distribution. As is well known from the debate over opinion polls, it is important to have a representative and unbiased sample. For the experimentalist, this means *not* rejecting data because they do not “*look right*”. The rejection of data, in fact, is something to be avoided unless there are overpowering reasons for doing so.

Given a data sample, one would then like to have a method for determining the *best* value of the true parameters from the data. The *best* value here is that which minimizes the variance between the estimate and the true value. In statistics, this is known as *estimation*. The estimation problem consists of two parts: (1) determining the best estimate and (2) determining the uncertainty on the estimate. There are a number of different principles which yield formulae for combining data to obtain a best estimate. However, the most widely accepted method and the one most applicable to our purposes is the principle of *maximum likelihood*. We shall very briefly demonstrate this principle in the following sections in order to give a feeling for how the results are derived. The reader interested in more detail or in some of the other methods should consult some of the standard texts given in the bibliography. Before treating this topic, however, we will first define a few terms.

### 4.4.1 Sample Moments

Let  $x_1, x_2, x_3, \dots, x_n$  be a sample of size  $n$  from a distribution whose theoretical mean is  $\mu$  and variance  $\sigma^2$ . This is known as the sample population. The *sample mean*,  $\bar{x}$ , is then defined as

$$\bar{x} = \frac{1}{n} \sum_{i=1}^n x_i, \quad (4.25)$$

which is just the arithmetic average of the sample. In the limit  $n \rightarrow \infty$ , this can be shown to approach the theoretical mean,

$$\mu = \lim_{n \rightarrow \infty} \frac{1}{n} \sum_{i=1}^n x_i. \quad (4.26)$$

Similarly, the *sample variance*, which we denote by  $s^2$  is

$$s^2 = \frac{1}{n} \sum_{i=1}^n (x_i - \bar{x})^2, \quad (4.27)$$

which is the average of the squared deviations. In the limit  $n \rightarrow \infty$ , this also approaches the theoretical variance  $\sigma^2$ .

In the case of multivariate samples, for example,  $(x_1, y_1), (x_2, y_2), \dots$ , the sample means and variances for each variable are calculated as above. In an analogous manner, the *sample covariance* can be calculated by

$$\text{cov}(x, y) = \frac{1}{n} \sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y}). \quad (4.28)$$

In the limit of infinite  $n$ , (4.28), not surprisingly, also approaches the theoretical covariance (4.10).

#### 4.4.2 The Maximum Likelihood Method

The method of maximum likelihood is only applicable if the form of the theoretical distribution from which the sample is taken is known. For most measurements in physics, this is either the Gaussian or Poisson distribution. But, to be more general, suppose we have a sample of  $n$  independent observations  $x_1, x_2, \dots, x_n$ , from a theoretical distribution  $f(x|\theta)$  where  $\theta$  is the parameter to be estimated. The method then consists of calculating the *likelihood* function,

$$L(\theta|x) = f(x_1|\theta)f(x_2|\theta)\dots f(x_n|\theta), \quad (4.29)$$

which can be recognized as the probability for observing the sequence of values  $x_1, x_2, \dots, x_n$ . The principle now states that this probability is a maximum for the observed values. Thus, the parameter  $\theta$  must be such that  $L$  is a maximum. If  $L$  is a regular function,  $\theta$  can be found by solving the equation,

$$\frac{dL}{d\theta} = 0. \quad (4.30)$$

If there is more than one parameter, then the partial derivatives of  $L$  with respect to each parameter must be taken to obtain a system of equations. Depending on the form of  $L$ , it may also be easier to maximize the logarithm of  $L$  rather than  $L$  itself. Solving the equation

$$\frac{d(\ln L)}{d\theta} = 0 \quad (4.31)$$

then yields results equivalent to (4.30). The solution,  $\hat{\theta}$ , is known as the maximum likelihood *estimator* for the parameter  $\theta$ . In order to distinguish the estimated value

from the true value, we have used a caret over the parameter to signify it as the estimator.

It should be realized now that  $\hat{\theta}$  is also a random variable, since it is a function of the  $x_i$ . If a second sample is taken,  $\hat{\theta}$  will have a different value and so on. The estimator is thus also described by a probability distribution. This leads us to the second half of the estimation problem: What is the error on  $\hat{\theta}$ ? This is given by the standard deviation of the estimator distribution. We can calculate this from the likelihood function if we recall that  $L$  is just the probability for observing the sampled values  $x_1, x_2, \dots, x_n$ . Since these values are used to calculate  $\hat{\theta}$ ,  $L$  is related to the distribution for  $\hat{\theta}$ . Using (4.9), the variance is then

$$\sigma^2(\hat{\theta}) = \int (\hat{\theta} - \theta)^2 L(\theta|x) dx_1 dx_2 \dots dx_n. \quad (4.32)$$

This is a general formula, but, unfortunately, only in a few simple cases can an analytic result be obtained. An easier, but only approximate method which works in the limit of large numbers, is to calculate the inverse second derivative of the log-likelihood function evaluated at the maximum,

$$\tilde{\sigma}^2(\hat{\theta}) \approx -\left(\frac{d^2 \ln L}{d\theta^2}\right)^{-1}. \quad (4.33)$$

If there is more than one parameter, the matrix of the second derivatives must be formed, i.e.,

$$U_{ij} = -\frac{\partial^2 \ln L}{\partial \theta_i \partial \theta_j}. \quad (4.34)$$

The diagonal elements of the inverse matrix then give the approximate variances,

$$\sigma^2(\hat{\theta}_i) \approx (U^{-1})_{ii}. \quad (4.35)$$

A technical point which must be noted is that we have assumed that the mean value of  $\hat{\theta}$  is the theoretical  $\theta$ . This is a desirable, but not essential property for an estimator, guaranteed by the maximum likelihood method only for infinite  $n$ . Estimators which have this property are *non-biased*. We will see one example in the following sections in which this is not the case. Equation (4.32), nevertheless, remains valid for all  $\hat{\theta}$ , since the error desired is the deviation from the true mean irrespective of the bias.

Another useful property of maximum likelihood estimators is invariance under transformations. If  $u = f(\theta)$ , then the best estimate of  $u$  can be shown to be  $\hat{u} = f(\hat{\theta})$ .

Let us illustrate the method now by applying it to the Poisson and Gaussian distributions.

#### 4.4.3 Estimator for the Poisson Distribution

Suppose we have  $n$  measurements of samples,  $x_1, x_2, x_3, \dots, x_n$  from a Poisson distribution with mean  $\mu$ . The likelihood function for this case is then

$$L(\mu|x) = \prod_{i=1}^n \frac{\mu^{x_i}}{x_i!} \exp(-\mu) = \exp(-n\mu) \prod_{i=1}^n \frac{\mu^{x_i}}{x_i!}. \quad (4.36)$$

To eliminate the product sign, we take the logarithm

$$L^* = \ln L = -n\mu + \sum x_i \ln \mu - \sum \ln x_i! . \quad (4.37)$$

Differentiating and setting the result to zero, we then find

$$\frac{dL^*}{d\mu} = -n + \frac{1}{\mu} \sum x_i = 0 , \quad (4.38)$$

which yields the solution

$$\hat{\mu} = \frac{1}{n} \sum x_i = \bar{x} . \quad (4.39)$$

Equation (4.39), of course, is just the sample mean. This is of no great surprise, but it does confirm the often unconscious use of (4.39).

The variance of  $\bar{x}$  can be found by using (4.33); however, in this particular case, we will use a different way. From (4.9) we have the definition

$$\sigma^2(\bar{x}) = E[(\bar{x} - \mu)^2] . \quad (4.40)$$

Applying this to the sample mean and rearranging the terms, we thus have

$$E[(\bar{x} - \mu)^2] = E\left[\left(\frac{1}{n} \sum x_i - \mu\right)^2\right] = \frac{1}{n^2} E[(\sum x_i - n\mu)^2] = \frac{1}{n^2} E[(\sum (x_i - \mu))^2] . \quad (4.41)$$

Expanding the square of the sum, we find

$$[\sum (x_i - \mu)]^2 = \sum_i (x_i - \mu)^2 + \sum_{i \neq j} (x_i - \mu)(x_j - \mu) . \quad (4.42)$$

If now the expectation value is taken, the cross term vanishes, so that

$$\sigma^2(\bar{x}) = \frac{1}{n^2} E[\sum (x_i - \mu)^2] = \frac{1}{n^2} \sum E[(x_i - \mu)^2] = \frac{n\sigma^2}{n^2} = \frac{\sigma^2}{n} . \quad (4.43)$$

As the reader may have noticed, (4.43) was derived without reference to the Poisson distribution, so that (4.43) is, in fact, a general result: the variance of the sample mean is given by the variance of the parent distribution, whatever it may be, divided by the sample size.

For a Poisson distribution,  $\sigma^2 = \mu$ , so that the error on the estimated Poisson mean is

$$\sigma(\hat{\mu}) = \sqrt{\frac{\mu}{n}} \approx \sqrt{\frac{\hat{\mu}}{n}} = \sqrt{\frac{\bar{x}}{n}} , \quad (4.44)$$

where have substituted the estimated value  $\hat{\mu}$  for the theoretical  $\mu$ .

#### 4.4.4 Estimators for the Gaussian Distribution

For a sample of  $n$  points, all taken from the same Gaussian distribution, the likelihood function is

$$L = \prod_{i=1}^n \frac{1}{\sigma \sqrt{2\pi}} \exp \left[ -\frac{(x_i - \mu)^2}{2\sigma^2} \right]. \quad (4.45)$$

Once again, taking the logarithm,

$$L^* = \ln L = -\frac{n}{2} \ln(2\pi\sigma^2) - \frac{1}{2} \sum \frac{(x_i - \mu)^2}{\sigma^2}. \quad (4.46)$$

Taking the derivatives with respect to  $\mu$  and  $\sigma^2$  and setting them to 0, we then have

$$\frac{\partial L^*}{\partial \mu} = \sum \frac{x_i - \mu}{\sigma^2} = 0 \quad (4.47)$$

and

$$\frac{\partial L^*}{\partial \sigma^2} = -\frac{n}{2\sigma^2} + \frac{1}{2} \sum \left( \frac{x_i - \mu}{\sigma} \right)^2 \frac{1}{\sigma^2} = 0. \quad (4.48)$$

Solving (4.47) first yields

$$\hat{\mu} = \frac{\sum x_i}{n} = \bar{x}. \quad (4.49)$$

The best estimate of the theoretical mean for a Gaussian is thus the sample mean, which again comes as no great surprise.

From the general result in (4.43), the uncertainty on the estimator is thus

$$\sigma(\bar{x}) = \frac{\sigma}{\sqrt{n}}. \quad (4.50)$$

This is usually referred to as the *standard error of the mean*. Note that the error depends on the sample number as one would expect. As  $n$  increases, the estimate  $\bar{x}$  becomes more and more precise. When only one measurement is made,  $n = 1$ ,  $\sigma(\bar{x})$  reduces to  $\sigma$ . For a measuring device,  $\sigma$  thus represents the *precision* of the instrument.

For the moment, however,  $\sigma$  is still unknown. Solving (4.48) for  $\sigma^2$  yields the estimator

$$\hat{\sigma}^2 = \frac{1}{n} \sum (x_i - \mu)^2 \approx \frac{1}{n} \sum (x_i - \bar{x})^2 = s^2, \quad (4.51)$$

where we have replaced  $\mu$  by its solution in (4.49). This, of course, is just the sample variance.

For finite values of  $n$ , however, the sample variance turns out to be a *biased estimator*, that is the expectation value of  $s^2$  does not equal the true value, but is offset from it by a constant factor. It is not hard to show, in fact, that  $E[s^2] = \sigma^2 - \sigma^2/n = (n-1)\sigma^2/n$ . Thus for  $n$  very large,  $s^2$  approaches the true variance as desired; however, for small  $n$ ,  $\sigma^2$  is underestimated by  $s^2$ . The reason is quite simple: for small samples, the occurrence of large values far from the mean is rare, so the sample variance tends to be weighted more towards smaller values. For practical use, a somewhat better estimate therefore, would be to multiply (4.51) by the factor  $n/(n-1)$ ,

$$\hat{\sigma}^2 = \frac{\sum (x_i - \bar{x})^2}{n-1}. \quad (4.52)$$

Equation (4.52) is unbiased, however, it is no longer the *best* estimate in the sense that its average deviation from the true value is somewhat greater than that for (4.51). The difference is small however, so that (4.52) still provides a good estimate. Equation (4.52) then is the recommended formula for estimating the variance. Note that unlike the mean, it is impossible to estimate the standard deviation from one measurement because of the  $(n-1)$  term in the denominator. This makes sense, of course, as it quite obviously requires more than one point to determine a dispersion!

The variance of  $\hat{\sigma}^2$  in (4.52) may also be shown to be

$$\sigma^2(\hat{\sigma}^2) = \frac{2\sigma^4}{n-1} \approx \frac{2\hat{\sigma}^4}{n-1} \quad (4.53)$$

and the standard deviation of  $\hat{\sigma}$

$$\sigma(\hat{\sigma}) = \frac{\sigma}{\sqrt{2(n-1)}} \approx \frac{\hat{\sigma}}{\sqrt{2(n-1)}}. \quad (4.54)$$

#### 4.4.5 The Weighted Mean

We have thus far discussed the estimation of the mean and standard deviation from a series of measurements of the same quantity with the same instrument. It often occurs, however, that one must combine two or more measurements of the same quantity with differing errors. A simple minded procedure would be to take the average of the measurements. This, unfortunately, ignores the fact that some measurements are more precise than others and should therefore be given more importance. A more valid method would be to weight each measurement in proportion to its error. The maximum likelihood method allows us to determine the weighting function to use.

From a statistics point of view, we have a sample  $x_1, x_2, \dots, x_n$ , where each value is from a Gaussian distribution having the same mean  $\mu$  but a different standard deviation  $\sigma_i$ . The likelihood function is thus the same as (4.45), but with  $\sigma$  replaced by  $\sigma_i$ . Maximizing this we then find the *weighted mean*

$$\hat{\mu} = \frac{\sum x_i / \sigma_i^2}{\sum 1/\sigma_i^2}. \quad (4.55)$$

Thus the weighting factor is the inverse square of the error, i.e.,  $1/\sigma_i^2$ . This corresponds to our logic as the smaller the  $\sigma_i$ , the larger the weight and vice-versa.

Using (4.33), the error on the weighted mean can now be shown to be

$$\sigma^2(\hat{\mu}) = \frac{1}{\sum 1/\sigma_i^2}. \quad (4.56)$$

Note that if all the  $\sigma_i$  are the same, the weighted mean reduces to the normal formula in (4.49) and the error on the mean to (4.50).

## 4.5 Examples of Applications

### 4.5.1 Mean and Error from a Series of Measurements

**Example 4.1** Consider the simple experiment proposed in Sect. 4.3.2 to measure the length of an object. The following results are from such a measurement:

17.62	17.62	17.615	17.62	17.61
17.61	17.62	17.625	17.62	17.62
17.61	17.615	17.61	17.605	17.61

What is the best estimate for the length of this object?

Since the errors in the measurement are instrumental, the measurements are Gaussian distributed. From (4.49), the best estimate for the mean value is then

$$\bar{x} = 17.61533$$

while (4.52) gives the standard deviation

$$\hat{\sigma} = 5.855 \times 10^{-3}$$

This can now be used to calculate the standard error of the mean (4.50),

$$\sigma(\bar{x}) = \hat{\sigma}/\sqrt{15} = 0.0015$$

The best value for the length of the object is thus

$$x = 17.616 \pm 0.002$$

Note that the uncertainty on the mean is given by the standard error of the mean and *not* the standard deviation!

### 4.5.2 Combining Data with Different Errors

**Example 4.2** It is necessary to use the lifetime of the muon in a calculation. However, in searching through the literature, 7 values are found from different experiments:

2.198 $\pm$ 0.001 $\mu$ s	2.203 $\pm$ 0.004 $\mu$ s	2.202 $\pm$ 0.003 $\mu$ s
2.197 $\pm$ 0.005 $\mu$ s	2.198 $\pm$ 0.002 $\mu$ s	2.1966 $\pm$ 0.0020 $\mu$ s
2.1948 $\pm$ 0.0010 $\mu$ s		

What is the best value to use?

One way to solve this problem is to take the measurement with the smallest error; however, there is no reason for ignoring the results of the other measurements. Indeed, even though the other experiments are less precise, they still contain valid information on the lifetime of the muon. To take into account all available information we must take the weighted mean. This then yields the mean value

$$\tau = 2.19696$$

with an error

$$\sigma(\tau) = 0.00061.$$

Note that this value is smaller than the error on any of the individual measurements. The best value for the lifetime is thus

$$\tau = 2.1970 \pm 0.0006 \mu\text{s}.$$

#### 4.5.3 Determination of Count Rates and Their Errors

**Example 4.3** Consider the following series of measurements of the counts per minute from a detector viewing a  $^{22}\text{Na}$  source,

2201	2145	2222	2160	2300
------	------	------	------	------

What is the decay rate and its uncertainty?

Since radioactive decay is described by a Poisson distribution, we use the estimators for this distribution to find

$$\hat{\mu} = \bar{x} = 2205.6 \quad \text{and}$$

$$\sigma(\hat{\mu}) = \sqrt{\frac{\bar{x}}{n}} = \sqrt{\frac{2205.6}{5}} = 21.$$

The count rate is thus

$$\text{Count Rate} = (2206 \pm 21) \text{ counts/min.}$$

It is interesting to see what would happen if instead of counting five one-minute periods we had counted the total 5 minutes without stopping. We would have then observed a total of 11028 counts. This constitutes a sample of  $n = 1$ . The mean count rate for 5 minutes is thus 11208 and the error on this,  $\sigma = \sqrt{11208} = 106$ . To find the counts per minute, we divide by 5 (see the next section) to obtain  $2206 \pm 21$ , which is identical to what was found before. Note that the error taken was the square root of the count rate in 5 minutes. A common error to be avoided is to first calculate the rate per minute and then take the square root of this number.

#### 4.5.4 Null Experiments. Setting Confidence Limits When No Counts Are Observed

Many experiments in physics test the validity of certain theoretical conservation laws by searching for the presence of specific reactions or decays forbidden by these laws. In such measurements, an observation is made for a certain amount of time  $T$ . Obviously, if one or more events are observed, the theoretical law is disproven. However, if no events are observed, the converse cannot be said to be true. Instead a limit on the lifetime of the reaction or decay is set.

Let us assume therefore that the process has some mean reaction rate  $\lambda$ . Then the probability for observing no counts in a time period  $T$  is

$$P(0|\lambda) = \exp(-\lambda T). \tag{4.57}$$

This, now, can also be interpreted as the probability distribution for  $\lambda$  when no counts are observed in a period  $T$ . We can now ask the question: What is the probability that  $\lambda$  is less  $\lambda_0$ ? From (4.1),

$$P(\lambda \leq \lambda_0) = \int_0^{\lambda_0} T \exp(-\lambda T) d\lambda = 1 - \exp(-\lambda_0 T), \quad (4.58)$$

where we have normalized (4.57) with the extra factor  $T$ . This probability is known as the *confidence level* for the interval between 0 to  $\lambda_0$ . To make a strong statement we can choose a high confidence level (CL), for example, 90%. Setting (4.58) equal to this probability then gives us the value of  $\lambda_0$ ,

$$\lambda_0 = -\frac{1}{T} \ln(1 - CL). \quad (4.59)$$

For a given confidence level, the corresponding interval is, in general, not unique and one can find other intervals which yield the same integral probability. For example, it might be possible to integrate (4.57) from some lower limit  $\lambda'$  to infinity and still obtain the same area under the curve. The probability that the true  $\lambda$  is *greater* than  $\lambda'$  is then also 90%. As a general rule, however, one should take those limits which cover the smallest range in  $\lambda$ .

**Example 4.4** A 50 g sample of  $^{82}\text{Se}$  is observed for 100 days for neutrinoless double beta decay, a reaction normally forbidden by lepton conservation. However, current theories suggest that this might occur. The apparatus has a detection efficiency of 20%. No events with the correct signature for this decay are observed. Set an upper limit on the lifetime for this decay mode.

Choosing a confidence limit of 90%, (4.59) yields

$$\lambda \leq \lambda_0 = -\frac{1}{100 \times 0.2} \ln(1 - 0.9) = 0.115 \text{ day}^{-1},$$

where we have corrected for the 20% efficiency of the detector. This limit must now be translated into a lifetime per nucleus. For 50 g, the total number of nuclei is

$$N = \frac{N_a}{82} \times 50 = 3.67 \times 10^{23},$$

which implies a limit on the decay rate per nucleus of

$$\lambda \leq \frac{0.115}{3.67 \times 10^{23}} = 3.13 \times 10^{-25} \text{ day}^{-1}.$$

The lifetime is just the inverse of  $\lambda$  which yields

$$\tau \geq 8.75 \times 10^{21} \text{ years} \quad 90\% \text{ CL},$$

where we have converted the units to years. Thus, neutrinoless double beta decay may exist but it is certainly a rare process!

**Example 4.5** Consider a near perfect electronic system for recording electronic pulses. Suppose we wish to measure its efficiency by sending in  $N$  pulses from a pulse generator and observing the number of pulses registered. Suppose that this number is also  $N$ . What can be said about the efficiency of the counter system from this measurement?

This experiment is equivalent to measuring the *inefficiency* of the system which is very small. Just as in Example 4.4, then, the question to ask is: what *lower limit* on the efficiency (or *upper limit* on the inefficiency) can be set from this result?

Let  $\varepsilon$  be the efficiency of the system. The probability of the system registering  $r$  counts when  $N$  pulses are injected is then given by the binomial distribution

$$P(N, r) = \frac{N!}{(N-r)! r!} \varepsilon^r (1-\varepsilon)^{N-r} .$$

The probability of detecting  $N$  pulses when  $N$  are injected is then

$$P(N, N) = \varepsilon^N .$$

Let us now try to invert this probability. With some reflection, in fact, we can see that the probability that the efficiency has some value  $\varepsilon = \varepsilon'$  when  $N$  pulses are counted is also given by

$$P(\varepsilon = \varepsilon') \propto \varepsilon'^N$$

except that  $\varepsilon$  is now the random variable instead of  $N$ . Normalizing the above probability distribution with respect to  $\varepsilon$ , we find

$$P(\varepsilon) = (N+1) \varepsilon^N .$$

This now allows us to calculate a confidence level CL for some lower limit  $\varepsilon_0$ ,

$$CL = \int_{\varepsilon_0}^1 P(\varepsilon') d\varepsilon' = 1 - \varepsilon_0^{N+1} .$$

Solving for  $\varepsilon_0$  yields the lower limit

$$\varepsilon_0 = (1 - CL)^{1/(N+1)} .$$

To illustrate this with some numbers, suppose  $N = 100$ . Choosing a 95% confidence level, we find that  $\varepsilon_0 = 0.9708$ . Thus we can say that the efficiency  $\varepsilon \geq 0.97$  with a 95% certainty!

#### 4.5.5 Distribution of Time Intervals Between Counts

A distribution which we will make use of later is the distribution of time intervals between events from a random source. Suppose we observe a radioactive source with a mean rate  $\lambda$ . The probability of observing no counts in a period  $T$  is then given by (4.57). In a manner similar to Sect. 4.5.4, we can interpret (4.57) as the probability den-

sity for the time interval  $T$  during which no counts are observed. Normalizing (4.57), we obtain the distribution

$$P(T) = \lambda \exp(-\lambda T) \quad (4.60)$$

for the time  $T$  between counts. Equation (4.60) is just an exponential distribution and can, in fact, be measured.

## 4.6 Propagation of Errors

We have seen in the preceding sections how to calculate the errors on directly measured quantities. Very often, however, it is necessary to calculate other quantities from these data. Clearly, the calculated result will then contain an uncertainty which is carried over from the measured data.

To see how the errors are propagated, consider a quantity  $u = f(x, y)$  where  $x$  and  $y$  are quantities having errors  $\sigma_x$  and  $\sigma_y$ , respectively. To simplify the algebra, we only consider a function of two variables here; however, the extension to more variables will be obvious. We would like then to calculate the standard deviation  $\sigma_u$  as a function of  $\sigma_x$  and  $\sigma_y$ . The variance  $\sigma_u^2$  can be defined as

$$\sigma_u^2 = E[(u - \bar{u})^2] \quad (4.61)$$

To first order, the mean  $\bar{u}$  may be approximated by  $f(\bar{x}, \bar{y})$ . This can be shown by expanding  $f(x, y)$  about  $(\bar{x}, \bar{y})$ . Now, to express the deviation of  $u$  in terms of the deviations in  $x$  and  $y$ , let us expand  $(u - \bar{u})$  to first order

$$(u - \bar{u}) \approx (x - \bar{x}) \frac{\partial f}{\partial x} \Big|_{\bar{x}} + (y - \bar{y}) \frac{\partial f}{\partial y} \Big|_{\bar{y}}, \quad (4.62)$$

where the partial derivatives are evaluated at the mean values. Squaring (4.62) and substituting into (4.61) then yields

$$E[(u - \bar{u})^2] \approx E \left[ (x - \bar{x})^2 \left( \frac{\partial f}{\partial x} \right)^2 + (y - \bar{y})^2 \left( \frac{\partial f}{\partial y} \right)^2 + 2(x - \bar{x})(y - \bar{y}) \frac{\partial f}{\partial x} \frac{\partial f}{\partial y} \right]. \quad (4.63)$$

Now taking the expectation value of each term separately and making use of the definitions (4.8, 9) and (4.10), we find

$$\sigma_u^2 \approx \left( \frac{\partial f}{\partial x} \right)^2 \sigma_x^2 + \left( \frac{\partial f}{\partial y} \right)^2 \sigma_y^2 + 2 \text{cov}(x, y) \frac{\partial f}{\partial x} \frac{\partial f}{\partial y}. \quad (4.64)$$

The errors therefore are added quadratically with a modifying term due to the covariance. Depending on its sign and magnitude, the covariance can increase or decrease the errors by dramatic amounts. In general most measurements in physics experiments are independent or should be arranged so that the covariance will be zero. Equa-

tion (4.64) then reduces to a simple sum of squares. Where correlations can arise, however, is when two or more parameters are extracted from the same set of measured data. While the raw data points are independent, the parameters will generally be correlated. One common example are parameters resulting from a fit. The correlations can be calculated in the fitting procedure and all good computer fitting programs should supply this information. An example is given in Sect. 4.7.2. If these parameters are used in a calculation, the correlation must be taken into account. A second example of this type which might have occurred to the reader is the estimation of the mean and variance from a set of data. Fortunately, it can be proved that the estimators (4.49) and (4.52) are statistically independent so that  $\rho = 0$ !

### 4.6.1 Examples

As a first example let us derive the formulas for the sum, difference, product and ratio of two quantities  $x$  and  $y$  with errors  $\sigma_x$  and  $\sigma_y$ .

i) Error of a Sum:  $u = x + y$

$$\sigma_u^2 = \sigma_x^2 + \sigma_y^2 + 2 \operatorname{cov}(x, y). \quad (4.65)$$

ii) Error of a Difference:  $u = x - y$

$$\sigma_u^2 = \sigma_x^2 + \sigma_y^2 - 2 \operatorname{cov}(x, y). \quad (4.66)$$

If the covariance is 0, the errors on both a sum and difference then reduce to the same sum of squares. The relative error,  $\sigma_u/u$ , however, is much larger for the case of a difference since  $u$  is smaller. This illustrates the disadvantage of taking differences between two numbers with errors. If possible, therefore, a difference should always be directly measured rather than calculated from two measurements!

iii) Error of a Product:  $u = xy$

$$\sigma_u^2 \approx y^2 \sigma_x^2 + x^2 \sigma_y^2 + 2 \operatorname{cov}(x, y) xy.$$

Dividing the left side by  $u^2$  and the right side by  $x^2 y^2$ ,

$$\frac{\sigma_u^2}{u^2} \approx \frac{\sigma_x^2}{x^2} + \frac{\sigma_y^2}{y^2} + 2 \frac{\operatorname{cov}(x, y)}{xy}. \quad (4.67)$$

iv) Error of a Ratio:  $u = x/y$

$$\sigma_u^2 \approx y^{-2} \sigma_x^2 + x^2 y^{-4} \sigma_y^2 - 2 \operatorname{cov}(x, y) xy^{-3}.$$

Dividing both sides by  $u^2$  as in (iii), we find

$$\frac{\sigma_u^2}{u^2} \approx \frac{\sigma_x^2}{x^2} + \frac{\sigma_y^2}{y^2} - 2 \frac{\operatorname{cov}(x, y)}{xy}, \quad (4.68)$$

which, with the exception of the sign of the covariance term is identical to the formula for a product. Equation (4.68) is generally valid when the relative errors are not too large. For ratios of small numbers, however, (4.68) is inapplicable and some additional considerations are required. This is treated in detail by *James and Roos* [4.1].

**Example 4.6** The classical method for measuring the polarization of a particle such as a proton or neutron is to scatter it from a suitable *analyzing* target and to measure the asymmetry in the scattered particle distribution. One can, for example, count the number of particles scattered to the left of the beam at certain angle and to the right of the beam at the same corresponding angle. If  $R$  is the number scattered to the right and  $L$  the number to the left, the asymmetry is then given by

$$\varepsilon = \frac{R - L}{R + L}.$$

Calculate the error on  $\varepsilon$  as a function of the counts  $R$  and  $L$ .

This is a straight forward application of (4.64). Taking the derivatives of  $\varepsilon$ , we thus find

$$\frac{\partial \varepsilon}{\partial R} = \frac{1}{R+L} + \frac{R-L}{(R+L)^2} = \frac{2L}{N_{\text{tot}}^2}$$

$$\frac{\partial \varepsilon}{\partial L} = \frac{1}{R+L} + \frac{R-L}{(R+L)^2} = \frac{-2R}{N_{\text{tot}}^2},$$

where the total number of counts  $N_{\text{tot}} = R + L$ . The error is thus

$$\sigma^2(\varepsilon) \approx \frac{4L^2}{N_{\text{tot}}^4} \sigma_R^2 + \frac{4R^2}{N_{\text{tot}}^4} \sigma_L^2.$$

The covariance is obviously 0 here since the measurements are independent. The errors on  $R$  and  $L$  are now given by the Poisson distribution, so that  $\sigma_R^2 = R$  and  $\sigma_L^2 = L$ . Substituting into the above, then yields

$$\sigma^2(\varepsilon) \approx 4 \frac{(L^2 R + R^2 L)}{N_{\text{tot}}^4} = 4 \frac{RL}{N_{\text{tot}}^3}.$$

If the asymmetry is small such that  $R \approx L \approx N_{\text{tot}}/2$ , we have the result that

$$\sigma(\varepsilon) \approx \sqrt{\frac{1}{N_{\text{tot}}}}.$$

## 4.7 Curve Fitting

In many experiments, the functional relation between two or more variables describing a physical process,  $y = f(x_1, x_2, \dots)$ , is investigated by measuring the value of  $y$  for various of  $x_1, x_2, \dots$ . It is then desired to find the parameters of a theoretical curve which best describe these points. For example, to determine the lifetime of a certain radioactive source, measurements of the count rates,  $N_1, N_2, \dots, N_n$ , at various times,  $t_1, t_2, \dots, t_n$ , could be made and the data fitted to the expression

$$N(t) = N_0 \exp(-t/\tau). \quad (4.69)$$

Since the count rate is subject to statistical fluctuations, the values  $N_i$  will have uncertainties  $\sigma_i = \sqrt{N_i}$  and will not all lie along a smooth curve. What then is the best curve or equivalently, the best values for  $t$  and  $N_0$  and how do we determine them? The method most useful for this is the method of *least squares*.

#### 4.7.1 The Least Squares Method

Let us suppose that measurements at  $n$  points,  $x_i$ , are made of the variable  $y_i$  with an error  $\sigma_i$  ( $i = 1, 2, \dots, n$ ), and that it is desired to fit a function  $f(x; a_1, a_2, \dots, a_m)$  to these data where  $a_1, a_2, \dots, a_m$  are unknown parameters to be determined. Of course, the number of points must be greater than the number of parameters. The method of least squares states that the best values of  $a_j$  are those for which the sum

$$S = \sum_{i=1}^n \left[ \frac{y_i - f(x_i; a_j)}{\sigma_i} \right]^2 \quad | \quad (4.70)$$

is a minimum. Examining (4.70) we can see that this is just the sum of the squared deviations of the data points from the curve  $f(x_i)$  weighted by the respective errors on  $y_i$ . The reader might also recognize this as the chi-square in (4.22). For this reason, the method is also sometimes referred to as *chi-square minimization*. Strictly speaking this is not quite correct as  $y_i$  must be Gaussian distributed with mean  $f(x_i; a_j)$  and variance  $\sigma_i^2$  in order for  $S$  to be a true chi-square. However, as this is almost always the case for measurements in physics, this is a valid hypothesis most of the time. The least squares method, however, is totally general and does not require knowledge of the parent distribution. If the parent distribution is known the method of maximum likelihood may also be used. In the case of Gaussian distributed errors this yields identical results.

To find the values of  $a_j$ , one must now solve the system of equations

$$\frac{\partial S}{\partial a_j} = 0. \quad (4.71)$$

Depending on the function  $f(x)$ , (4.71) may or may not yield an analytic solution. In general, numerical methods requiring a computer must be used to minimize  $S$ .

Assuming we have the best values for  $a_j$ , it is necessary to estimate the errors on the parameters. For this, we form the so-called covariance or *error matrix*,  $V_{ij}$ ,

$$(V^{-1})_{ij} = \frac{1}{2} \frac{\partial^2 S}{\partial a_i \partial a_j}, \quad (4.72)$$

where the second derivative is evaluated at the minimum. (Note the second derivatives form the *inverse* of the error matrix). The diagonal elements  $V_{ii}$  can then be shown to be the variances for  $a_i$ , while the offdiagonal elements  $V_{ij}$  represent the covariances between  $a_i$  and  $a_j$ . Thus,

$$V = \begin{pmatrix} \sigma_1^2 & \text{cov}(1, 2) & \text{cov}(1, 3) & \dots \\ . & \sigma_2^2 & \text{cov}(2, 3) & \dots \\ . & . & \sigma_3^2 & \dots \\ . & . & . & \dots \end{pmatrix} \quad (4.73)$$

and so on.

### 4.7.2 Linear Fits. The Straight Line

In the case of functions linear in their parameters  $a_j$ , i.e., there are no terms which are products or ratios of different  $a_j$ 's, (4.71) can be solved analytically. Let us illustrate this for the case of a straight line

$$y = f(x) = ax + b, \quad (4.74)$$

where  $a$  and  $b$  are the parameters to be determined. Forming  $S$ , we find

$$S = \sum \frac{(y_i - ax_i - b)^2}{\sigma_i^2}. \quad (4.75)$$

Taking the partial derivatives with respect to  $a$  and  $b$ , we then have the equations

$$\begin{aligned} \frac{\partial S}{\partial a} &= -2 \sum \frac{(y_i - ax_i - b)x_i}{\sigma_i^2} = 0, \\ \frac{\partial S}{\partial b} &= -2 \sum \frac{(y_i - ax_i - b)}{\sigma_i^2} = 0. \end{aligned} \quad (4.76)$$

To simplify the notation, let us define the terms

$$\begin{aligned} A &= \sum \frac{x_i}{\sigma_i^2} & B &= \sum \frac{1}{\sigma_i^2} \\ C &= \sum \frac{y_i}{\sigma_i^2} & D &= \sum \frac{x_i^2}{\sigma_i^2} \\ E &= \sum \frac{x_i y_i}{\sigma_i^2} & F &= \sum \frac{y_i^2}{\sigma_i^2}. \end{aligned} \quad (4.77)$$

Using these definitions, (4.76) becomes

$$\begin{aligned} 2(-E + aD + bA) &= 0, \\ 2(-C + aA + bB) &= 0. \end{aligned} \quad (4.78)$$

This then leads to the solution,

$$a = \frac{EB - CA}{DB - A^2} \quad b = \frac{DC - EA}{DB - A^2}. \quad (4.79)$$

Our work is not complete, however, as the errors on  $a$  and  $b$  must also be determined. Forming the inverse error matrix, we then have

$$V^{-1} = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix}, \quad \text{where} \quad (4.80)$$

$$A_{11} = \frac{1}{2} \frac{\partial^2 S}{\partial a^2}, \quad A_{22} = \frac{1}{2} \frac{\partial^2 S}{\partial b^2}, \quad A_{12} = A_{21} = \frac{1}{2} \frac{\partial^2 S}{\partial a \partial b}.$$

Inverting (4.80), we find

$$V = \frac{1}{A_{11}A_{22} - A_{12}^2} \begin{pmatrix} A_{22} & -A_{12} \\ -A_{12} & A_{11} \end{pmatrix} \quad (4.81)$$

so that

$$\begin{aligned} \sigma^2(a) &= \frac{A_{22}}{A_{11}A_{22} - A_{12}^2} = \frac{B}{BD - A^2}, \\ \sigma^2(b) &= \frac{A_{11}}{A_{11}A_{22} - A_{12}^2} = \frac{D}{BD - A^2}, \\ \text{cov}(a, b) &= \frac{-A_{12}}{A_{11}A_{22} - A_{12}^2} = \frac{-A}{BD - A^2}. \end{aligned} \quad (4.82)$$

To complete the process, now, it is necessary to also have an idea of the *quality of the fit*. Do the data, in fact, correspond to the function  $f(x)$  we have assumed? This can be tested by means of the chi-square. This is just the value of  $S$  at the minimum. Recalling Sect. 4.2.4, we saw that if the data correspond to the function and the deviations are Gaussian,  $S$  should be expected to follow a chi-square distribution with mean value equal to the degrees of freedom,  $v$ . In the above problem, there are  $n$  independent data points from which  $m$  parameters are extracted. The degrees of freedom is thus  $v = n - m$ . In the case of a linear fit,  $m = 2$ , so that  $v = n - 2$ . We thus expect  $S$  to be close to  $v = n - 2$  if the fit is *good*. A quick and easy test is to form the *reduced chi-square*

$$\frac{\chi^2}{v} = \frac{S}{v}, \quad (4.83)$$

which should be close to 1 for a *good fit*.

A more rigorous test is to look at the probability of obtaining a  $\chi^2$  value greater than  $S$ , i.e.,  $P(\chi^2 \geq S)$ . This requires integrating the chi-square distribution or using cumulative distribution tables. In general, if  $P(\chi^2 \geq S)$  is greater than 5%, the fit can be accepted. Beyond this point, some questions must be asked.

An equally important point to consider is when  $S$  is very small. This implies that the points are *not* fluctuating enough. Barring falsified data, the most likely cause is an overestimation of the errors on the data points. If the reader will recall, the error bars represent a  $1\sigma$  deviation, so that about 1/3 of the data points should, in fact, be expected to fall outside the fit!

**Example 4.7** Find the best straight line through the following measured points

$x$	0	1	2	3	4	5
$y$	0.92	4.15	9.78	14.46	17.26	21.90
$\sigma$	0.5	1.0	0.75	1.25	1.0	1.5

Applying (4.75) to (4.82), we find

$$a = 4.227 \quad b = 0.878$$

$$\sigma(a) = 0.044 \quad \sigma(b) = 0.203 \quad \text{and}$$

$$\text{cov}(a, b) = -0.0629.$$

To test the *goodness-of-fit*, we must look at the chi-square

$$\chi^2 = 2.078$$

for 4 degrees of freedom. Forming the reduced chi-square,  $\chi^2/v \approx 0.5$ , we can see already that this is a good fit. If we calculate the probability  $P(\chi^2 > 2.07)$  for 4 degrees of freedom, we find  $P \approx 97.5\%$  which is well within acceptable limits.

**Example 4.8** For certain nonlinear functions, a *linearization* may be affected so that the method of linear least squares becomes applicable. One case is the example of the exponential, (4.69), which we gave at the beginning of this section. Consider a decaying radioactive source whose activity is measured at intervals of 15 seconds. The total counts during each period are given below.

$t$ [s]	1	15	30	45	60	75	90	105	120	135
$N$ [cts]	106	80	98	75	74	73	49	38	37	22

What is the lifetime for this source?

The obvious procedure is to fit (4.69) to these data in order to determine  $\tau$ . Equation (4.69), of course, is nonlinear, however it can be linearized by taking the logarithm of both sides. This then yields

$$\ln N = \frac{-t}{\tau} + \ln N_0.$$

Setting  $y = \ln N$ ,  $a = -1/\tau$  and  $b = \ln N_0$ , we see that this is just a straight line, so that our linear least-squares procedure can be used. One point which we must be careful about, however, is the errors. The statistical errors on  $N$ , of course, are Poissonian, so that  $\sigma(N) = \sqrt{N}$ . In the fit, however, it is the logarithm of  $N$  which is being used. The errors must therefore be transformed using the propagation of errors formula; we then have

$$\sigma^2(\ln N) = \left( \frac{\partial \ln N}{\partial N} \right)^2 \sigma^2(N) = \frac{1}{N^2} N = N^{-1}.$$

Using (4.75) to (4.82) now, we find

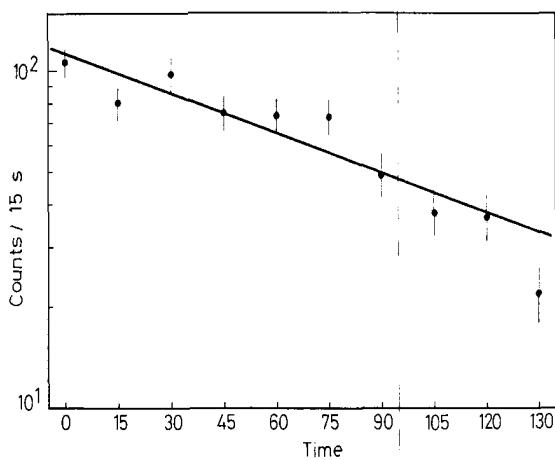
$$\begin{aligned} a &= -1/\tau = -0.008999 & \sigma(a) &= 0.001 \\ b &= \ln N_0 = 4.721 & \sigma(b) &= 0.064. \end{aligned}$$

The lifetime is thus

$$\tau = 111 \pm 12 \text{ s}.$$

The chi-square for this fit is  $\chi^2 = 15.6$  with 8 degrees of freedom. The reduced chi-square is thus  $15.6/(8 \approx 1.96)$ , which is somewhat high. If we calculate the probability  $P(\chi^2 > 15) \approx 0.05$ , however, we find that the fit is just acceptable. The data and the best straight line are sketched in Fig. 4.7 on a semi-log plot.

While the above fit is acceptable, the relatively large chi-square should, nevertheless, prompt some questions. For example, in the treatment above, background counts



**Fig. 4.7.** Fit to data of Example 4.8. Note that the error bars of about 1/3 of the points do not touch the fitted line. This is consistent with the Gaussian nature of the measurements. Since the region defined by the errors bars ( $\pm 1\sigma$ ) comprises 68% of the Gaussian distribution (see Fig. 4.5), there is a 32% chance that a measurement will exceed these limits!

were ignored. An improvement in our fit might therefore be obtained if we took this into account. If we assume a constant background, then the equation to fit would be

$$N(t) = N_0 \exp(-t/\tau) + C.$$

Another hypothesis could be that the source has more than one decay component in which case the function to fit would be a sum of exponentials. These forms unfortunately cannot be linearized as above and recourse must be made to nonlinear methods. In the special case described above, a non-iterative procedure [4.2 – 6] exists which may also be helpful.

#### 4.7.3 Linear Fits When Both Variables Have Errors

In the previous examples, it was assumed that the independent variables  $x_i$  were completely free of errors. Strictly speaking, of course, this is never the case, although in many problems the errors on  $x$  are small with respect to those on  $y$  so that they may be neglected. In cases where the errors on both variables are comparable, however, ignoring the errors on  $x$  leads to incorrect parameters and an underestimation of their errors. For these problems the *effective variance method* may be used. Without deriving the result which is discussed by Lybanon [4.7] and Orear [4.8] for Gaussian distributed errors, the method consists of simply replacing the variance  $\sigma_i^2$  in (4.70) by

$$\sigma_i^2 \rightarrow \sigma_y^2 + \left( \frac{df}{dx} \right)^2 \sigma_x^2, \quad (4.84)$$

where  $\sigma_x$  and  $\sigma_y$  are the errors on  $x$  and  $y$  respectively. Since the derivative is normally a function of the parameters  $a_j$ ,  $S$  is nonlinear and numerical methods must be used to minimize  $S$ .

#### 4.7.4 Nonlinear Fits

As we have already mentioned, nonlinear fits generally require a numerical procedure for minimizing  $S$ . Function minimization or maximization<sup>2</sup> is a problem in itself and

<sup>2</sup> A minimization can be turned into a maximization by simply adding a minus sign in front of the function and vice-versa.

a number of methods have been developed for this purpose. However, no one method can be said to be applicable to all functions, and, indeed, the problem often is to find the right method for the function or functions in question. A discussion of the different methods available, of course, is largely outside the scope of this book. However, it is nevertheless worthwhile to briefly survey the most used methods so as to provide the reader with a basis for more detailed study and an idea of some of the problems to be expected. For practical purposes, a computer is necessary and we strongly advise the reader to find a ready-made program rather than attempt to write it himself. More detailed discussions may be found in [4.9–11].

**Function Minimization Techniques.** Numerical minimization methods are generally iterative in nature, i.e., repeated calculations are made while varying the parameters in some way, until the desired minimum is reached. The criteria for selecting a method, therefore, are speed and stability against divergences. In general, the methods can be classified into two broad categories: *grid* searches and *gradient* methods.

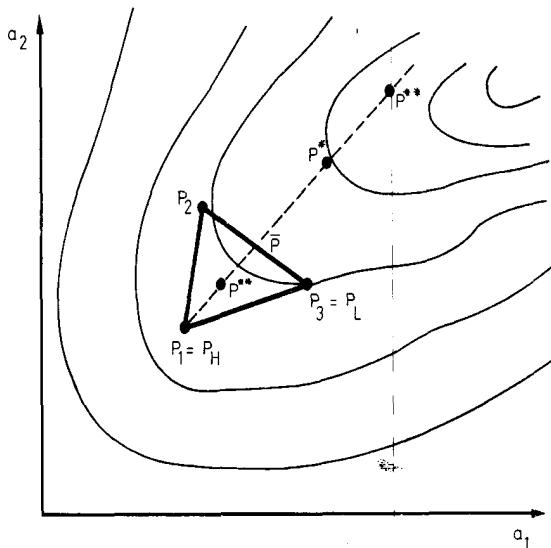
The grid methods are the simplest. The most elementary procedure is to form a grid of equally spaced points in the variables of interest and evaluate the function at each of these points. The point with the smallest value is then the approximate minimum. Thus, if  $F(x)$  is the function to minimize, we would evaluate  $F$  at  $x_0, x_0 + \Delta x, x_0 + 2\Delta x$ , etc. and choose the point  $x'$  for which  $F$  is smallest. The size of the grid step,  $\Delta x$ , depends on the accuracy desired. This method, of course, can only be used over a finite range of  $x$  and in cases where  $x$  ranges over infinity it is necessary to have an approximate idea of where the minimum is. Several ranges may also be tried.

The elementary grid method is intrinsically stable, but it is quite obviously inefficient and time consuming. Indeed, in more than one dimension, the number of function evaluations becomes prohibitively large even for a computer! (In contrast to the simple grid method is the *Monte Carlo* or *random* search. Instead of equally spaced points, random points are generated according to some distribution, e.g., a uniform density.)

More efficient grid searches make use of variable stepping methods so as to reduce the number of evaluations while converging onto the minimum more rapidly. A relatively recent technique is the *simplex* method [4.12]. A simplex is the simplest geometrical figure in  $n$  dimensions having  $n + 1$  vertices. In  $n = 2$  dimensions, for example, the simplex is a triangle while in  $n = 3$  dimensions, the simplex is a tetrahedron, etc. The method takes on the name simplex because it uses  $n + 1$  points at each step. As an illustration, consider a function in two dimensions, the contours of which are shown in Fig. 4.8. The method begins by choosing  $n + 1 = 3$  points in some way or another, perhaps at random. A simplex is thus formed as shown in the figure. The point with the highest value is denoted as  $P_H$ , while the lowest is  $P_L$ . The next step is to replace  $P_H$  with a better point. To do this,  $P_H$  is reflected through the center of gravity of all points except  $P_H$ , i.e., the point

$$\bar{P} = \sum_i \frac{P_i - P_H}{n}. \quad (4.85)$$

This yields the point  $P^* = \bar{P} + (\bar{P} - P_H)$ . If  $F(P^*) < F(P_L)$ , a new minimum has been found and an attempt is made to do even better by trying the point  $P^{**} = \bar{P} + 2(\bar{P} - P_H)$ . The best point is then kept. If  $F(P^*) > F(P_H)$  the reflection is brought backwards to  $P^{**} = \bar{P} - \frac{1}{2}(\bar{P} - P_H)$ . If this is not better than  $P_H$ , a new



**Fig. 4.8.** The simplex method for function minimization

simplex is formed with points at  $P_i = (P_i + P_L)/2$  and the procedure restarted. In this manner, one can imagine the triangle in Fig. 4.8 “falling” to the minimum. The simplex technique is a good method since it is relatively insensitive to the type of function, but it can also be rather slow.

*Gradient* methods are techniques which make use of the derivatives of the function to be minimized. These can either be calculated numerically or supplied by the user if known. One obvious use of the derivatives is to serve as guides pointing in the direction of decreasing  $F$ . This idea is used in techniques such as the method of *steepest descent*. A more widely used technique, however, is *Newton's method* which uses the derivatives to form a second-degree Taylor expansion of the function about the point  $x_0$ ,

$$F(x) \approx F(x_0) + \frac{\partial F}{\partial x} \Big|_{x_0} (x - x_0) + \frac{1}{2} \frac{\partial^2 F}{\partial x^2} \Big|_{x_0} (x - x_0)^2. \quad (4.86)$$

In  $n$  dimensions, this is generalized to

$$F(x) \approx F(x_0) + g^T (x - x_0) + \frac{1}{2} (x - x_0)^T G (x - x_0), \quad (4.87)$$

where  $g_i$  is the vector of first derivatives  $\partial F / \partial x_i$  and  $G_{ij}$  the matrix of second derivatives  $\partial^2 F / \partial x_i \partial x_j$ . The matrix  $G$  is also called the *hessian*. In essence, the method approximates the function around  $x_0$  by a quadratic surface. Under this assumption, it is very easy to calculate the minimum of the  $n$  dimensional parabola analytically,

$$x_{\min} = x_0 - G^{-1} g. \quad (4.88)$$

This, of course, is not the true minimum of the function; but by forming a new parabolic surface about  $x_{\min}$  and calculating its minimum, etc., a convergence to the true minimum can be obtained rather rapidly. The basic problem with the technique is that it requires  $G$  to be everywhere positive definite, otherwise at some point in the iteration a maximum may be calculated rather than a minimum, and the whole process diverges. This is more easily seen in the one-dimensional case in (4.86). If the second derivative is negative, then, we clearly have an inverted parabola rather than the desired well-shape figure.

Despite this defect, Newton's method is quite powerful and algorithms have been developed in which the matrix  $G$  is artificially altered whenever it becomes negative. In this manner, the iteration continues in the right direction until a region of positive-definiteness is reached. Such variations are called *quasi-Newton* methods.

The disadvantage of the Newton methods is that each iteration requires an evaluation of the matrix  $G$  and its inverse. This, of course, becomes quite costly in terms of time. This problem has given rise to another class of methods which either avoid calculating  $G$  or calculate it once and then "update"  $G$  with some correcting function after each iteration. These methods are described in more detail by *James* [4.11].

In the specific case of least squares minimization, a common procedure used with Newton's method is to *linearize* the fitting function. This is equivalent to approximating the hessian in the following manner. Rewriting (4.70) as

$$S = \sum_k s_k^2, \quad (4.89)$$

where  $s_k = [y_k - f(x_k)]/\sigma_k$ , the hessian becomes

$$\begin{aligned} \frac{\partial^2 S}{\partial x_i \partial x_j} &= \frac{\partial}{\partial x_i} \frac{\partial}{\partial x_j} \sum_k s_k^2 \\ \frac{\partial^2 S}{\partial x_i \partial x_j} &= \frac{\partial}{\partial x_i} \sum_k 2s_k \frac{\partial s_k}{\partial x_j} = 2 \sum_k \frac{\partial s_k}{\partial x_i} \frac{\partial s_k}{\partial x_j} + s_k \frac{\partial^2 s_k}{\partial x_i \partial x_j}. \end{aligned} \quad (4.90)$$

The second term in the sum can be considered as a second order correction and is set to zero. The hessian is then

$$G_{ij} \approx 2 \sum \frac{\partial s_k}{\partial x_i} \frac{\partial s_k}{\partial x_j}. \quad (4.91)$$

This approximation has the advantage of ensuring positive-definiteness and the result converges to the correct minimum. However, the covariance matrix will not in general converge to the correct covariance values, so that the errors as determined by this matrix may not be correct.

As the reader can see, it is not a trivial task to implement a nonlinear least squares program. For this reason we have advised the use of a ready-made program. A variety of routines may be found in the NAG library [4.13], for example. A very powerful program allowing the use of a variety of minimization methods such a simplex, Newton, etc., is *Minuit* [4.14] which is available in the CERN program library. This library is distributed to many laboratories and universities.

**Local vs Global Minima.** Up to now we have assumed that the function  $F$  contains only one minimum. More generally, of course, an arbitrary function can have many local minima in addition to a global, absolute minimum. The methods we have described are all designed to locate a local minimum without regard for any other possible minima. It is up to the user to decide if the minimum obtained is indeed what he wants. It is important, therefore, to have some idea of what the true values are so as to start the search in the right region. Even in this case, however, there is no guarantee that the process will converge onto the closest minimum. A good technique is to fix those parameters which are approximately known and vary the rest. The result can then be

used to start a second search in which all the parameters are varied. Other problems which can arise are the occurrence of overflow or underflow in the computer. This occurs very often with exponential functions. Here good starting values are generally necessary to obtain a result.

**Errors.** While the methods we have discussed allow us to find the parameter values which minimize the function  $S$ , there is no prescription for calculating the errors on the parameters. A clue, however, can be taken from the linear one-dimensional case. Here we saw the variance of a parameter  $\theta$  was given by the inverse of the second derivative (4.72),

$$\sigma^2 = \left| \frac{1}{2} \frac{\partial^2 S}{\partial \theta^2} \right|^{-1}. \quad (4.92)$$

If we expand  $S$  in Taylor series about the minimum

$$\begin{aligned} S(\theta) &= S(\theta^*) + \frac{1}{2} \frac{\partial^2 S}{\partial \theta^2} (\theta - \theta^*)^2 \\ &= S(\theta^*) + \frac{1}{\sigma^2} (\theta - \theta^*)^2. \end{aligned} \quad (4.93)$$

At the point  $\theta = \theta^* + \sigma$ , we thus find that

$$S(\theta^* + \sigma) = S(\theta^*) + 1. \quad (4.94)$$

Thus the error on  $\theta$  corresponds to the distance between the minimum and where the  $S$  distribution increases by 1.

This can be generalized to the nonlinear case where the  $S$  distribution is not generally parabolic around the minimum. Finding the errors for each parameter then implies finding those points for which the  $S$  value changes by 1 from the minimum. If  $S$  has a complicated form, of course, this is not always easy to determine and once again, a numerical method must be used to solve the equation. If the form of  $S$  can be approximated by a quadratic surface, then, the error matrix in (4.73) can be calculated and inverted as in the linear case. This should then give an estimate of the errors and covariances.

## 4.8 Some General Rules for Rounding-off Numbers for Final Presentation

As a final remark in this chapter, we will suggest here a few general rules for the rounding off of numerical data for their final presentation.

The number of digits to be kept in a numerical result is determined by the errors on that result. For example, suppose our result after measurement and analysis is calculated to be  $x = 17.615334$  with an error  $\sigma(x) = 0.0233$ . The error, of course, tells us that the result is uncertain at the level of the second decimal place, so that all following digits have absolutely no meaning. The result therefore should be rounded-off to correspond with the error.

Rounding off also applies to the calculated error. Only the first significant digit has any meaning, of course, but it is generally a good idea to keep two digits (but not more) in case the results are used in some other analysis. The extra digit then helps avoid a cumulative round-off error. In the example above, then, the error is rounded off to  $\sigma = 0.0233 \rightarrow 0.023$ ; the result,  $x$ , should thus be given to three decimal places.

A general method for rounding off numbers is to take all digits to be rejected and to place a decimal point in front. Then

- 1) if the fraction thus formed is less than 0.5, the least significant digit is kept as is,
- 2) if the fraction is greater than 0.5, the least significant digit is increased by 1,
- 3) if the fraction is exactly 0.5, the number is increased if the least significant digit is odd and kept if it is even.

In the example above, three decimal places are to be kept. Placing a decimal point in front of the rejected digits then yields 0.334. Since this is less than 0.5, the rounded result is  $x = 17.615 \pm 0.023$ .

One thing which should be avoided is rounding off in steps of one digit at a time. For example, consider the number 2.346 which is to be rounded-off to one decimal place. Using the method above, we find  $2.346 \rightarrow 2.3$ . Rounding-off one digit at a time, however, yields

$$2.346 \rightarrow 2.35 \rightarrow 2.4 !$$