Frequentist and Bayesian confidence intervals

Günter Zech

Universität Siegen, D-57068 Siegen
zech@physik.uni-siegen.de

Abstract. Frequentist (classical) and Bayesian approaches to the construction of confidence limits are compared. Various examples which illustrate specific problems are presented. The Likelihood Principle and the Stopping Rule Paradox are discussed. The performance of the different methods is investigated relative to the properties coherence, precision, bias, universality, simplicity. A proposal on how to define error limits in various cases are derived from the comparison. They are based on the likelihood function only and follow in most cases the general practice in high energy physics. Classical methods are not recommended because they violate the Likelihood Principle, they can produce inconsistent results, suffer from lack of precision and generality. Also the extreme Bayesian approach with arbitrary choice of the prior probability density or priors deduced from scaling laws is rejected.

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Contents

1 Introduction .......................................................... 3
  1.1 Scope of this article .................................................. 3
  1.2 A first glance at the problem ....................................... 5

2 Classical confidence limits .......................................... 7
  2.1 Visualization .......................................................... 7
  2.2 Classical confidence limits in one dimension – definitions ... 9
    2.2.1 Central intervals ................................................... 10
    2.2.2 Equal probability density intervals ........................... 10
    2.2.3 Minimum size intervals .......................................... 10
    2.2.4 Symmetric intervals .............................................. 10
    2.2.5 Selective intervals ............................................... 11
    2.2.6 One-sided intervals .............................................. 11
    2.2.7 Which definition is the best? .................................. 11
  2.3 Two simple examples ................................................ 12
  2.4 Digital measurements ............................................... 13
  2.5 External constraints ................................................ 14
  2.6 Classical confidence limits with several parameters .......... 14
  2.7 Nuisance parameters ............................................... 16
    2.7.1 Factorization and restructuring ................................ 17
    2.7.2 Global limits .................................................... 18
    2.7.3 Other methods ................................................... 18
2.8 Upper and lower limits .................................................. 19
2.9 Upper limits for Poisson distributed signals ......................... 19
  2.9.1 Rate limits with uncertainty in the luminosity .............. 20
  2.9.2 Poisson limits with background ................................ 20
  2.9.3 Limits with re-normalized background ....................... 23
  2.9.4 Uncertainty in the background prediction .................... 24
2.10 Discrete parameters .................................................. 24

3 Unified approaches ....................................................... 26
  3.1 Basic ideas of the unified approach .............................. 26
  3.2 Difficulties with two-sided constraints ......................... 27
  3.3 External constraint and distributions with tails ............... 27
  3.4 Artificial correlations of independent parameters ............ 29
  3.5 Several bounded parameters ...................................... 30
  3.6 Upper Poisson limits ............................................... 30
  3.7 Restriction due to unification ................................... 30
  3.8 Alternative unified methods ...................................... 32

4 Likelihood ratio limits and Bayesian confidence intervals ......... 33
  4.1 Inverse probability ................................................. 33
  4.2 Interval definition .................................................. 34
    4.2.1 Bayesian intervals ........................................... 34
    4.2.2 Likelihood ratio intervals ................................. 35
  4.3 Problems with likelihood ratio intervals ....................... 36
  4.4 The prior parameter density and the parameter choice ........ 37
  4.5 External constraints .............................................. 39
  4.6 Several parameters and nuisance parameters ................... 40
  4.7 Upper and lower limits .......................................... 40
  4.8 Discrete parameters .............................................. 42

5 The Likelihood Principle and information ............................ 42
  5.1 The Likelihood Principle .......................................... 42
  5.2 Some objections to the Likelihood Principle ................... 44
    5.2.1 The likelihood function does not explore the full sample space 44
    5.2.2 Inference of Gaussian parameters from a single observation 45
  5.3 The Stopping Rule Paradox ....................................... 46
  5.4 Stein's example .................................................... 49
    5.4.1 The paradox and its solution ............................... 50
    5.4.2 Classical treatment .......................................... 51
  5.5 Stone's example .................................................... 52
  5.6 Goodness-of-fit tests ............................................. 53
  5.7 Randomization ..................................................... 53
  5.8 Precision and consistency ....................................... 54
1 Introduction

1.1 Scope of this article

The progress of experimental sciences to a large extent is due to the assignment of uncertainties to experimental results. A measurement is incomplete and more or less useless, unless an error interval is attributed to it. The precision of measurements has to be known i) to combine data from different experiments, ii) to deduce secondary parameters from it and iii) to test predictions of theories. Different statistical methods have to be judged on their ability to fulfill these tasks.

In the language of statistics a measurement and its error are an estimate of a parameter and an estimate of a parameter interval - the confidence interval. Both are to be inferred from a data sample or a single element drawn from a statistical distribution which depends on that parameter. The statistical data sample collected in an experiment is called an observation which we distinguish from a measurement.\footnote{For example, an observation of ten decay times of a certain particle species constitutes a sample drawn from an exponential distribution with unknown slope parameter. The estimate of this parameter provides the measurement of the mean life of the particle. When we perform a least square fit of some function containing unknown parameters (which we want to measure) to experimental data points (the observation), our probability distribution is a $\chi^2$-distribution provided that the individual deviations of the data points follow Gaussians. The observation, - think of the reading of a meter, a drift time, a mass distribution, a number of observed events - has no error assigned to it. The statistical uncertainty is embedded in the probability distribution function describing it. Often the observation and the measurement are numerically identical. In other cases, an observation summarizes many experimental numbers and the measurement is the outcome of a sophisticated data analysis.}
Parameter inference is a relatively non-controversial subject, but there is still no consensus on how to define confidence intervals for the parameters among the different schools of statistics, represented by frequentists and Bayesians. One of the reasons for a continuing debate between these two parties is that statistics is partially an experimental science, as stressed by Jaynes [1], and partially a mathematical discipline as expressed by Fisher: The first sentence in his famous book on statistics [2] is “The science of statistics is essentially a branch of Applied Mathematics”. Thus one expects from statistical methods not only to handle all kind of practical problems but also to be deducible from few axioms and to provide correct solutions for sophisticated exotic examples, requirements which are not even fulfilled by old and reputed sciences like physics.

Corresponding to the two main lines of statistical thought, we are confronted with different kinds of error interval definitions, the classical (or frequentist) one and some more or less Bayesian inspired ones. The majority of particle physicists intellectually favor to the first but in practice use the second. Both methods are mathematically consistent. In most cases their results are very similar but there are also situations where they differ considerably. These cases exhibit either low event numbers, large measurement errors or parameters restricted by physical limits, like positive mass, $|\cos| \leq 1$, positive rates etc..

Some standard is badly needed. For example, there exist at present at least eight different methods to the single problem to compute an upper limit for Poisson distributed events.

The purpose of this article is not to repeat all the philosophical arguments in favor of the Bayesian or the classical school. They can be found in many textbooks for example in Refs. [3, 4, 5] and more or less profound articles and reports [6, 7]. Further references are given in an article by Cousins [7]. I am convinced that methods from both schools are valid and partially complementary. Pattern recognition, noise suppression, analysis of time series are fields where Bayesian methods dominate, goodness-of-fit techniques are based on classical statistics.

We restrict our discussion to the evaluation of parameters of an otherwise completely defined theory and of the confidence intervals of these parameters. They are deduced from a comparison of the theoretical predictions to a clean, unbiased data sample. In this context, goodness-of-fit tests are not relevant.

The situation in physics is different from that in social, medical or economic sciences where usually crude models have to be used which cannot be parametrized in a unique way and thus forbid the use of a likelihood function.

In this report, the emphasis is mainly put on performance and less on the mathematical and statistical foundation. An exception is a discussion of the Likelihood Principle which is fundamental for modern statistics. The intention is to apply the procedures to problems to be solved in physics and to judge them on the basis of their usefulness. Even though the challenge is in real physics cases it is in simple examples that we gain clarity and insight. Thus simple examples are selected which illustrate the essential problems.

To judge the different definitions of confidence intervals, we introduce the following set of criteria:

1. Error intervals and one-sided limits have to measure the precision of an experiment.
2. They should be selective (exclude wrong parameter values, powerful in classical notation \[8\]).

3. They have to be unique and consistent: Equally precise measurements have equal errors intervals. More precise measurements provide smaller intervals than less precise measurements.

4. Subjective input has to be avoided.

5. The procedure should allow us to combine results from different experiments with minimum loss of information.

6. The interval should provide a firm basis for decisions, like excluding a theory or stopping data taking in an experiment.

7. The method should be as general as possible. Ad hoc solutions for special cases should be avoided.

8. Last not least, we emphasize simplicity and transparency.

Most of these points have acquired little attention in the ongoing debate in the physics community, and the professional statistical literature which is dominated by applications in economics, medicine, biology and sociology hardly touches our problems.

The present discussion focuses on upper limit determinations and here especially on the Poisson case relevant in rare or exotic particle searches. However, upper limits should not be regarded isolated from the general problem of error assignment.

In the following section we will confront the classical method with examples which demonstrate its main difficulties and limitations. Section 3 deals with the unified approach proposed by Feldman and Cousins \[9\]. In Sect. 4 we investigate methods based on the likelihood function and discuss related problems. Section 5 is devoted to the Likelihood Principle and Sect. 6 contains a systematic comparison of the methods with respect to the issues mentioned above. Section 7, finally, concludes with some recommendations. Part of the content of this report has been presented in Ref. \[11\].

We emphasize low statistics experiments. For simplicity, we will usually assume that a likelihood function of the parameters of interest is available and that it has at most one significant maximum. For some applications (averaging of results) not only an interval has to be estimated but also a parameter point. Normally, the maximum likelihood estimate is chosen. In classical approaches, the intervals do not necessarily contain the likelihood estimate and special prescriptions for the combination of results are necessary.

In the first part of this report we will use undefined statistical terms like precision and inconsistency and hope that they will become clear from the context in which they are applied. We will come back to them in Sect. 5.

1.2 A first glance at the problem

Before we start to discuss details, let us look in a very qualitative way at the main difference between a frequentist approach (respecting the coverage principle, see Sect. 2) and methods based on the likelihood function (respecting the Likelihood Principle, see Sect. 5).
As a simple example we imagine an observation $x$ of a variate (random variable) $X$ and a probability distribution function (pdf) $f(X|\theta)$ depending on an unknown parameter $\theta$ which we estimate from $x$. How should we select the range of parameters which we consider compatible with the data? In Fig. 1 we display an observation $x$. The two pdfs correspond to two specific parameter values $\theta_1$ and $\theta_2$.

A parameter value $\theta$ is supported by an observation $x$ if the observation is located where its probability density $f(x|\theta)$ is high. If we had to choose between $\theta_1$ and $\theta_2$, intuitively we would prefer $\theta_1$, corresponding to the narrow peak because the probability density $f(x|\theta_1)$, i.e. the likelihood of $\theta_1$, is larger than the likelihood $f(x|\theta_2)$ and would include $\theta_1$ in a confidence interval with higher priority than the competitor $\theta_2$.

Classical confidence limits (CCL) rely on tail probabilities. A parameter value is accepted inside the confidence interval if the observation is not too far in the tail of the corresponding pdf. Essentially, the integral over the tail beyond $x$ determines whether $\theta$ is included. Classical methods would preferentially accept the parameter $\theta_2$ corresponding to the wide peak, the observation being less than one standard deviation off, and not $\theta_1$. Thus, they may exclude parameter values that correspond to higher likelihood than those which they include.

Which of the two approaches is the better one? Given $x$ with no additional information we certainly would bet for $\theta_1$ with betting odds corresponding to the likelihood ratio $f(x|\theta_1)/f(x|\theta_2)$ in favor of $\theta_1$. However, we then clearly favor precise predictions over crude ones. Assume $\theta_2$ applies. The chance to accept it inside a certain likelihood interval is smaller than the corresponding chance for $\theta_1$. The choice based on the likelihood function is unfair to $\theta_2$.

The classical limits exhibit an integration in the sample space, thus depending on the probability density of data that have not been observed. Bayesians object to using such irrelevant information. (Why should we care about the probability density $f(x'|\theta)$ at $x'$ when we have observed $x$?) They rely on the likelihood function, transform it into a probability density of the parameter and usually integrate the result to compute probabilities or moments. Thus their conclusions depend on the somewhat arbitrary choice of the parameter space. This is not acceptable to frequentists.

The simplest and most common procedure is to avoid the integration and to define intervals based solely on the likelihood function. It depends only on the local probability density of the observed data and does not include subjective or irrelevant elements. Admittedly, restricting interval estimation to the information contained in the likelihood function - which is a mere parametrization of the data - does not permit to deduce probabilities or confidence levels in the probabilistic sense.

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2 We use capital letters for variates and small letters for observations of the variate.

3 For the definition of statistical terms see Ref. [11].

4 In most cases we do not distinguish between discrete and continuous probability distribution functions.

5 We consider only uniform prior densities. There is no loss of generality, see Sect. 4.
Fig. 1. The likelihood is larger for parameter $\theta_1$, but the observation is less than 1 st. dev. off $\theta_2$. Classical approaches include $\theta_2$ and exclude $\theta_1$ within a 68.3% confidence interval.

2 Classical confidence limits

The defining property of classical confidence limits (CCL) is coverage: If a large number $n$ of experiments perform measurements of a parameter with confidence level $\alpha$, in the limit $n \to \infty$, the fraction $\alpha$ of the limits has to contain the true value of the parameter inside the confidence limits.

In the following we show how confidence limits fulfilling the coverage requirement can be constructed.

2.1 Visualization

We illustrate the concept of CCL for an observation consisting of a vector $(x_1, x_2)$ and a two-dimensional parameter space (see Fig. 2). In a first step we associate to each point $\theta_1, \theta_2$ in the parameter space a closed probability contour in the sample space containing an observation with probability $\alpha$. (The probability contour is not necessarily a curve of constant probability. Given $\alpha$, there is an infinite number of ways to define probability contours. Specific choices will be discussed below.) For example, the probability contour labeled $a$ in the sample space corresponds to the parameter values of point $A$ in the parameter space. The curve (confidence contour) connecting all points in the parameter space with probability contours in the sample space passing through the actual observation $x_1, x_2$ encloses the confidence region of confidence level (C.L.) or coverage $\alpha$. This construction guarantees that all parameter values contained in the confidence region...
Fig. 2. Two parameter classical confidence limit for an observation $x_1, x_2$. The dashed contours labeled with small letters in the sample space correspond to probability contours of the parameter pairs labeled with capital letters in the parameter space.

Fig. 3. Two parameter classical confidence limit. The dashed probability contours labeled with small letters contain an estimate of the true value (capital letter) with probability $\alpha$ that contain the observation inside their probability contour. As a consequence, whatever the values of the parameters realized in nature are, measurements will produce with probability $\alpha$ a confidence contour which contains these parameters.
Frequently, an observation is composed of many independent single observations which are combined to an estimate $\hat{\theta}$ of the parameter. Then the two plots of Fig. 2 can be combined to a single graph (see Fig. 3).

Figures 2 and 3 demonstrate some of the requirements necessary for the construction of a simply connected, non-empty confidence region with coverage exactly equal to $\alpha$:

1. The sample space must be continuous. (Discrete distributions, thus all digital measurements and in principle also Poisson processes are excluded.)
2. The probability contours should enclose a simply connected region.
3. The parameter space has to be continuous.
4. The parameter space should be infinite.

The restriction (1) usually is overcome by relaxing the requirement of exact coverage. The probability contours are enlarged to contain at least the fraction $\alpha$ of observations. In most cases, confidence limits with minimum overcoverage are chosen. This makes sense only when the density of points in the sample space is relatively large.

A possibility to conserve exact coverage is to randomize the confidence belts. The sample points are associated to the probability region of one or another parameter according to an appropriate probability distribution. This method is quite popular in some research fields and discussed extensively in the statistical literature but will not be followed here. It introduces an additional unnecessary uncertainty. A procedure cannot be optimum when decisions depend on the outcome of coin tossing.

Discrete parameter spaces can lead to empty intervals if an observation is not included in any of the probability contours.

Confidence intervals may be located in a region forbidden by physical constraints. Mathematical constrains, like $\cos \leq 1$, can produce empty intervals in the standard classical approaches. This problem is absent in unified approaches (see Sect. 3).

Frequentists usually require that confidence intervals do not contain regions where the parameter is not defined. Then instead of unphysical intervals empty intervals are obtained. Unphysical intervals, however, are more informative. From the two statements “$m = 0$ with 68% confidence” and “$-2eV < m < -1eV$ with 68% confidence”, the second one is more valuable.

There is considerable freedom in the choice of the probability contours but to ensure coverage their definition has to be independent of the result of the experiment. Usually, the contours are locations of constant probability density.

### 2.2 Classical confidence limits in one dimension – definitions

For each possible value of the parameter $\theta$ we fix a probability interval $[X_1(\theta), X_2(\theta)]$ fulfilling

$$P(X_1 \leq X \leq X_2|\theta) = \int_{X_1}^{X_2} f(X|\theta) dX = \alpha$$
Table 1. Some choices for classical confidence intervals

| Central Interval | $P(X \leq X_1|\theta) = P(X \geq X_2|\theta) = (1-\alpha)/2$ |
|------------------|----------------------------------------------------------|
| Equal Probability Densities | $f(X_1|\theta) = f(X_2|\theta)$ |
| Minimum Size | $\theta_{\text{high}} - \theta_{\text{low}}$ is minimum |
| Symmetric | $\theta_{\text{high}} - \hat{\theta} = \hat{\theta} - \theta_{\text{low}}$ |
| Likelihood Ratio Ordering | $f(X_1|\theta)/f(X_1|\theta_{\text{best}}) = f(X_2|\theta)f(X_2|\theta_{\text{best}})$ |
| One-Sided | $\theta_{\text{low}} = -\infty$ or $\theta_{\text{high}} = \infty$ |

where $f(X|\theta)$ is the pdf. Using the construction explained above, we find for an observation $x$ the confidence limits $\theta_{\text{low}}$ and $\theta_{\text{high}}$ from

$$x_1(\theta_{\text{high}}) = x$$
$$x_2(\theta_{\text{low}}) = x$$

The definitions do not fix the limits completely. Additional constraints have to be added. Some sensible choices are listed in Table 1. (We only consider distributions with a single maximum.)

2.2.1 Central intervals. The standard choice is central intervals. For a given parameter value it is equally likely to fall into the lower tail and into the upper tail of the distribution. The Particle Data Group (PDG) [12] advocates central intervals, though the edition from the year 2000 also proposes intervals based on the likelihood ratio ordering. Central intervals are invariant against variable and parameter transformations. Their application is restricted to the simple case with one variate and one parameter. When central intervals are considered together with a point estimation (measurement, parameter fit), the obvious parameter choice corresponds to the zero interval length limit ($\alpha = 0$) which in most cases would not coincide with the maximum likelihood estimate.

2.2.2 Equal probability density intervals. Equal probability density intervals are preferable because in the majority of the cases they are shorter and less biased than central intervals and the concept is also applicable to the multidimensional case. They coincide with central intervals for symmetric distributions. A disadvantage is the non-invariance of the definition under variate transformations (see Sect. 6.4).

2.2.3 Minimum size intervals. Of course we would like the confidence interval to be as short as possible [13]. The construction of minimum size intervals, if possible at all, is a difficult task [3, 13]. In Appendix B we illustrate how pivotal quantities can be used to compute such intervals. Clearly, these intervals depend by definition on the parameter choice. When we determine the mean lifetime of a particle the minimum size limits for the lifetime will not transform into limits of the decay constant with the same property.

2.2.4 Symmetric intervals. Often it is reasonable to quote symmetric errors relative to an estimate $\hat{\theta}$ of the parameter. Again this type of interval is difficult to construct and not invariant under parameter transformations.
2.2.5 Selective intervals. One could try to select confidence intervals which minimize the probability to contain wrong parameter values \( \alpha \). These intervals are called shortest by Neyman and most selective by Kendall and Stuart \( [14] \). Since this condition cannot be fulfilled for two-sided intervals independent of the value of the true parameter, Neyman has proposed the weaker condition that the coverage for all wrong parameter values has to be always less than \( \alpha \). It defines the shortest unbiased or most selective unbiased (MSU) intervals.

Most selective unbiased intervals can be constructed \([15]\) with the likelihood ratio ordering (not to be mixed up with likelihood ratio intervals). Here the probability contour (in the sample space) of a parameter corresponds to constant \( R \), defined by

\[
R(X|\theta) = \frac{f(X|\theta)}{f(X|\theta_{\text{best}})}
\]

where \( \theta_{\text{best}} \) is the maximum likelihood estimate for a fictitious observation \( X \). Qualitatively this means that preferentially those values of \( X \) are added to the probability interval of \( \theta \) where competitive values of the parameter have a low likelihood. Selective intervals have the attractive property that they are invariant under transformations of variables and parameters independent of their dimension. Usually the limits are close to likelihood ratio intervals (see Sect. 4.2) and shorter than central intervals \([8, 3, 17]\). The construction of the limits is quite tedious unless a simple sufficient statistic can be found. In the general case, where sufficiency requires a full data sample of say 1000 events, one has to find likelihood ratio contours in a 1000-dimensional space. For this reason, MSU intervals have not become popular in the past and were assumed to be useful only for the so-called exponential family \([16]\) of pdfs where a reduction of the sample space by means of sufficient statistics is admitted. Nowadays, the computation has become easily feasible on PCs. However, the programming effort is not negligible.

The likelihood ratio ordering is applied in the unified approach \([9]\) which will be discussed in Sect. 3.

2.2.6 One-sided intervals. One-sided intervals define upper and lower limits. Here, obviously the limit should be a function of a sufficient statistic or equivalently of the likelihood.

2.2.7 Which definition is the best? No general answer can be given. The choice may be different when we are interested in the uncertainty of a measurement of a particle track or in the verification of a theory. The former case one may prefer criteria based on the mean squared deviation of the limits from the true parameter value \([18]\). If probability arguments dominate, Neyman’s MSU intervals are most attractive. Their only disadvantage is the complicated numerical evaluation of the limits.

To simplify the discussion, in the following section (except for the first example) we do not apply the Neyman construction but follow the more popular line using central or

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\(7\) These intervals are closely related to uniformly most powerful and uniformly most powerful unbiased tests \([14]\).

\(8\) The likelihood ratio ordering minimizes the probability of errors of the second kind for one sided intervals. For two-sided intervals this probability can only be evaluated using relative prior probabilities of the parameters located at the two sides of the confidence interval. \([8, 3, 17]\).
Fig. 4. Position measurement from drift time. The error is due to diffusion. Classical confidence intervals are shown together with the likelihood function.

Fig. 5. Likelihood ratio ordering. The likelihood ratios are equal at the limits of the shaded probability interval.

equal probability intervals. The MSU prescription will be treated separately in Sect. 3 dealing with the unified approach.

2.3 Two simple examples

Example 1 To illustrate the concept of classical confidence levels in one dimension we consider an electron moving in a gaseous detector. The observed drift time is converted to a distance $x$. The uncertainty is due to diffusion. The probability density is

$$f(X) = \frac{1}{\sqrt{2\pi c\theta}} \exp \left[ -\frac{(X - \theta)^2}{2c\theta} \right]$$
where \( c \) is a known constant. Fig. 4 shows an observation, the likelihood function and the confidence limits for a central interval and for a MSU interval. The likelihood ratio ordering is indicated in Fig. 5 for \( \theta = 1 \). The 68.3% probability interval covers the region of \( x \) where the likelihood ratio is largest. The dip at \( X = 0 \) is due to the fact that \( f(0|\theta_{\text{best}}) = f(0|\theta = 0) = \infty \). The MSU (likelihood ratio ordering) interval is shorter than the central interval and very close to the likelihood ratio interval which is bound by parameter values of equal likelihood (see Sect. 4.2).

We now turn to problematic situations.

**Example 2** We extract the slope of a linear distribution

\[
f(X|\theta) = \frac{1}{2}(1 + \theta X)
\]

with \(-1 < X < 1\). Our data sample consists of two events observed at symmetric locations, \( x_1, x_2 \). From the observed sample mean \( s = (x_1 + x_2)/2 \) we construct the central limits

\[
\int_{-1}^{s} g(s'|\theta_{\text{high}}) ds' = \int_{s}^{1} g(s'|\theta_{\text{low}}) ds' = \frac{1 - \alpha}{2}
\]

where \( g(s|\theta) \) is the distribution of the sample mean of two observations each following \( f(X|\theta) \). For the specific result a) \( x_1 = -0.5, x_2 = 0.5 \), we find \( s = 0 \) and \( \theta_{\text{low}} = -0.44, \theta_{\text{high}} = 0.44 \) with C.L. = 0.683. If instead the result of the observation had been b) \( x_1 = 0, x_2 = 0 \) or c) \( x_1 = -1, x_2 = 1 \) the same confidence limits would have been obtained as in case a).

We realize that experimental data which are non-informative as in case b) can provide stringent limits. This is compensated by relatively loose limits for informative observations as in case c) and a well defined coverage is obtained.

The reason for the poor behavior is that the first moment of the linear distribution is not a sufficient statistic. The limits do not exhaust the experimental information.

In the quoted example the behavior can be improved also in classical statistics by working in the two-dimensional space of \( x_1, x_2 \).

For a sample of size \( n \) in the above example, probability contours have to be defined in a \( n \)-dimensional space because no simple sufficient statistic is available. The computation of the limits becomes complex but is easily feasible with present PCs with non-negligible programming effort.

### 2.4 Digital measurements

**Example 3** A particle track is passing at the unknown position \( \mu \) through a proportional wire chamber. The registered coordinate \( x \) is set equal to the wire location \( x_w \). The probability density

\[
f(X|\mu) = \delta(X - x_w)
\]

is independent of the true location \( \mu \). Thus it is impossible to define a classical confidence interval, except a trivial one with full overcoverage. This difficulty is common to all digital measurements because they violate condition 1 of Sect. 2.1. Thus a large class of measurements cannot be handled in classical statistics.
Even frequentists use the obvious Bayesian solution (see Sect. 4) to this problem. True values near the wire are always covered, those near the border never.

2.5 External constraints

One of the main objections to classical confidence limits is related to situations where the parameter space is restricted by external constraints. To illustrate the problem, we take up an often quoted example:

Example 4 A physical quantity like the mass of a particle with observations following normal distributions is constrained to positive values. Figure 6 shows typical central confidence bounds which extend into the unphysical region. In extreme cases an observation which due to a statistical fluctuation is located in the unphysical region may produce a 90% confidence interval which does not cover physical values at all.\footnote{In classical statistics the situation is usually described by a zero-length interval. I prefer unphysical intervals which retain more of the experimental information.}

An similar situation for the standard classical method is also encountered in the following example corresponding to the distribution of Example 2.

Example 5 For a sample of 100 events following the distribution of Eq. (2), a likelihood analysis gives a best value for the slope parameter of $\hat{\theta} = 0.92$ (see Fig. 7). When we try to compute central classical 68.3% confidence bounds we get $\theta_{\text{low}} = 0.82$ and find no upper bound inside the allowed range $-1 \leq \theta \leq 1$. We cannot compute a limit above 1 either because slopes $\theta > 1$ are not acceptable since they would produce negative probabilities for small values of $X$.

Frequentists may solve this problem by choosing asymmetric probability intervals (excluding central and equal probability intervals) which then should be defined before the measurement is done.

Another difficulty arises for parameters which are restricted from both sides:

Example 6 A particle passes through a small scintillator and another position sensitive detector with Gaussian resolution. Both boundaries of the classical error interval are in the region forbidden by the scintillator signal (see Fig. 8). The classical interval is twice as large as the r.m.s. width. One would restrict it to the allowed region, but the error interval is meaningless.

2.6 Classical confidence limits with several parameters

In case several parameters have to be determined, the notion of central intervals no longer makes sense and the construction of intervals of minimal size is exceedingly complex. It is advisable to use curves of equal probability or likelihood ratio boundaries to define the probability region.

Very disturbing confidence intervals may be obtained in several dimensions when one tries to minimize the size of the interval. Here, a standard example is the case of the simple normal distribution in more than two dimension where occasionally ridiculously tiny intervals are obtained [19].
Fig. 6. Confidence limits for a measurement with Gaussian errors and a physical boundary. The left side shows 68.3% confidence intervals, the right side 90% upper limits. The observed values of $\theta$ are $-1$ (top) and $+1$ (bottom). The labels refer to classical (c), unified classical (cu) and Bayesian (b).
2.7 Nuisance parameters

In most experimental situations we have to estimate several parameters but are interested in only one of them. The other parameters, the nuisance parameters, have to be eliminated. A large number of research articles have been published on the subject. A detailed discussion and references can be found in Basu’s work [20].

A formal way to eliminate the nuisance parameter without violating the exact coverage principle is the following: For a given pdf $f(X|\theta, \nu)$ where $\theta$ is the parameter of
interest and $\nu$ the nuisance parameter. We search for a statistic $Y_\nu$ which is ancillary in $\nu$ (contains no information on $\nu$) and use the pdf $f(Y_\nu|\theta)$ to determine the confidence interval. Usually $Y_\nu$ will not be sufficient for $\theta$ and the approach is not optimum since part of the experimental information has to be neglected. The implementation of this approach is not straightforward. Of practical interest are the following methods.

### 2.7.1 Factorization and restructuring.

It is easy to eliminate the nuisance parameter if the pdf factorizes in a function $f_\nu$ of the nuisance parameter $\nu$ and a function $f_\theta$ of the parameter of interest $\theta$.

$$f(X|\theta, \nu) = f_\theta(X|\theta)f_\nu(X|\nu) \quad (3)$$

Then the limits for $\theta$ are independent of a specific choice of $\nu$. If this condition is not realized, one may try to restructure the problem looking for another parameter $\eta(\theta, \nu)$ which fulfills the condition.

$$f(X|\theta, \eta) = f_\theta(X|\theta)f_\eta(X|\eta)$$

Then again fixing the new parameter $\eta$ to an arbitrary value has no influence on the confidence limits for the parameter of interest and we may just forget about it.

The following example is taken from Edwards [21].

**Example 7** The absorption of a piece of material is determined from the two rates $r_1, r_2$ registered with and without the absorber. The rates follow Poisson distributions with mean values $\theta_1, \theta_2$:

$$f(R_1, R_2) = \frac{e^{-(\theta_1+\theta_2)}\theta_1^{R_1}\theta_2^{R_2}}{R_1!R_2!}$$

We are interested in the ratio $\phi = \theta_1/\theta_2$ which is directly related to the absorption parameter. By a clever choice of the nuisance parameter $\nu$

$$\nu = \frac{\theta_1}{\theta_2}$$

we get

$$f = e^{-\nu R_1 + R_2} \frac{(1 + 1/\phi)^{R_1}(1 + \phi)^{R_2}}{R_1!R_2!}$$

$$= f_\nu(R_1 + R_2|\nu)f_\phi(R_1, R_2|\phi)$$

where the dependence of $f$ on the interesting parameter $\phi$ and the function of the nuisance parameter $\nu$ factorize. The sum $R_1 + R_2$ which is proportional to the measuring time, obviously contains no information about the absorption parameter. It is ancillary and we can condition on $R_1 + R_2$. It is interesting to notice that $f_\phi$

$$f_\phi = \frac{(1 + 1/\phi)^{R_1}(1 + \phi)^{R_2}}{R_1!R_2!}$$

is not a function of the absorption ratio $R_1/R_2$ only.\footnote{An interesting application is the determination of $\epsilon'$ from a double ratio of CP violating kaon decays.}
Fig. 9. Likelihood contours for Example 8. For better visualization the discrete values of the nuisance parameter “number of events” are connected.

A lot of effort has been invested to solve the factorization problem [22]. The solutions usually yield the same results as integrating out the nuisance parameter.

That restructuring is not always possible is seen in the following example.

**Example 8** The mean decay rate $\gamma$ is to be determined from a sample of 20 events which contain an unknown number of background events with decay rate $\gamma_b = 0.2$. Likelihood contours for the two parameters $\gamma$ and the number of signal events are shown in Fig. 9. There is no obvious way to disentangle the parameters.

2.7.2 **Global limits.** A possible but not satisfactory solution to eliminate a nuisance parameter is to compute a conservative limit. How this can be done is indicated by the dashed lines in the right hand graph of Fig. 2 for the two parameter case: A global confidence interval is computed for all parameters including the nuisance parameters. The projection of the contour onto the parameter of interest provides a conservative confidence interval for this parameter.

Looking again at Fig. 2, we realize that by squeezing the confidence ellipse in the direction of the parameter of interest and by stretching it in the other direction, the confidence level probably can be maintained but a narrower projected interval could be obtained. To perform this deformation in a consistent way such that minimum overcoverage is guaranteed is certainly not easy. An example is discussed in Sect. 2.9.

2.7.3 **Other methods.** Another popular method used by classical statisticians [23, 24] to eliminate the nuisance parameter is to estimate it away, to replace it by the best estimate. This proposal does not only violate the coverage principle but is clearly incorrect when the parameters are correlated. The stronger the correlation between the parameters is, the smaller the confidence interval will become. In the limit of full correlation it will approach zero!


2.8 Upper and lower limits

Frequently, we want to give upper or lower limits for a physical parameter. Then, of course, we use one sided bounds.

**Example 9** In a measurement of the neutrino mass the result is \( \hat{m} = (-2 \pm 2) \text{eV} \) with Gaussian errors independent of the true value. A 90% confidence upper limit \( m_u \) is defined classically by

\[
0.9 = \int_{\hat{m}}^{\infty} \eta(X|m_u, 2) dX
\]

where \( \eta \) denotes the normal distribution centered at \( m_u \) with width 2. The upper 90% confidence limit is \( m_u < 0.6 \text{eV} \). For a measurement \( \hat{m} = (-4 \pm 2) \text{eV} \) the limit would be \( m_u < -1.4 \text{eV} \) in the unphysical region. This is a frequently discussed problem. The fact that we confirm with 90% confidence something which is obviously wrong does not contradict the concept of classical confidence limits. The coverage is guaranteed for an ensemble of experiments and the unphysical interval occur only in a small fraction of them. Whether such confidence statements are of any use is a different story.\(^{11}\)

2.9 Upper limits for Poisson distributed signals

In particle physics, by far the most frequent case is the calculation of upper limits for the mean of Poisson distributed numbers, \( P(k|\mu) = e^{-\mu}\mu^k/k! \). (To conform to the notations used in physics, we do not consistently apply the convention to use capital letters for variates.) As stated above, for discrete data the frequentist approach has to accept overcoverage. (Remember, we do not consider randomization.) In the approximation with minimum overcoverage the upper limit \( \mu \) with confidence \( \alpha \) for \( n \) observed events is given by:

\[
\alpha = \sum_{i=n+1}^{\infty} P(i|\mu) \\
1 - \alpha = \sum_{i=0}^{n} P(i|\mu)
\]

In words, this means: If the limit corresponded to the true parameter value \( \mu \), the probability to observe \( n \) events or less were equal to \( 1 - \alpha \).

In the majority of search experiments no event \( (n = 0) \) is found. The classical 90% upper confidence limit is then \( \mu = 2.3 \) as shown in Fig. 10.

Now assume the true value is \( \mu = 0 \). Obviously, no event will be found in repeated experiments and the coverage is 100% independent of the nominal confidence value. It is impossible to avoid the complete overcoverage. Published exotic particle searches are much more often right than indicated by the given confidence level.

\(^{11}\)Savage et al. \[^{[25]}\]: “The only use I know for a confidence interval is to have confidence in it.”
2.9.1 Rate limits with uncertainty in the luminosity. A rate is obtained by dividing the number of observed events by the luminosity or flux which usually is not exactly known. We are only interested in the ratio, the flux is a nuisance parameter which is to be eliminated. In Refs. [7, 23] it was claimed, that the flux uncertainty improves the frequentist limit. This would be an inconsistent result. We apply the procedure outlined above in Sect. 2.72 and obtain a conservative global limit.

Example 10  We observe zero events \( n = 0 \) of a certain type and measure the flux \( f = 1 \pm 0.05 \) and want to compute an upper limit for the rate. To simplify the problem for the present purpose, we assume that the observed flux follows a Gaussian distribution with width independent of the mean value. The event number is Poisson distributed. As usual, we first have to construct probability contours in the sample space. Figure 11 left shows 90% probability contours for three different combinations of true flux and true rate. Each combination is chosen such that the observation \( n = 0, f = 1 \) is located at the border of the probability region. In the upper plot the range for the observed flux was selected smaller than in the lower plot. The corresponding confidence contours are displayed at the right hand side. The global limits for the rate are indicated by a dashed line. There is an infinite number of ways to construct the 90% probability region. Each of them will lead to a different global limit. The construction belonging to the lower plots obviously is superior to the first because it gives a more restrictive limit. An optimization has not been done. In any case the limit is considerably worse than in an experiment without uncertainty in the flux in contradiction to Refs. [4, 23].

2.9.2 Poisson limits with background. The situation becomes complex when the experimental data contain background indistinguishable from signal. Assuming the background expectation \( b \) is precisely known the probability to find \( k \) events (background
Fig. 11. Probability contours (left) and confidence regions (right) for a Poisson rate with flux uncertainty. The conservative 90% upper limit of the rate is indicated by the dashed line. The lower plots with 3 st. dev. limits in the flux provide more restrictive 90% limits than the upper 2 st. dev. flux limits.

The probability of observing a total of $k$ events in the data, given the true rate $\mu$ and the background distribution $Q(j|b)$ (plus signal) is

$$W(k) = \sum_{i=0}^{k} \sum_{j=1}^{k} P(i|\mu)Q(j|b)\delta_{i+j,k}$$

(4)

$$= \sum_{i=0}^{k} P(i|\mu)Q(k-i|b)$$

(5)

with $Q(j|b)$ the background distribution. (We sum over all combinations of background $j$ and signal $i$ which add up to $k$ events.) Usually the background also follows a Poisson
distribution.

\[ W(k) = \sum_{i=0}^{k} P(i|\mu)P(k-i|b) \]  
\[ = P(k|\mu+b) \]  

Then the probability to find less than or equal to \( n \) events is

\[ 1 - \alpha = \sum_{k=0}^{n} W(k) \]  
\[ = \sum_{k=0}^{n} P(k|\mu+b) \]

Solving the last equation for \( \mu \), we get the upper limit with confidence \( \alpha \). Apparently, for \( n \) given, the limit becomes more restrictive the larger is \( b \).

In experiments with large background, occasionally, due to background fluctuations, the numerical evaluation produces even negative limits or zero length limits. The limits then do not represent the precision of the experiment which certainly is not infinite.

It is instructive to study the case where no event is observed but where background is expected:

**Example 11** In a garden there are apple and pear trees near together. Usually during night some pears fall from the trees. One morning looking from his window, the proprietor who is interested in apples find that no fruit is lying in the grass. If there were any, since it is still quite dark, he would be unable to distinguish apples from pears. He concludes that the mean rate of falling apples per night is less the 2.3 with 90% confidence level. His wife who is a classical statistician tells him that his rate limit is too high because he has forgotten to subtract the expected pears background. He argues, “there are no pears”, but she insists and explains him that if he ignores the pears that could have been there but weren’t, he would violate the coverage requirement. In the meantime it has become bright outside and pears and apples - which both are not there - would now be distinguishable. Even though the evidence has not changed, the classical limit has.

The 90% confidence limits for zero events observed and background expectation \( b = 0 \) is \( \mu = 2.3 \). For \( b = 2 \) it is \( \mu' = 0.3 \) much lower. Classical confidence limits are different for two experiments with exactly the same experimental evidence relative to the signal (no signal event seen). This conclusion is absolutely unacceptable. The classical procedure is inconsistent in this case: The two experimental results \( n = 0, b = 0 \) and \( n = 0, b = 0 \) warrant the same conclusion for the rate \( \mu \) but lead to different interval sizes.

Frequentists argue that in the classical approach the long-term properties of many experiments are well defined. This is not in contradiction to the fact that there are severe problems in the evaluation of single experiments with low statistics. We will come back to this discussion in Sect. 6.

Feldman and Cousins consider the objections to the classical result as “based on a misplaced Bayesian interpretation of classical intervals” [9]. It is hard to detect a
Table 2. 90 percent confidence limits in frequentist and Bayesian approaches for \( n \) observed events and background expectation \( b \)

| n=0, b=0 | n=0, b=1 | n=0, b=2 | n=0, b=3 | n=2, b=2 |
|---------|---------|---------|---------|---------|
| standard classical | 2.30 | 1.30 | 0.30 | -0.70 | 3.32 |
| unified classical | 2.44 | 1.61 | 1.26 | 1.08 | 3.91 |
| uniform Bayesian | 2.30 | 2.30 | 2.30 | 2.30 | 3.88 |

Bayesian origin in a generally accepted principle in science, namely, two observations containing the same information should give identical results. The criticism here is not that CCLs are inherently wrong but that their application to the computation of upper limits when background is expected does not make sense, i.e. these limits do not measure the precision of the experiment which is the only purpose of error intervals. This is also illustrated in the following example which is a more scientific replicate of Example 11:

**Example 12** An experiment is undertaken to search for events predicted by some exotic theory. In a pre-defined kinematic region no event is found. A search in a corresponding control region predicts \( b \) background events. An upper limit is computed. After the limit has been published a student discovers a new kinematical cut which completely eliminates all background. The improved analysis produces a much less stringent classical limit than the original one!

The 90% upper limits for some special cases are collected in Table 2. The upper rate limit for no event found but three background events expected is negative.

### 2.9.3 Limits with re-normalized background

To avoid the unacceptable situation, I had proposed \cite{26} a modified frequentist approach to the calculation of the Poissonian limits. It takes into account that the background \( k \) has to be less or equal to the number \( n \) of observed events. For example, if \( n = 1 \), we know for sure that the background is either 0 or 1. Then only the probability ratio \( Q(1)/Q(0) \) is relevant, \( Q(k > 1) \) is irrelevant for the inference of the signal from the available data. The a priori background distribution for the condition \( k \leq n \) is then:

\[
Q'(k|b) = \frac{Q(k|b)}{\sum_{i=1}^{n} Q(i|b)}
\]

We replace \( Q \) by \( Q' \) in Eq. (5) and obtain for the Poisson case:

\[
1 - \alpha = \frac{\sum_{k=0}^{n} P(k|\mu + b)}{\sum_{k=0}^{n} P(k|b)}
\] (9)

The interpretation is: The probability \( 1 - \alpha \) to observe less or equal \( n \) events (signal + background) for a signal mean equal \( \mu \), a background mean equal \( b \) with the restriction that the background does not exceed the observed number is given by Eq. (9). The resulting limits respect the Likelihood Principle (see Sect. 5) and thus are consistent. The standard classical limits depend on the background distribution for background larger than the observed event number. This information which clearly is irrelevant for estimating the signal is ignored in the modified approach (Equ. 9).
The formula 9 accidentally coincides with that of the uniform Bayesian method. Interesting applications of the method with some variations are found in Refs. 27, 28, 29, 30.

Formula 9 has been criticized by Highland [31] because the method does not respect the coverage requirement. This is correct, but coverage had not be claimed in my paper. A reply is given in Ref. 32 and a further discussion can be found in Ref. 33.

In view of the unavoidable complete overcoverage for \( \mu = 0 \) of all classical methods, the moderate overcoverage of the Relation 9 which avoids inconsistencies seems to be acceptable to many pragmatic frequentists.

### 2.9.4 Uncertainty in the background prediction.

Often the background expectation \( b \) is not known precisely. We have to distinguish two cases.

a) The pdf \( g(b) \) of \( b \) is known. Then we can integrate over \( b \) and obtain for the conventional classical expression

\[
1 - \alpha = \int g(b) \sum_{k=0}^{n} P(k|\mu + b) db
\]

and the modified frequentist Formula 9 becomes

\[
1 - \alpha = \frac{\int g(b) \sum_{k=0}^{n} P(k|\mu + b) db}{\int g(b) \sum_{k=0}^{n} P(k|b) db}
\]

b) We know only the likelihood function of \( b \) for example if it is estimated from side bands or from other measurements with limited statistics. Then \( b \) is a nuisance parameter. Thus the methods outlined in Sect. 2.7 have to be applied. Again, I would not support the proposal of Cousins [23], “replace the nuisance parameter by the best estimate” since the result often violates the coverage principle, the coverage is not necessarily greater than or equal to \( \alpha \) for all values of the signal. The “global” method (Sect. 2.72) should be used to eliminate the nuisance parameter.

### 2.10 Discrete parameters

For discrete parameters usually it does not make much sense to give error limits but we would like to define relative confidence values for the parameters.

**Example 13** Two theories \( H_1, H_2 \) predict the time of an earthquake with Gaussian resolution:

\[
H_1 : t_1 = (7.50 \pm 2.25) \ h \\
H_2 : t_2 = (50 \pm 100) \ h
\]

The event actually takes place at time \( t_m = 10 \ h \). The predictions together with the observation are displayed in Fig. 12 top. The prediction of \( H_2 \) is rather vague but includes the observation within half a standard deviation. \( H_1 \) is rather precise but misses the observation within the errors. There is no obvious way to associate classical confidence levels to the two possible solutions. A rational extension of the frequentist methods applied
Fig. 12. Predictions from two discrete hypothesis $H_1, H_2$ and observation (top) and log-likelihood for $H_3$, a parametrization of $H_1$ and $H_2$ (bottom). The likelihood ratio strongly favors $H_1$ which is excluded by the classical confidence limits.

To continuous parameters would be to compare the tail probabilities of the two hypotheses. Tail probabilities, however, are quite misleading as will be illustrated below in Example 14. They would support $H_2$ contrary to our intuition which is clearly in favor of $H_1$. For this reason classical statisticians prefer to apply the Neyman-Pearson test based on the likelihood ratio, in our case equal to 26 in favor of $H_1$.

A similar example is analyzed in detail in an article by Jeffreys and Berger [34]. It is interesting to consider the modified example:
Example 14  Another theory, $H_3(t_3)$, depending on the unknown parameter $t_3$ predicts the Gaussian probability density

$$f(T) = \frac{25}{\sqrt{2\pi t_3^2}} \exp \left( -\frac{625(T - t_3)^2}{2t_3^4} \right)$$

for the time $T$. The classical confidence limits for the same observation as above, $t_m = 10\ h$, are $7.66 \ h < t_3 < \infty$, is slightly excluding $t_1$ but in perfect agreement with $t_2$. Fig. 12 bottom shows the corresponding likelihood function and the classical confidence limit.

The probability density of our example has been constructed such that it includes $H_1$ and $H_2$ for the specific values of $t_3$ equal $t_1, t_2$. Thus the likelihood ratio $f(t_1)/f(t_2)$ is identical to that of the previous example. Let us assume that the alternative theories $H_1$ and $H_2$ (which are both compatible with $H_3$) were developed after $H_3$. $H_1$ which is by far more likely than $H_2$ could have been excluded on the basis of the observation and the classical confidence limits.

A decision in favor of one of two alternative hypothesis, according to the Neyman-Pearson Lemma should be based on the likelihood ratio only. Here, frequentists usually do not consider the full sample space and do not compute the coverage for the two hypotheses.

What happens, when we add to the first two discrete parameter values a third, forth, fifth parameter and so on? We may construct a transition from the discrete case to the continuous one by adding more and more hypotheses. At a certain point, frequentists would switch from characterizing the situation by likelihood ratios to using coverage intervals.

The two classical concepts, confidence limit and Neyman-Pearson test, lack a common basis. Frequentists would argue that there are two different methods for two different goals. The question is then: What are there two different goals exactly and why are we interested in the likelihood ratio in one situation and in coverage in the other?

3 Unified approaches

Feldman and Cousins [9] have proposed a new approach to the computation of classical confidence bounds which avoids the occurrence of non-null (or alternatively non-physical) confidence regions, one of the most problematic features of the conventional classical confidence limits. In addition it unifies the two procedures “computation of confidence intervals” and “computation of one-sided confidence limits”. The unified treatment has already been adopted by several experiments and is recommended by the Particle Data Group [12]. However, as shown below, it has serious drawbacks.

3.1 Basic ideas of the unified approach

The unified approach has two basic ingredients:

1) It unifies the two procedures “computation of a two-sided interval” and “computation of an upper limit”. The scientist fixes the confidence level before he looks at the data and then the data provide either an error interval or a lower or upper limit, depending on the possibility to obtain an error interval within the allowed physical region. The method thus avoids a violation of the coverage principle which is obvious in the
commonly used procedure where the selection of one or two sided bounds is based on the data and personal prejudice.

2) It uses the *likelihood ratio ordering* principle (see Sect. 2.2) which has the attractive property to be invariant against transformations of the sample space variables. In addition, unphysical intervals or limits are avoided. Here the trick is to require that the quantity $\theta_{best}$ of relation (1) is inside the range allowed by the laws of physics. As discussed in Sect. 2, the likelihood ordering corresponds to MSU intervals and is an old concept. What is new is the application to cases where the parameter range is restricted by external bounds.

In practice, the main impact of this method is on the computation of upper limits. Experiments have “improved” their upper limits by switching to the unified approach [35, 36].

The new approach has attractive properties, however, all those problems like the treatment of nuisance parameters which are intrinsic to the philosophy of classical statistics remain unsolved.

Kendall and Stuart [37] write in connection with the likelihood ratio ordering (notation slightly modified) “For the likelihood ratio method to be useful ... the distribution of $R(X|\theta)$ has to be free of nuisance parameters.”

Additional complications are introduced by the requirement that $\theta_{best}$ has to be inside the allowed parameter space [10]. Pathological cases have also been presented by Punzi [38] and Bouchet [39].

### 3.2 Difficulties with two-sided constraints

One of the advantages of the unified approach is the improved handling of physical bounds. This is shown in Fig. 6 for a Gaussian with external bounds. The unified intervals avoid unphysical values of the parameter but unfortunately this problem persists when a parameter is bounded from both sides.

**Example 15** We resume Example 6, Fig. 8. A particle track is measured by a combination of a proportional wire chamber and a position detector with Gaussian resolution. Let us assume an observation $\hat{x} = 0$ of a parameter $\mu$ with a physical bound $-1 < \mu < 1$ and a Gaussian resolution of $\sigma = 1.1$. The Bayesian r.m.s. error computed by integrating the likelihood function is 0.54. Since there are two boundaries the procedure applied in Example 4 no longer works. Requiring a 68.3% confidence level produces at the same time an upper and a lower limit. It is impossible to fulfill the coverage requirement, except if the complete range of $x$ is taken (complete coverage).

A similar example is discussed in the classical book by Kendall and Stuart [40]: “It may be true, but would be absurd to assert $-1 \leq \mu \leq +2$ if we know already that $0 \leq \mu \leq 1$. Of course we could truncate our interval to accord with the prior information. In our example, we could assert $0 \leq \mu \leq 1$: the observation would have added nothing to our knowledge.”

### 3.3 External constraint and distributions with tails

Difficulties occur also for location parameters with one-sided physical bounds when the resolution function has tails. In the unified approach, unphysical confidence intervals
Fig. 13. Probability distribution (top) and corresponding likelihood ratio (center) for the superposition of two Gaussians in the unified approach. Since regions are added to the probability interval using the likelihood ratio as an ordering scheme, disconnected intervals (shaded) are obtained. A Breit-Wigner pdf shows a similar behavior (bottom) are avoided by adding preferentially those parts of the sample space to the probability region which are located in the unphysical region. However, the corresponding likelihood ratio ordering may produce disconnected probability regions and consequently also disconnected confidence intervals if the pdf decreases slowly in the unphysical part of the sample space. Disconnected confidence intervals do not make sense for measurements following smooth probability distributions with a single maximum.

**Example 16** We consider the superposition of a narrow and a wide Gaussian. (It is
Frequentist and Bayesian confidence intervals

quite common that distributions have non-Gaussian tails.)

\[ f(X|\mu) = \frac{1}{\sqrt{2\pi}} \left\{ 0.9 \exp\left(-\frac{(X-\mu)^2}{2}\right) + \exp\left(-\frac{(X-\mu)^2}{0.02}\right) \right\} \]  \hspace{1cm} (10)

with the additional requirement of positive parameter values \( \mu \). This pdf is shown in Fig. 13 top for \( \mu = 1 \). The likelihood ratio for an observation \( x = 1 \) is displayed in the center of Fig. 13. Adding \( X \)-values to the probability interval according to the likelihood ratio produces disconnected probability interval regions which do not make sense. It is impossible to construct simply connected confidence intervals.

The same difficulty arises for the Breit-Wigner distribution, where again the likelihood ratio is shown in Fig. 13 bottom for an observation \( x = 1 \).

In fact, it is only a very special class of distributions for which we can guarantee that we do not get disconnected confidence intervals. For pdfs depending on \( |X-\theta| \) like those we just discussed, disconnected probability intervals are avoided if the likelihood ratio \( R = f(X|\theta)/f(X|\theta_{\text{best}}) \) decreases monotonically from the center of the distribution towards the tails. The requirement \( \frac{dR}{dX} < 0 \) for \( X > \theta \) is equivalent to

\[
\frac{d}{dX} \ln f(X|\theta_{\text{best}}) > \frac{d}{dX} \ln f(X|\theta)
\]

\[
\frac{d}{dX} \ln f(X|\theta + \Delta) > \frac{d}{dX} \ln f(X|\theta)
\]

\[
\frac{d}{dX} \ln f(X - \Delta|\theta) > \frac{d}{dX} \ln f(X|\theta)
\]

\[
\frac{d}{dX} \frac{\ln f(X|\theta) - \ln f(X - \Delta|\theta)}{\Delta} < 0
\]

where we have set \( \Delta = \theta_{\text{best}} - \theta \). All values of \( \Delta \) can occur. In the limit \( \Delta \to 0 \) we get

\[
\frac{d^2 \ln f}{dX^2} < 0
\]

Thus, the problem is absent for pdfs with convex logarithms. Integrating the last relation twice, we find that near physical boundaries the unified approach in the present form is essentially restricted to Gaussian like pdfs.

### 3.4 Artificial correlations of independent parameters

Since the confidence intervals are defined through coverage, one has to be careful in the interpretation of error bounds near physical boundaries: Artificial correlations between parameters are introduced.

**Example 17** The uncorrelated variates \( X, Y \) follows a two dimensional Gaussian. The two variances are equal and known, the center \( \mu_x, \mu_y \) is unknown. Figure 14 shows schematically the circular probability contour for the conventional classical approach and the modified contour of the unified approach which has shrunk in \( X \) due to the boundary in \( Y \). An observation \( x, y \) near the boundary will lead to confidence contours which reflect this modified shape. The error for \( \mu_x \) shrinks due to the unphysical \( \mu_y \) region.

Probably one would try to avoid the artificially introduced correlation and treat the two coordinates independently but even a slight real correlation would inhibit this possibility.
3.5 Several bounded parameters

The prescription to restrict the value $\theta_{best}$ to the physically allowed region is easily extended to the situation where we have to determine confidence limits for several bounded parameters. However, this case has not been studied and very strange results might be obtained in some cases. Feldman and Cousins [9] apply their method to a two-dimensional toy model and show that the method works technically. A thorough study is still missing.

3.6 Upper Poisson limits

Table 2 contains 90% C.L. upper limits for Poisson distributed signals with background. For the case $n = 0, b = 3$ the uniform approach avoids the unphysical limit of the conventional classical method but finds a limit which is more restrictive than that of a much more sensitive experiment with no background expected and twice the flux! Compared to the conventional approach, the situation has improved - from a Bayesian point of view - but the basic problem is not solved and the inconsistencies discussed in Sect. 2.9 persist.

Figure 15 compares the coverage and the interval lengths of the unified method with the Bayesian one with uniform prior (to be discussed below). The nominal coverage is 90%. Unavoidably for $\mu = 0, b = 0$ there is maximum over-coverage and in the range $0 \leq \mu \leq 2.2$ the average coverage is 96%.

3.7 Restriction due to unification

Let us assume that in a search for a Susy particle a positive result is found which however is compatible with background within two standard deviations. Certainly, one would prefer to publish an upper limit to a measurement, contrary to the prescription of the unified method. The authors defend their method arguing that a measurement with a given error interval always can be interpreted as a limit - which is true.
Fig. 15. Coverage and confidence interval width for the unified approach and the Bayesian case. The Bayesian curves are computed according to the unification prescription.
### 3.8 Alternative unified methods

Recently modified versions of the unified treatment of the Poisson case have been published [41, 42, 38, 43, 44].

The results of Giunti [41] are nearer to the uniform Bayesian ones, but wider than those of Feldman and Cousins.

Roe and Woodroffe [42] re-invented the method proposed by myself ten years earlier [26] and added the unification principle. The authors introduced the concept of “ancillary variable” for the background and condition on its upper limit given by \( n \). Since this number obviously is not an ancillary statistic, their concept fails to provide the required coverage properties. In their second paper [43] they present a Bayesian method which is claimed to have good coverage properties, but this is also true for the standard Bayesian approach.

Punzi [38] modifies the definition of confidence intervals such that they fulfill the Likelihood Principle. This approach is in some sense attractive but the intervals become quite wide and it is difficult to interpret them as standard error bounds.

Ciampolillo [45] uses the likelihood statistic which maximizes the likelihood inside the physically allowed region as estimator. In most cases it coincides with the parameter or parameter set which maximizes the likelihood function. Usually, the maximum likelihood estimator is not a sufficient statistic and thus will not provide optimum precision (see Example 2). Similarly, Mandelkern and Schulz [44] use an estimator confined to the physical domain. Both approaches lead to intervals which are independent of the location of the observation within the unphysical region. I find it quite unsatisfactory.
that two observations following Gaussian pdfs \( x_1 = -0.1 \) and \( x_2 = -2 \) with the bound \( \mu > 0 \) and width \( \sigma = 1 \) yield the same confidence interval. Certainly, our betting odds would be different in the two cases.

In summary, from all proposed unified methods only the Feldman/Cousins approach has a simple statistical foundation. Zech/Roe/Woodroofe’s method is not correct from a classical frequentist point of view, Punzi’s method is theoretically interesting but not suited for error definitions, and the other prescriptions represent unsatisfactory ad-hoc solutions.

The Figs. 16 and 17 compare upper limits, coverage and interval lengths for some approaches for \( b = 0 \) and \( b = 3 \). (Part of the data has been taken from Ref. [42].) The likelihood functions for \( n = 0, b = 0 \) and \( n = 0, b = 3 \) are of course identical up to an irrelevant constant factor. Apparently, Feldman and Cousins avoid under-coverage while the other approaches try to come closer to the nominal confidence level but in some cases are below. The interval widths are similar for all methods.

4 Likelihood ratio limits and Bayesian confidence intervals

4.1 Inverse probability

Bayesians treat parameters as random variables (see also Appendix A). The combined probability density \( f(X, \theta) \) of the variate \( X \) and the parameter \( \theta \) can be conditioned on the outcome of one of the two variates using Bayes theorem:

\[
\begin{align*}
  f(X, \theta) &= f_x(X|\theta)\pi_\theta(\theta) = f_\theta(\theta|X)\pi_x(X) \\
  f_\theta(\theta|X) &= \frac{f_x(X|\theta)\pi_\theta(\theta)}{\pi_x(X)} \tag{11}
\end{align*}
\]

where the functions \( \pi \) are the marginal densities. The density \( \pi_\theta(\theta) \) in this context usually is called prior density of the parameter and gives the probability density for \( \theta \) prior to the observation \( x \) of \( X \). For a given observation \( x \) the conditional density \( f_x \) can be identified with the likelihood function. The marginal distribution \( \pi_x \) is just a multiplicative factor independent of \( \theta \) and is eliminated by the normalization requirement.

\[
\begin{align*}
  f_\theta(\theta|x) &\propto L(x, \theta)\pi_\theta(\theta) \\
  f_\theta(\theta|x) &= \frac{L(x, \theta)\pi_\theta(\theta)}{\int_{-\infty}^{\infty} L(x, \theta)\pi_\theta(\theta)d\theta} \tag{12}
\end{align*}
\]

The prior density \( \pi_\theta \) has to guarantee that the normalization integral is finite.

In the literature \( f_\theta \) often is called inverse probability to emphasize the change of role between \( X \) and \( \theta \).

The relation (12) contains one parameter and one observation, but \( x \) can also be interpreted as a “vector” \( (x_1, x_2, ..) \), a set of individual observations of independent and identically distributed (i.i.d.) variates, following the same distribution \( f_0(X|\theta) \)

\[
f(X|\theta) = \prod_i f_0(X_i|\theta)
\]

or any kind of statistic and \( \theta \) may be a set of parameters.
Fig. 17. Top: Coverage as a function of the Poisson rate for expected background $b = 3$. The nominal coverage is 90%. The labels refer to \[9\] (f), Bayesian (b), \[41\] (g) and \[42\] (r). Bottom: Interval length as a function of the observed number of events

4.2 Interval definition

4.2.1 Bayesian intervals. Having the probability density of the parameter in hand, it is easy to compute mean values, r.m.s. errors or probabilities for upper or lower bounds (see Fig. 18).

There is again some freedom in defining the Bayesian limits. One possibility would be
to quote the mean and the variance of the parameter, another possibility is to compute intervals of a given probability\textsuperscript{12}. The first possibility emphasizes error propagation, the second is better adapted to hypothesis testing. In the latter case, the interval boundaries correspond to equal probability density of the parameter\textsuperscript{13} (equal likelihood for a uniform prior). Again a lack of standardization is apparent for the choice of the interval.

4.2.2 Likelihood ratio intervals. Since the likelihood function itself represents the information of the data relative to the parameter of interest and is independent of the problematic choice of a prior it makes sense to publish this function or to parametrize it. Usually, the log-likelihood, in this context called support function\textsuperscript{16} or support-by-data an expression introduced by Hacking\textsuperscript{17}, is mathematically more convenient than the likelihood function itself.

For continuous parameters, usually likelihood limits are given. For a single parameter, the two equivalent conditions

\begin{align}
L_{\text{max}} / L(\theta_{\text{low}}) &= L_{\text{max}} / L(\theta_{\text{high}}) = e^\Delta \\
\ln L(\theta_{\text{low}}) &= \ln L_{\text{max}} - \Delta = \ln L(\theta_{\text{high}})
\end{align}

where $L_{\text{max}}$ is the maximum of the function in the allowed parameter range $\theta_{\text{min}} < \theta < \theta_{\text{max}}$, fix a likelihood ratio interval $\theta_{\text{low}} < \theta < \theta_{\text{high}}$ (see Fig. 18). The values $\Delta = 0.5$ and $\Delta = 2$ define one and two standard deviation likelihood limits (support intervals). In the one parameter case limit where $f(X)$ is a Gaussian (the width being independent of the parameter) these bounds correspond to classical C.L.s. of 0.683 and 0.954 confidence.

The one-dimensional likelihood limits transform into boundaries in several dimensions. For example for two parameters we get the confidence contour in the $\theta_1 - \theta_2$ plane.

$$\ln L(x; \theta_1, \theta_2) = \ln L_{\text{max}} - \Delta$$

\textsuperscript{12}In the literature the expression \textit{degree of belief} is used instead of probability to emphasize the dependence on a prior density. For simplicity we will stick to the expression confidence level.

\textsuperscript{13}Central intervals are wider and restricted to one dimension.
The value of $\Delta L$ is again equal to 0.5 (2) for the 1st. dev. (2 st. dev.) case. The contour is invariant under transformations of the parameter space.

Upper Poisson limits are usually computed from Bayesian probability intervals. D’Agostini [48] emphasizes the likelihood ratio as a sensible measure of upper limits, for example in Higgs searches. In this way the dependence of the limit on the prior of the Bayesian methods is avoided.

### 4.3 Problems with likelihood ratio intervals

Many of the situations where the classical methods find difficulties are also problematic for likelihood ratio intervals.

- The elimination of nuisance parameters is as problematic as in the frequentist methods.
- Digital measurements have constant likelihood functions and cannot be handled.
- The error limits for functions with long tails (like the Breit-Wigner pdf) are misleading.
- When the likelihood function has its mathematical maximum outside the physical region ($L_{\text{max}}$ is then at the edge of the physical region), the resulting one-sided likelihood ratio interval for $\Delta = 0.5$ may be unreasonably short.
- The same situation occurs when the maximum is near the border of the allowed sample space.

A frequently discussed example is:

**Example 18** The width $\theta$ of a uniform distribution

$$f(X|\theta) = \frac{1}{\theta}, \quad 0 < X < \theta$$

is estimated from $n$ observations $x_i$. The likelihood function is

$$L = \theta^{-n}, \quad \theta \geq x_{\text{max}}$$

with a $1/\sqrt{\text{e}}$ likelihood ratio interval of $x_{\text{max}} < \theta < x_{\text{max}} e^{1/(2n)}$ which for $n = 10$ is only about half of the classical and the Bayesian widths. (This example is relevant for the determination of the time zero $t_0$ from a sample of registered drift times.)

We will come back to likelihood ratio intervals in sections 6 and 7. In the following we concentrate on the Bayesian method with uniform prior but free choice of parameter.
4.4 The prior parameter density and the parameter choice

The Bayesian method would be ideal if we knew the prior of the parameter. Clearly the problem is in the prior parameter density and some statisticians completely reject the whole concept of a prior density. The following example demonstrates that at least in some cases the Bayesian way is plausible.

Example 19 An unstable particle with known mean life \( \tau \) has decayed at time \( \theta \). We are interested in \( \theta \). An experiment with Gaussian resolution \( s, \eta(t|\theta, s) \) finds the value \( t \). The prior density \( \pi(\theta) \) for \( \theta \) is proportional to \( \exp(-\theta/\tau) \). Using (12) we get

\[
f_\theta(\theta) = \frac{\eta(t|\theta, s)e^{-\theta/\tau}}{\int_0^\infty \eta(t|\theta, s)e^{-\theta/\tau}d\theta}
\]

However, there is no obvious way to fix the prior density in the following example:

Example 20 We find a significant peak in a mass spectrum and associate it to a so far unknown particle. To compute the probability density of the mass \( M \) we need to know the a priory mass density \( \pi(M) \).

There are all kind of intermediate cases:

Example 21 When we reconstruct particle tracks from wire chamber data, we always assume a flat track density (uniform prior) between two adjacent wires. Is this assumption which is deduced from experience justified also for very rare event types? Is it valid independent of the wire spacing?

In absence of quantitative information on the prior parameter density, there is no rigorous way to fix it. Some Bayesians use scaling laws to select a specific prior or propose to express our complete ignorance about a parameter by the choice of a uniform prior distribution (Bayes’ Principle). An example for the application of scaling is presented in Appendix C. Some scientists invoke the Principle of Maximum Entropy to fix the prior density.

I cannot find convincing these arguments, but nevertheless I consider it very sensible to choose a flat prior as is common practice. This attitude is shared by most physicists. I do not know of any important experimental result in particle physics analyzed with a non-uniform prior. In Example 21 it is quite legitimate to assume a uniform track density at the scale of the wire spacing.

Similarly for a fit of the \( Z^0 \)-mass there are no reasons to prefer a priori a certain mass within the small range allowed by the measurement. This fact translates also into the quasi independence of the result of the parameter selection. Assuming a flat prior for the mass squared would not noticeably alter the result.

The constant prior density is what physicists use in practice. The probability density is then obtained by normalizing the likelihood function. The obvious objection to this recipe is that it is not invariant against parameter transformations. A flat prior of \( \theta_1 \) is

\[14\] A different point of view is expressed in Refs. 8, 13.

\[15\] Normalizing the likelihood function means technically \( L(\theta)/\int_{-\infty}^{\infty} L(\theta)d\theta \) and is the Bayesian pdf for \( \theta \) obtained from a uniform prior \( \pi(\theta) = \text{const} \).
incompatible with a flat prior of $\theta_2$ unless the relation between the two parameters is linear since we have to fulfill

$$\pi_1(\theta_1)d\theta_1 = \pi_2(\theta_2)d\theta_2$$

The formal contradiction often is unimportant in practice unless the intervals are so large that a linear relation between $\theta_1$ and $\theta_2$ is a bad approximation.

One should also note that fixing the prior density to be uniform does not really restrict the Bayesian choice: There is the additional freedom to select the parameter. A parameter $\theta_1$ with arbitrary prior can be transformed into a parameter $\theta_2(\theta_1)$ with a constant prior density. Thus, for example, a physicist who would like to choose a prior density $\pi_\tau \propto 1/\tau^2$ for the mean life $\tau$ is advised to use instead the decay parameter $\gamma = 1/\tau$ with a constant prior density. In the following we will stick to the convention of a uniform prior but allow for a free choice of the parameter.

The convention to use uniform prior pdfs is convenient because it simplifies the presentation of results. It is enough to state the parameter and the interval. The scientist has to select a parameter space for which he has no strong a priori preference for specific parameter values.

An example where the parameter choice matters is the following:

**Example 22** The decay time of a particle is recorded. The single observation $t$ is used to estimate its mean life $\tau$. Using a flat prior we find the posterior parameter density

$$f(\tau) \sim \frac{1}{\tau} e^{-t/\tau}$$

which is not normalizable.

Thus a flat prior density is not always a sensible choice for an arbitrarily selected parameter. In the preceding example the reason is clear: A flat prior density would predict the same probability for a mean life of an unknown particle in the two intervals $0 < \tau < 1ns$ and $1s < \tau < 1s + 1ns$ which obviously is a fairly exotic choice. When we choose instead of the mean life the decay constant $\gamma$ with a flat prior, we obtain

$$f(\gamma) = \int_0^\infty \frac{\gamma e^{-\gamma t}}{\gamma e^{-\gamma t}d\gamma} = t^2 e^{-\gamma t}$$

The second choice is also supported by the more Gaussian shape of the likelihood function of $\gamma$ as illustrated in Fig. 19 for the observation of two decays. The figure gives also the distributions of the likelihood estimators to indicate how frequent they are.

One possible criterion for a sensible parameter choice is the shape of the likelihood function. One could try to find a parameter with approximately Gaussian shaped likelihood function and use a constant prior.

We resume the digital position measurement by a proportional wire chamber (Example 21). The likelihood is constant inside the interval allowed by the measuring device. It does not make sense to transform the parameter to obtain a Gaussian shape. Here it is common practice to use a constant prior probability and to associate to the central value the r.m.s. error interval $\pm2mm/\sqrt{12}$ of a flat probability distribution.
Fig. 19. Distribution of the max. likelihood estimates for the mean life (a) and the decay constant (b) for two decays. The corresponding likelihood functions are shown in (c) and (d) for estimates equal to one.

4.5 External constraints

Bayesians account for external constraints by using vanishing prior functions in the unphysical region which is equivalent to normalizing the parameter density to the relevant parameter interval as is illustrated in Fig. 20. The same procedure is applied to the Gaussian of Example 4 in Fig. 6.
4.6 Several parameters and nuisance parameters

The extension of the Bayesian scheme to several parameters is straightforward. Nuisance parameters can be integrated out. To do so, in principle, we have to choose the full prior density of all parameters.

\[ f(\theta|x) \sim \int L(\theta, \phi, x) \pi(\theta, \phi) d\phi \]

Even in case the likelihood function of the parameters factorizes we cannot separate the parameters without making the additional assumption that also the prior density can be written as a product of independent priors.

Since we have decided to accept only uniform prior densities the difficulty is absent.

4.7 Upper and lower limits

Bayesians compute the upper limits \( \mu \) from the tail of the inverse probability density which for a constant prior is the normalized likelihood function.

\[ \alpha = \int_\mu^\infty L(\mu')d\mu'/ \int_{-\infty}^\infty L(\mu')d\mu' \]  

(15)

For the Poisson process with Poisson distributed background we get the limit \( \mu \) from

\[ \alpha = \int_\mu^\infty P(n|\mu' + b)d\mu' = 1 - \frac{\sum_{i=0}^{n} P(i|\mu + b)}{\sum_{i=0}^{n} P(i|b)} \]

which is identical to the frequentist formula with normalization to possible background [26], and, for zero background expectation to the classical limit. Figure 21 compares the classical 90% confidence limits to the Bayesian ones for 4 expected background events as a function of the number \( n \) of observed events. The width of the horizontal bins indicates
Fig. 21. 90% c.l. upper limits in the Poisson case for the classical and the Bayesian approach. The expected background is 4, the parameter $n$ is the number of observed events. The unphysical limits of the classical approach for $n < 2$ are suppressed. The integrated probability corresponds to the true value $\mu = 0$.

the frequency of the occurrence of a certain number $n$ of observed events for the specific case where $\mu = 0$. The unphysical limits of the classical approach for $n = 0, 1$ occur in about 9% of the cases.

It is easy to generalize the Bayesian procedure for arbitrarily distributed background with the probability $Q(m|b)$ to obtain $m$ background events for a given expectation $b$.

$$L(\mu) = \sum_{i=0}^{n} P(i|\mu) Q(n - i|b)$$

The likelihood function has to be inserted in Equ. 15. The background parameter $b$ may follow another distribution $g(b)$.

$$L(\mu) = \sum_{i=0}^{n} P(i|\mu) \int_{-\infty}^{\infty} Q(n - i|b)g(b)db$$

The latter expression is useful if the background mean has an uncertainty for example when it is deduced from the sidebands of an experimental histogram.
4.8 Discrete parameters

The discrete case is automatically included in the continuous one if we allow for δ-functions. The probability for hypothesis \( i \) is given by

\[
P_i = \frac{L_i \pi_i}{\sum_i L_i \pi_i}
\]

where the likelihoods are multiplied by the prior probabilities. The confidence level for an interval translates into the confidence attributed to a hypothesis. Usually, one would set the priors all equal and obtain the simple likelihood ratio used in Example 13. Another example (quoted in Ref. [7]) follows:

**Example 23** The Mark II collaboration reported a measurement of the number of neutrinos \( N_\nu = 2.8 \pm 0.6 \) which is slightly lower than the known number of three neutrino generations. They take advantage of the negative fluctuation of their result and derive from the tail distribution the 95\% classical confidence limit \( N_\nu < 3.9 \). A Bayesian would quote the ratio of the likelihoods for the hypothesis of three and four neutrino species, \( L(3|2.8 \pm 0.6)/L(4|2.8 \pm 0.6) = 7.0 \) (assuming Gaussian distributed errors) which in principle could be multiplied by prior probabilities. The difference between these results is considerable: The classical tail limit indicates a factor 20 in favor of the three neutrino hypothesis. The likelihood ratio certainly is better suited to describe the experimental situation.

5 The Likelihood Principle and information

In this article I hope to convince the reader that all parameter and interval inference should be based solely on the likelihood function. To this end we start with a discussion of the Likelihood Principle which plays a key role in modern statistics.

5.1 The Likelihood Principle

Many statisticians (Fisher, Barnard, Birnbaum, Hacking, Basu and others) have contributed to the development of the Likelihood Principle (LP). References, derivations and extensive discussions are found in a summary of Basu’s articles [53] and the book by Berger and Wolpert [52].

We assume that our observation \( x \) follows a given probability density \( f(X|\theta) \) with unknown parameter \( \theta \).

The Likelihood Principle states:

*The information contained in an observation \( x \) with respect to the parameter \( \theta \) is summarized by the likelihood function \( L(\theta|x) \).*

In other words, \( L(\theta|x) \) of the actual observation is all what matters for the parameter inference.

A multiplicative constant \( c(x) \) in \( L \) (corresponding to an additive constant not depending on \( \theta \) in the log-likelihood) is irrelevant. Methods not respecting the LP – inference not based on \( L \) alone – do not use the full information contained the data sample.\(^{16}\)

\(^{16}\)Information as used here is not to be mistaken with the technical meaning given to this word by Fisher [54].
The LP asserts that the information relative to a parameter is identical in two experiments with proportional likelihood functions and identical parameter space, even when the pdfs are different (see Stein’s example below). Parameter inference should be based on the likelihood function alone.

The Poisson problem, with zero events observed but background expected, is a nice example illustrating the LP. The likelihood function is independent of the background expectation but the pdf depends on it. According to the LP, the information relative to the signal is independent of the background expectation. Classical confidence intervals are in conflict with the LP, likelihood ratio limits and Bayesian intervals are in agreement with it.

The LP relies on the strict validity of the probability density which is used, a condition usually fulfilled in exact sciences. It is less useful in social, economical and medical applications where only approximative theoretical descriptions are available. Methods based on the likelihood function often are very sensitive to unknown biases, background and losses.

The LP can be derived from the Sufficiency Principle:

If \( T' = T(x_1', x_2', \ldots, x_n') \) is a sufficient statistic in an experiment and if \( T'' = T(x_1'', x_2'', \ldots, x_n'') \) the same value is obtained in another experiment, both experiments following \( f(X_1, X_2, \ldots, X_n | \theta) \) the evidence for \( \theta \) is the same in both experiments.

and the Weak Conditioning Principle (in sloppy notation):

Performing the mixed experiment where randomly one of the experiments \( E_1 \) and \( E_2 \) is selected is equivalent to performing directly the selected experiment.

We illustrate the Weak Conditioning Principle with a simple example: An experiment \( E_1 \) has two position sensitive detectors \( D_1 \) with low resolution and \( D_2 \) with high resolution. The efficiency of \( D_2 \) is low. When \( D_2 \) has seen a particle, only the measurement of \( D_2 \) is used. For this specific measurement the experiment with both detectors is equivalent to the experiment \( E_2 \) with only one detector \( D_2 \). The Weak Conditioning Principle requires that inference of the position should be the same in both experiments. The presence of a detector which is not used should not matter.

However, there exist reservations against the proof of the LP and some prominent statisticians do not believe in it. Barnard and Birnbaum, originally promoters of the LP, ultimately came close to rejecting it or to strongly restrict its applicability. One of the reasons for rejecting the LP is its incompatibility with classical concepts. We will come back to some of the most disturbing examples. Other criticism is related to questioning the Sufficiency Principle and to unacceptable consequences of the LP in specific cases. Most statisticians, frequentists and Bayesians, usually accept that the likelihood function summarizes the experimental information but some statisticians like Barnard feel that parameter inference should include system information like the pdf or, if relevant, the condition applied to stop data taking (see below).

Independent of the formal proof, the LP can be justified by simple arguments.

The LP almost follows from the optimal performance of the likelihood ratio test for a discrete hypothesis. It is hardly avoidable if the concept of a prior probability density for the parameter is accepted. Then Bayes’ theorem can be used to deduce the probability density \( g(\theta | x) \) of the parameter \( \theta \) conditioned on the outcome \( x \) of an experiment (see

\[ ^{17} \text{A statistic } t \text{ is sufficient for a parameter } \theta, \text{ if the distribution of a sample given } T \text{ does not depend on } \theta. \]
Bayes’ theorem is a simple consequence of probability calculus and accepted by all statisticians. For known prior information \( \pi(\theta) \), the distribution \( g(\theta|x) \) contains all we know about \( \theta \). We can compute the expectation value for the mean, all other moments and probabilities for arbitrary intervals\(^{18} \). Since \( \pi \) does not depend on \( x \) the full sample information is contained in \( L \). If we accept that \( L(\theta|x) \) contains the full sample information about \( \theta \) regardless of the known prior, then we also have to accept that if \( \pi(\theta) \) is unknown, all information is contained in the likelihood function.

There are two possibilities to escape these conclusions based on Bayes’ Theorem:

- We can deny the existence of the prior density. In deed, at first glance it is not obvious what meaning we should attribute for example to a prior density of the muon neutrino mass but to derive LP it is not necessary to assume that the prior \( \pi \) is known, it is sufficient to assume that it exists, that God has chosen this mass at random according to an arbitrary distribution \( \pi(\theta) \) which we do not know, or in other words that in the big bang a random process has fixed the particle masses. Such an assumption would certainly not affect our scientific analysis techniques.

- We can argue that \( g(\theta|x) \) is not all we want to know about \( \theta \). In this case we have to demonstrate that the information missing in \( g \) is relevant to inference of \( \theta \).

There is one point of caution: The integral \( \int L(\theta|x)\pi(\theta)dx\,d\theta \) has to be finite and the prior parameter density has to be normalizable. Thus in some cases the assumption of an improper uniform prior extending over an infinite parameter range can lead to problematic results. In practice, this is not a problem. For example, restricting the Higgs mass to positive values below the Planck mass would be acceptable to every educated scientist.

The formal proof of the LP does not require the existence of a prior.

5.2 Some objections to the Likelihood Principle

5.2.1 The likelihood function does not explore the full sample space. One of the objection to the validity of LP is that the likelihood function cannot contain all relevant information because it is not possible to compute frequentist confidence intervals from the likelihood function alone.

In some occasions, like in Example 19, we know the prior density and inference on the parameter \( \theta \) can be based on Bayes’ Theorem. Bayes’ Theorem allows us, using Eq. (11) or equivalently Eq. (16) to compute the full pdf \( g(\theta) \) and the probabilities to contain \( \theta \) for arbitrary intervals. On the other hand the information \( L(\theta|x), \pi(\theta) \) entering in Equ. 16 is not sufficient to compute the coverage of these intervals. As a consequence, coverage intervals must rely on elements of information which are irrelevant to \( g(\theta) \). Full information relative to \( \theta \) does not imply full information relative to coverage. This conclusion is independent on whether we know the prior or not. The fact that coverage

\(^{18}\)It is interesting to notice that the sample pdf does not enter in Relation 16.
cannot be computed from the likelihood function is not a valid argument against the LP.

Another argument against the frequentist objection is the following: Assuming that information relevant for parameter inference is missing in the likelihood function of small samples, we hardly can imagine that by combining the likelihood functions of many small samples to a large sample the missing information is recovered. Therefore also the likelihood function of large samples should be insufficient to compute coverage intervals. However, in the limit of large samples, the likelihood function usually approximates a Gaussian and allows the derivation of frequentist intervals without requiring the pdf.

The violation of the LP by classical methods does not imply that those are wrong. The latter address a different question. Their goal is to provide coverage while the application of the LP is restricted to parameter inference.

5.2.2 Inference of Gaussian parameters from a single observation. Inferring the mean $\mu$ and the width $\sigma$ of a Gaussian from a single observation $x$ we realize that the likelihood function is infinite for $\mu = x, \sigma = 0$ which implies this solution with certainty if we apply the LP. This was one of the examples that had cast doubt on Birnbaum’s believe in the LP [57]. However, close inspection reveals that this situation cannot occur. No measurement can be described by a Gaussian with zero variance.

**Example 24** When we turn Birnbaum’s Gaussian pdf into a more realistic pdf

$$f(x|\theta, \sigma) = \frac{1}{\sqrt{2\pi(\sigma^2 + s^2)}} \exp\left[-\frac{(x-\mu)^2}{2(\sigma^2 + s^2)}\right]$$

where we interpret $s$ as the known experimental resolution, we still get a maximum of the likelihood function at $\mu = x, \sigma = 0$. For $s = 1$ and an observation at $x = 0$ we find for the log-likelihood

$$\ln L = -0.5 \ln(\sigma^2 + 1) - \frac{\mu^2}{2(\sigma^2 + 1)} + \text{const.}$$

which has a narrow peak but also a long tails in $\sigma$ and does not contradict our intuition. Figure 22 shows the likelihood contours.

**Example 25** We may modify Birnbaum’s example further, fix the parameter $\mu$ to $\mu = 0$ and assume $x = 0$. This observation which hits exactly the prediction is likely if the value of $\sigma$ is small. The log-likelihood function is shown in Figure 22. The 1, 2 and 3 st. dev. likelihood ratio limits are $\sigma_1 < 1.31, \sigma_2 < 7.32$ and $\sigma_3 < 90$. Classical intervals would include all values of $\sigma$ independent of the confidence level since the observation is obviously compatible with any $\sigma$.

The LP does not contradict the frequentist result. It just states that all information on $\sigma$ is in the likelihood function. Certainly, we learn something about $\sigma$ when we observe a $x - \mu = 0$, information which is completely lost in frequentist intervals but partially conserved in likelihood ratio intervals.
Fig. 22. One, two and three st. dev. likelihood ratio contours (left) and log-likelihood for $\mu = 0$ as a function of $\sigma$, Example 24

Fig. 23. Rate measurement. The time sequence is stopped when 3 events are observed within 1 second (indicated by a bar) and a new measurement is started. Since the combination of many conditioned measurements is equivalent to a long unconditioned measurement, this stopping rule cannot introduce a bias

5.3 The Stopping Rule Paradox

The likelihood function is independent of the sequence of independent and identically distributed observations. Thus, since according to the LP parameter, inference should solely be based on the observed sample it should be independent of any sequential sampling plan \cite{50}. For example, stopping data taking in an experiment after a “golden event” has been observed should not introduces a bias. This contradicts our naive intuition and corresponds to the so-called Stopping Rule Paradox. Similarly, some people believe that one can bias the luck in a casino by playing until the balance is positive and stopping then.

The Stopping Rule Principle is of considerable importance for experimental tech-
Frequentist and Bayesian confidence intervals

Fig. 24. Likelihood for the decay rate. Left hand: Four events are observed in one time unit. The classical error limits depend on the stopping condition i.e. fixed time interval or fixed event number. Right hand: Same evaluation for one event.

Frequentists claim that stopping rules introduce biases and consequently deny the LP. One has to admit that the Stopping Rule Principle is hard to digest.

It is easy to see that there is no bias in the example quoted above: Let us imagine that we record experimental observations for infinitely long time where many “golden event” are recorded. The experiment now is cut into many sub-experiments, each stopping after a “golden event” and the sub-experiments are analyzed separately. Since nothing has changed, the sub-experiments cannot be biased and since the sum of the log-likelihoods of the subsamples is equal to the log-likelihood of the full sample it is also guaranteed that combining the results of a large number of experiments performed with an arbitrary stopping rule asymptotically give the correct result. Of course the condition that the subsamples are unbiased is necessary but not sufficient for the validity of the Stopping Rule Principle. The effect of the stopping rule “stop when 3 events are found within 1 second” is presented in Fig. 23.

In the following example we explicitly study a specific stopping rule.

Example 26 In a rate measurement 4 events have been observed within the time interval $t$. Does the uncertainty on the rate $\theta$ depend on the two different experimental conditions: a) The observation time had been fixed. b) The experiment had been stopped after 4 events. In case a) the uncertainty is due to the event number fluctuation and in b) to the time variation. The LP denies any difference, only the data actually seen matter, while for a classical treatment also the data that could have been observed are important. The likelihood functions $L_a, L_b$ derived from the Poisson distribution and the decay time distribution, respectively, are proportional to each other and depend only on

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19Edwards, Lindman, Savage [59]: “The irrelevance of stopping rules to statistical inference restores a simplicity and freedom to experimental design that had been lost by classical emphasis on significance levels ... Many experimenters would like to feel free to collect data until they have either conclusively proved their point, conclusively disproved it, or run out of time, money, or patience.”
the observation time and the number of events seen (see Fig. 24):

\[ L_a(\theta, n) = P(n, \theta t) = e^{-\theta t} \frac{(\theta t)^4}{4!} \propto \theta^4 e^{-\theta t} \]

\[ L_b(\theta, t) = \frac{t^3 \theta^4}{3!} e^{-\theta t} \propto \theta^4 e^{-\theta t} \]

This example is well suited to explain the essence of the LP. Followers of the LP would bet the same amount of money that \( \theta \) is located in a certain arbitrarily selected interval in both experiments.

The stopping rule may be tested by a Monte Carlo simulation. In the previous example we could select two arbitrary rate values \( \theta_1 \) and \( \theta_2 \) and simulate a large number of the two kinds of experiments. For the experiments of type a) only results with 4 events found are retained and the ratio of successes \( R_a \) for the two values of \( \theta \) is formed. For the experiments of type b) a small time slice around \( t \) is fixed and \( R_b \) is formed from the number of cases where four events are recorded. The two ratios should be equal if the information relative to the parameter is the same in both variants. Actually, a simulation is not necessary. The quantities \( R_a \) and \( R_b \) are the likelihood ratios which agree because the likelihood functions are the same up to a constant factor. The stopping rule does not favor one or the other of the \( \theta \) values. There is no bias.

A classical treatment produces inconsistent results for the two equivalent experiments. The error limits depend on the way we are looking at the data (Fig. 24).

The intuitive explanation for the independence of inference of a sequential stopping rule indicates also its limitations. The stopping rule has to be simple in the sense that the different pieces obtained by cutting an infinitely long chain of observations cannot be classified differently. Experiments stopped when the result is significant, when for a long time no event has been recorded or when money has run out should be analyzed ignoring the reason for stopping data taking.

The following example cited in the statistical literature is more subtle. Basu presents a detailed discussion [60].

**Example 27** We sample data \( x_i \) following a Gaussian with unknown mean \( \theta \) and width equal to one. The mean \( \bar{x} \) is formed after each observation. The experiment is stopped after observation \( n \) when one of the following conditions is fulfilled:

\[ |\bar{x}| > \frac{2}{\sqrt{n}}, \text{ or } n = 1000 \quad (17) \]

The idea behind this construction is to discriminate the value \( \theta = 0 \) which will be off by 2 st. dev. in all cases where the first condition is realized. (One may want to stop clinical trials when a 2 st. dev. significance is reached for the effectiveness of a certain drug.) The second condition is introduced to avoid extremely large samples for \( \theta = 0 \) (non-performable experiments). Let us assume that an experiment produces an event of size \( n = 100 \) and \( |\bar{x}| = 0.21 > 2/\sqrt{100} \). When we ignore the stopping condition a frequentist would exclude the parameter value \( \theta = 0 \) with > 95% confidence (tail probability). Knowing the stopping rule, he would realize that the first of the two conditions 17 has been fulfilled and probably be willing to accept \( \theta = 0 \) as a possible value. Wouldn’t we
include the stopping condition into our considerations? Basu [60] and also Berger and Wolpert [52] deny this and argue that our intuition is misled. In fact, the likelihood at $\theta = 0$ is not really reduced by the stopping rule, it is the integrated tail which is small, because the likelihood function becomes narrower with increasing $n$.

In the last example certainly is not easy to accept the likelihood solution and it is less the problem to understand that $\theta = 0$ is not excluded but rather to accept that some value different from zero has a very large value of the likelihood even when $\theta = 0$ is correct.

The stopping rule changes the experiment and some rules are not very useful. But this is not in contradiction to the fact, once the data are at hand, knowing the stopping rule does not help to improve the inference of the parameter of interest.

### 5.4 Stein’s example

In 1960, L. J. Savage emphasized [61]: “If the LP were untenable, clear-cut counter-examples by now would have come forward. But such examples seem, rather, to illuminate, strengthen, and confirm the principle.” One year later C. Stein [62] came up with his famous example which we will discuss in this section. Since then, other more or less exotic counter-examples have been invented to disprove the LP. The corresponding distributions exhibit strange infinities and are far from what we can expect in physics. Nevertheless, they are very instructive.

Stein has been introduced the probability density

$$f(X, \theta) = \frac{a}{X} \exp \left\{ -100 \frac{(\theta - X)^2}{2X^2} \right\}, \quad \text{for } 0 \leq X \leq b\theta$$

where for simplicity we have fixed the slope parameter in the exponent.

The functional form resembles a Gaussian with width proportional to the mean value as shown in Fig. 25a and 25b but it has a long tail towards large values of $X$ which completely dominates the distribution. The range of $X$ is restricted by the cutoff parameter $b$ to obtain a normalizable density. Since the $1/X$ term almost insures convergence the upper limit of $X$ may be rather large for not too large $a$. The two constants $a$, $b$ are fixed by the normalization condition and the requirement that $X$ exceeds $\theta$ by at least a factor of ten in 99% of the cases.

$$\int_0^{b\theta} f(X, \theta)dX = 1$$

$$\int_{10\theta}^{b\theta} f(X, \theta)dX = 0.99 \quad (18)$$

The cutoff parameter is huge $b\theta > 10^{10^{10^{52}}}$ and $a \approx 0.04$. Figure 25a,b are plots of Stein’s function with the specific choice $\theta = 5$. Only about 1% of the $X$-values lie inside the bell shaped part ($X < 50$) of the probability density, the remaining part is located in the long right hand tail.
Fig. 25. Stein’s test function (a,b) with a long tail towards large \( x \). The maximum is close to the parameter value. The Gaussian likelihood function for an observation \( x = 8 \) is shown in (c).

5.4.1 The paradox and its solution. For a single observation \( x \) the likelihood function for the Stein pdf is:

\[
L(\theta) \sim \exp \left\{ -100 \left( \frac{\theta - x}{2x^2} \right)^2 \right\}, \quad \text{for} \quad x/b < \theta < \infty
\]

It is proportional to the likelihood function of a Gaussian centered at \( x \), with width \( s = x/10 \) and restricted to positive \( \theta \). It is displayed in Fig. 25c for \( x = 8 \). (There is a small difference in the validity range of \( \theta \) for the Gaussian and Stein’s distribution which numerically is of no importance.)

If the likelihood function contains the full information relative to the parameter, the inferences on \( \theta \) should be the same for the very different distributions, the Gaussian and the Stein function. However, one might conclude from Eq. (18) that the Stein parameter \( \theta \) is 10 times smaller than the observation \( x \) in 99% of the cases, while the Gaussian case would favor a parameter in the vicinity of the observation [62]. It seems silly to select the same confidence interval in both cases.

The solution of Stein’s paradox can be summarized as follows:

- The LP does not relate different probability densities. It just states that the like-
likelihood function contains the full information relative to the unknown parameter. Thus there is no contradiction in the fact that the same likelihood belongs to two different probability densities.

- The assertion “from $X > 10\theta$ in 99% of the cases for given $\theta$, independent of the value of $\theta$, follows that for given $x$ we have $\theta < x/10$ in 99% of the case, independent of the value of $x$” is not conclusive.

- Related to the last point: The same $\theta$ interval corresponds to very different coverages in the two cases, Gaussian and Stein pdf. Coverage, however, is a frequentist concept which is not computable from the likelihood function. This is not specific to Stein’s example and thus not relevant here.

It is easily seen that for any proper (normalizable) prior density the inferences for the Gaussian and the Stein cases should be identical while the classical intervals are rather strange in some cases.

Let us look at an example: We select a uniform prior function $\pi(\theta) = 0.1$ and $0 < \theta < 10$. In most cases one would get $x$ much larger than $\theta$, say $x = 10^{1000}$. Obviously, we cannot learn much from such an observation, a fact which translates into a likelihood function which is completely flat in the allowed $\theta$ range:

$$L = \exp \left\{ -100 \frac{(\theta - x)^2}{2x^2} \right\}$$

$$\sim \exp \left\{ -100\theta/x \right\} \approx 1$$

The same result would be obtained for a Gaussian pdf, except that the occurrence of very large $x$ is rare.

Now assume $x = 5$. Then

$$L(\theta) \sim \exp \left\{ -\frac{(\theta - 5)^2}{2 \cdot 0.5^2} \right\}, \quad \text{for } 5/b < \theta < 10$$

is a Gaussian of width $s = 0.5$ and we guess that $\theta$ is near to $x$. In both cases, for the Gaussian pdf and the Stein pdf the results derived from the likelihood function are very reasonable. The difference between the two is that in the former case likelihood functions centered around small $x$ are frequent and in the latter those centered at large $x$, but for a given observation this is irrelevant. The reader is invited to invent other prior densities and to search for inconsistencies in the Bayesian treatment.

The argument of Stein relies on the following frequentist observation. Assume $\theta$ values are selected in a range $\theta < \theta_{\max}$. Then in 99% of all cases the likelihood function would favor $\hat{\theta} \approx x > 10\theta_{\max}$, an estimate which is considerably worse than the classical one. The flaw of the argument is due to the inconsistency in selecting specific test parameters $\theta$ and using a uniform prior of $\theta$ extending to some $10^{(10^{20})}\theta_{\max}$.

### 5.4.2 Classical treatment.

What would a classical treatment give for central 99% confidence intervals?
\[
\int_{x}^{0.005} f(X, \theta_{\text{low}}) dX = 0.005 \Rightarrow \theta_{\text{low}} \ll x
\]
\[
\int_{0}^{x} f(X, \theta_{\text{high}}) dX = 0.005 \Rightarrow \theta_{\text{high}} \ll x
\]

For any reasonably small \(x\) both limits would be nearly zero. For very large \(x\) the classical procedure produces a rather wide \(\theta\) interval. Qualitatively the classical interval fails to contain the true value in the 1% cases where the observation falls into the bell shaped part of the distribution but produces a safe result in the remaining 99% where \(x\) is located in the tail. Thus the correct coverage is guaranteed but in some cases ridiculous error limits have to be quoted. This is the well known problem of classical statistics: It can produce results that are known to be wrong. In the remaining cases the interval will be enormously wide and extend to extremely large values.

**Example 28** A SUSY particle has a mass of \(\theta = 1\) eV. A physicist who does not know this value designs an experiment to measure the mass in the range from 0.001 eV < \(\theta < 1\) TeV through a quantity \(x\) depending on \(\theta\) according to the Stein distribution. (It is certainly not easy to determine a parameter \(\theta\) over 15 orders of magnitude from a quantity \(x\) which may vary over \(10^{20}\) orders of magnitude.) A 99% confidence level is envisaged. A frequentist analysis of the data will provide wrong limits \(0 < \theta \ll 0.1\) eV in 1% of the cases and huge, useless intervals in the remaining ones (except for a tiny fraction). In contrast, a Bayesian physicist will obtain a correct and useful limit in 1% of the cases and a result similar to the classical one in the remaining cases.

It is impossible to invent a realistic experimental situation where the Bayesian treatment of the Stein problem produces wrong results. The Stein function plays with logarithmic infinities, which cannot occur in reality. Limiting the uniform prior to a reasonable range or using other normalizable prior densities avoids the paradoxical conclusion of Stein. Experimental conditions always forbid improper prior densities.

**5.5 Stone’s example**

Another nice example has been presented by M. Stone \[63\] which is presented here in simplified form. The Stone example is much closer to problems arising in physics than the rather exotic Stein Paradox.

**Example 29** A drunken sailor starts from a fixed intersection of streets and proceeds at random through the square net of streets oriented along the directions N, W, S, E (see Fig. 26\[21\]). At a certain intersection \(x\) he stops. The problem is to guess the last crossing before the stop, i.e. the direction. We name the four possible origins n, w, s, e. Starting in a random direction from e, the probability to arrive at \(x\) is 1/4. Thus the likelihood for e is also 1/4. The same likelihoods apply for the other three locations. With a “non-informative” prior for the locations, one has to associate equal probabilities to all four possibilities. This is in contradiction to the correct intuition that a position between the starting point and the stop is more likely than 1/4.

\[^{20}\text{Any other normalizable prior would produce very similar results.}\]

\[^{21}\text{The analogy to physics is not between the sailor and drunken physicists but between his random walk and diffusion.}\]
The example does not directly involve the LP but it questions inference based solely on the likelihood function. Here, the solution is rather simple: There is information about the prior and it is clearly not uniform. (In the original version of the example the prior has an even stronger influence.) Including the prior information, and using the constant likelihood we obtain a correct result.

It is not clear, what a classical solution of the problem would look like.

The fact, that so far no simple counter-example to the LP has been found provides strong support to this principle.

5.6 Goodness-of-fit tests

Significance tests cannot be based on the LP since there is no parameter differentiating between the hypothesis at hand and the rather diffuse alternatives. For this reason they have been criticized especially by Bayesians and some statisticians adhering to the LP. However, as long as no better alternatives are available, classical methods should be used. Goodness-of-fit tests like the Neyman-Pearson or Kolmogorov tests are very useful and cannot easily be replaced by likelihood based recipes. Note that also here the subjectivity problem is present. The binning has to be chosen according to the Bayesian expectation of possible deviations. A rough binning neglects narrow deviations and with fine binning in the Neyman-Pearson test the statistical fluctuations hide systematic deviations. Also the fact that we use one-sided tests has a Bayesian origin.

The approach to significance tests and classical confidence limits is very similar, but significance tests are not related logically to interval estimation.

5.7 Randomization

Randomization is an important tool in many statistical applications like clinical tests and survey studies. For example, we might select randomly fifty CERN physicists and ask them their opinion on closing down the LEP machine. It might turn out that by accident the majority of the selected physicists are involved in LEP experiments. This post-
experimental information has to be ignored in a frequentist approach in contradiction to the LP but explains the outcome.

Strong criticism of randomization is expressed by Basu [67] and it seems obvious that with a good unbiased judgement one should be able to get better performance than by random selection. Yet, there are cases where this classical procedure is very useful - think of Monte Carlo simulation - and especially for experiments with large statistics the Bayesian objections are less convincing. This point of view is shared by prominent Bayesians like Savage [61]: “The theory of personal probability ... does lead to new insight into the role and limitations of randomization but does by no means deprive randomization of its important function in statistics.”

In conclusion, there are useful frequentist concepts which are not respecting the LP. We should neither exclude these methods nor use them as an argument against the LP. Goodness-of-fit tests and randomization methods have no bearing whatsoever on parameter interval estimation for a given pdf.

5.8 Precision and consistency

Following the LP we can fix an ordering principle for precision.

Two measurements $E_1$, $E_2$ of the same parameter are equally precise if their likelihood functions $L_1(\theta)$ and $L_2(\theta)$ are proportional to each other. $E_1$ is more precise than $E_2$ if they have the maximum at the same parameter value $\theta_{\text{max}}$ and if $L_1(\theta) < cL_2(\theta)$ for all other values of $\theta$ where the normalization constant $c$ is fixed by $L_1(\theta_{\text{max}}) = cL_2(\theta_{\text{max}})$. The narrower the likelihood function is, the more precise is the measurement. This requirement should be acceptable to all statisticians. We could extend our modest requirement to a general definition but then it would single out a specific statistical method.

A statistical approach is inconsistent if it associates different error intervals to equally precise measurements or if it produces smaller error intervals for less precise measurements than for more precise ones.

6 Comparison of the methods

The quality of a confidence interval is measured

- in the classical approach by coverage, the average number of intervals containing the true value of a parameter,
- by the likelihood ratio in likelihood ratio intervals,
- by the probability obtained by integrating likelihood times uniform prior over the interval.

Likelihood ratio and Bayesian intervals are related numerically. The standard likelihood ratio intervals corresponds to 68.3% Bayesian probability in the parameter space where the likelihood function is Gaussian and the prior is uniform.
6.1 Difference in philosophy

Before we compare the frequentist methods with the likelihood based approaches in detail, let us come back to the example (see Fig. 1) presented in the introduction which is repeated in more detail as Example 13/14.

Frequentists test the compatibility of data with a parameter and independent of details of the theoretical prediction, they want to be right in a specified fraction of cases. The confidence level is a kind of “inclusion probability” of the correct parameter value inside the interval and is fixed. The “exclusion probability” of wrong parameter values which depends on the width of the probability distribution is at least partially ignored in the classical approaches. In the language of discrete parameters one could say that the “error of the second kind” is not fully considered. The wider the distribution is, the likelier it is to include a wrong parameter in the confidence interval.

Since the confidence interval is based on an integration of the pdf it depends on data that potentially could have been observed. The probability to observe the actual value \( x \) is not enough for classical reasoning. Intuitively, one would find the two parameter values \( \theta_1 \) and \( \theta_2 \) which satisfy \( f(x|\theta_1) = f(x|\theta_2) \) equally acceptable, but the non locality of the frequentist coverage introduces a difference.

On the other hand in concepts based on the likelihood function only the value of the pdf at the observed data is important. The methods are local in the sample space. To illustrate the idea behind it, it is simpler to argue with discrete variables.

Example 30 Assume, we have a bag with many dice of seven different kinds, all differently biased, except for die type “7” which is unbiased. We do not know the number of dies of each kind. Each of the biased dies favors a different number with probability \( \frac{1}{2} \). The remaining numbers have probabilities of \( \frac{1}{10} \). One of the dies of unknown type is selected and thrown. We observe the number “3” and have to estimate the type.

The following table contains the probabilities \( p(3|\text{type}) \) to observe “3” for the seven dies. Obviously, we would select die “3” and we would not care about the probabilities \( p(1), p(2), p(4), p(5), p(6) \) for alternative outcomes. Thus we would base our decision on the observation only and not consider the remaining sample space.

| die type | 1 | 2 | 3 | 4 | 5 | 6 | 7 |
|----------|---|---|---|---|---|---|---|
| \( p(3|\text{type}) \) | 0.1 | 0.1 | 0.5 | 0.1 | 0.1 | 0.1 | 1/6 |

If we would repeat the experiment many times with the same die, we would always select one of the first six die types and never die “7”. Thus a frequentist would argue that the procedure is inadmissible because the procedure does not provide equal coverage to all hypotheses. A Bayesian would not care about long term coverage. He wants to make the optimum decision in the present case and select the die which gives the largest likelihood. Why is long term coverage not an issue? The Bayesian updates his information by multiplying the likelihoods of the individual trials and after some 20 experiments, he then, if “7” applies would probably find for die “7” a higher likelihood than for the other dies.

Let us look at another very extreme example.

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22 Error of the second kind: Accepting a hypothesis when it is false.
Example 31 An electronic code reader is able to identify the number 0.45301. For any other input number it will produce a random output $\theta$ between zero and one. Both, the sample variable $X$ and the parameter $\theta$ are restricted to the interval $[0,1]$. For the sake of the argument, let us assume that the device has infinite resolution, and that numbers have an infinite number of digits.

$$f(X|\theta) = \begin{cases} 
\delta(X - \theta) & \text{for } \theta = 0.45301 \\
1 & \text{for } \theta \neq 0.45301 
\end{cases}$$

The observation is $x = 0.45301$. The classical confidence interval would be the full interval $0 \leq \theta \leq 1$. The Bayesian result would be $\theta = 0.45301 \pm 0$ with 100% confidence. I believe, everybody would intuitively support the Bayesian conclusion.

Classical confidence intervals are not well qualified for decision making. Even advocates of the classical concept admit that for decision making classical limits may not be optimum 1. The question is then, what else should they be used for? Frequentists, however, argue that the intention of inference is not necessarily to optimize decisions. Kendall and Stuart 68 write: “Some writers have gone so far as to argue that all estimation and hypothesis-testing are, in fact, decision-making operations. We emphatically disagree, both that all statistical inquiry emerges in decisions and that the consequences of many decisions can be evaluated numerically.”

Narsky 69 who compares several different approaches to the estimation of upper Poisson limits, states: “There is no such thing as the best procedure for upper limit estimation. An experimentalist is free to choose any procedure she/he likes, based on her/his belief and experience. The only requirement is that the chosen procedure must have a strict mathematical foundation.” This opinion is typical for many papers on confidence limits. However, “the real test of the pudding is in its eating” and not in the beauty of the cooking recipe. We should state what we aim for and should not forget that what we measure has practical implications, hopefully!

6.2 Relevance, consistency and precision

A. W. F. Edwards writes 21: “Relative support (He refers to a hypothesis or a parameter) must be consistent in different applications, so that we are content to react equally to equal values, and it must not be affected by information judged intuitively to be irrelevant.” We can check whether we consider information as “irrelevant” when we consider betting odds. When the amount of money we are ready to bet that $\theta$ is in a certain interval is independent of part of the available information, then this information is considered irrelevant.

The most obvious example for the violation of this principle in all classical approaches is the Poisson case with background expected but where no event is observed (Examples 11, 12). Other examples are related to the dependence of classical results on the sampling plan (Example 26) For this reason alone, classical limits are to be discarded as a useful description of uncertainty.

Formally, the inconsistency of classical limits, the fact that different limits are obtained in equivalent situations manifests itself as a violation of the LP which requires equal parameter inference for equal likelihood functions. In the Poisson case 32 for $n$ events found and $b$ background events expected, the likelihood function for the signal
parameter $\mu$ is

$$L(\mu) \sim \sum_{b'=0}^{n} P(b'|b)P(n-b'|\mu)$$

and for $n = 0$ it reduces to

$$L(\mu) \propto e^{-\mu}$$

independent of the background expectation. In Fig. 16 the likelihood function is compared to the classical and Bayesian results.

Similarly, different stopping rules which produce identical likelihood functions lead to different classical limits (Example 26). Another example is presented by Berger and Berry [70].

In the previous section we discussed the notion of precision and established an ordering principle. This principle is violated in classical statistics in our standard Poisson example: An experimental result of zero events $n = 0$ found with background expectation $b = 0$ is clearly more exclusive than a result $n = 1$ with $b = 3$. This obvious conclusion based on common sense is confirmed by the formal argument that the measurement observing $n = 0$ is the more precise because the likelihood function $L(\theta|n = 0, b = 0)$ is steeper than $L(\theta|n = 1, b = 3)$ for all values of $\theta$. The corresponding 90% upper confidence limits 2.44 and 1.88 of the unified approach [3] invert the sequence of precision.

All problems in the frequentist approach have the same origin: The limits depend on the full sample pdf. However, there is no reason why we should care about the probability of events that have not occurred.

These statements should not be misunderstood. The classical approach in itself is not inconsistent but it does not provide a consistent measure of uncertainty.

The deficiency of classical upper limits is also recognized by some frequentists. They accept that the classical confidence intervals are not always useful measures of precision. But, what else should they be used for? To cure the problem, Feldman and Cousins [3] propose to supplement the confidence limit by an additional quantity called sensitivity. However, they do not explain how to combine the two quantities to produce a sensitive measure for the relative precision of different experimental results and how to use the confidence interval to check the compatibility of the measurement with a theoretical prediction.

Bayesian methods are in agreement with the LP and respect the consistency property. Problems may occur for probability densities with multiple maxima when the prior density is updated with increasing event number [71]. These exotic cases are not relevant in real physics problems and cannot be handled by classical methods either. Complicated situations should be represented by likelihood maps.

In the limit that the assumption of a uniform prior density is correct, likelihood ratio intervals are optimum: For a given interval length the probability to contain the true parameter value is maximum. In other words, avoiding the notion of prior density, the likelihood interval contains the parameter values best supported by the data.

\footnote{Obviously, frequentists realize that important information is not contained in the frequentist limits interval.}
Classical methods hardly emphasize precision. Nevertheless they discuss “minimum length” and “likelihood ratio” intervals. Clearly, classical intervals cannot be optimum when they violate the LP because then they ignore available information. For example, it is easy to improve negative Poisson limits or unphysical intervals. Qualitatively, the intervals from the unified approach are expected to be superior to other classical intervals with respect to precision.

Frequentists sometimes argue that the performance of different approaches should not be compared looking at specific examples but that it is the average performance which is relevant. On the other hand, also the average performance is improved if more reasonable solutions are implemented in individual disturbing cases. Why should it harm to modify intervals like zero length intervals which with certainty do not include the true value?

6.3 Coverage

In the classical approach we have the attractive property that a well known fraction of experimental results contain the true value of a measured parameter within the quoted error limits. As explained in the introductory example, coverage is a democratic principle which gives different true parameter values the same chance to be included in a confidence interval.

Major criticism of the classical concepts is related to the requirement of pre-experimental definition of the analysis methods necessary to guarantee coverage. Conditioning on the actual observation is forbidden. However as shown by Kiefer [72], conditioning and coverage are not always exclusive.

On the other hand for an individual experiment we cannot deduce from the computed coverage a probability that the result is true and it is the latter we need to make decisions.

Example 32 An experimenter tosses a coin to decide whether the Higgs mass is larger or less than 100 GeV and finds that it is larger. The confidence level is 50%. It would be stupid to deduce from this “observation” a probability of 50% for the Higgs mass to be larger than the arbitrarily selected mass value of 100 GeV. Confidence is deduced from zero information.

The admiration of coverage by many physicists is due to an illusion: They inadvertently mix coverage with the probability that the true value of the parameter is located inside the confidence interval even if they intellectually realize the difference. In reality, the only possible way to derive such a probability is to invent a Bayesian prior to multiply it with the likelihood function and to integrate the product over the confidence interval. We cannot do any better. On the other hand, coverage is not a useless quality as some Bayesians claim. Coverage intervals retain a large fraction of the information contained in the likelihood function.

Coverage is a property of an ensemble of experiments and makes sense if an experiment is repeated many times. Let us assume that we have 10 experiments measuring with different precision a particle mass and providing 90% confidence intervals each. It will not be probable that more than one or two of the limits will not contain the true value.

Insurance companies may rely on coverage.
value. This will certainly give us an idea where the true value may be located, but a quantitative evaluation is difficult.

Although it is quite rare in physics applications that we have an ensemble of similar experiments, let us assume that this is the case. What would we do with our results? We would probably not be satisfied contemplating the different confidence intervals but try to combine them\textsuperscript{25}. If possible, we would go back to the original data, combine them to a high statistics experiment and then forget about the individual data sets. Thus, we have again a single experiment. There is no obvious reason to consider ensembles. Otherwise we would subdivide high statistics experiments in many low statistics measurements. In conclusion, the problem of parameter inference can be discussed on the basis of single experiments.

The violation of coverage due to the separate treatment of upper limits and intervals was the main motivation for the development of the unified approach. In the years before the adoption of this new scheme, rare decay searches usually presented Bayesian upper limits - not intervals - when the result was compatible with background. It is hard to detect negative consequences from the former procedure to the progress of physics.

The main problems with the coverage paradigm are the following:

- Coverage often is only approximate. There is complete overcoverage in Poisson distributed data with mean zero and in digital measurements.
- The usual treatment of nuisance parameters\textsuperscript{23} can lead to undercoverage.
- It is difficult to retain coverage when results are averaged.
- The principle is not universally applied. When the prior density is known, like in Example 19 the coverage requirement is put aside.

Classical confidence cannot be attributed to intervals based on the likelihood function. The PDG\textsuperscript{12} gives the advice to determine the true coverage by a Monte Carlo simulation. It is not possible to associate a single classical confidence level to an arbitrary interval. Of course, coverage as a function of the true value can be computed but it is not very economic to first compress a measurement into an estimate and an error interval and the to complement it by a function.

### 6.4 Invariance under variate and parameter transformations

We consider the following non-linear parameter transformation $\theta' = u(\theta)$ since linear transformations do not pose problems.

\[ \hat{\theta}' = u(\hat{\theta}) \]
\[ \theta'_{\text{low}} = u(\theta_{\text{low}}) \]
\[ \theta'_{\text{high}} = u(\theta_{\text{high}}) \]

Clearly, the probabilities $P(\theta_{\text{low}} < \theta < \theta_{\text{high}})$ and $P(\theta'_{\text{low}} < \theta' < \theta'_{\text{high}})$ are the same.

In addition, we may transform the sample space variables and consequently also the probability densities $f(X) \longrightarrow g(X')$.\textsuperscript{25}Insurance companies cannot do this.
Invariance means that i) the probability and ii) the interval limits are the same independent of the initial choice of the parameter $\theta$ or $\theta'$ for which we compute the confidence interval and independent of the sample variable to which the definition applies.

a) In the frequentist scheme both conditions are satisfied with the likelihood ratio ordering used in the unified approach and in the conventional scheme when central intervals are chosen, a choice which is restricted to the single variate case. Equal probability density intervals defined in $X$ usually differ from probability density intervals in $X'$. Shortest confidence intervals depend on the parameter choice.

General transformations of a multi-dimensional sample space may lead to concave probability contours and ruin the whole concept.

Conceptually the parameter and sample variable dependence is acceptable: The parameters and the sample variables have to be chosen pre-experimentally in a reasonable way independent of the result of the experiment similarly to all the other analysis procedures in the classical method. Nevertheless, it is disturbing that a physicist’s choice to determine a confidence interval from a mass squared distribution instead from a simple mass distribution may produce different limits. Thus the likelihood ratio ordering which is free of this problem is certainly to be preferred to the other classical methods.

b) Likelihood ratio intervals are strictly invariant under parameter transformations. The support by data is independent of the choice of the parameter. It is also invariant against transformations of the sample variable.

c) The Bayesian method conserves probability if the prior is transformed according to:

$$\pi'(\theta')d\theta' = \pi(\theta)d\theta$$

Of course not both prior densities $\pi$ and $\pi'$ can be uniform. The invariance of the probability is guaranteed, but the size of the interval depends on the primary parameter choice for which we required $\pi(\theta) = \text{const}$. With our requirement of using uniform priors, the Bayesian prescription is not invariant under transformations of the parameter.

The fact that the choice of a parameter space affects the result of an analysis is quite common. Very useful parameters like root mean square errors are not invariant. The success of inference procedures like pattern recognition strongly relies on the adequate selection of the observation space. We use Dalitz plots to detect resonances above a smooth background, $r - \phi$ plots to find particle tracks in collider experiments, rapidity, $q^2$, $x$ distributions etc.. Part of data analysis skills consists in selecting the right variables and often results rely on an educated choice.

I find it rather natural that a scientist chooses not only the selection criteria but also the parameter and sample space variables. In many cases there is quite some common agreement on a reasonable choice (for example $1/p$ for tracking, $m^2$ for neutrino mass limits, $\gamma$ for the decay rate).

6.5 Error treatment

Error propagation is simple when the distributions are Gaussian and the functions are linear. All other cases are difficult to handle and very little guidance can be found in the literature. A detailed discussion of the problem is beyond the scope of this article.

26 This happens, for example, if the probability contours in the sample space are locations of constant pdf.
Error propagation requires not only an error interval, but also a parameter estimation. The usual choice for the latter is the maximum likelihood estimate. To classical methods other choices are better adapted. Central intervals are well compatible with the estimate which we obtain when we shrink the confidence interval to zero width. These estimates, however, usually are not very efficient estimators.

The errors - better called uncertainties - of a measurement are usually not accurately known and this is also not necessary. A precision of about 10% is good enough in most cases. Thus, we should be satisfied with reasonable approximations.

6.5.1 Error definition. In the classical schemes error intervals are typically 68.3% confidence intervals. They are well defined, except for the arbitrariness of the definition of the probability intervals.

Physicists usually publish the asymmetric likelihood ratio limits which provide approximate information of the shape of the likelihood function.

The Bayesian probability distributions for parameters gives full freedom (which is a disadvantage) in defining the error. An obvious choice is to use mean value, variance, and, when necessary skewness and kurtosis of the parameter probability density. This method has the advantage that tails in the likelihood function are taken into account.

A comparison of error bounds of lifetime measurements from the different methods is presented in Fig. 27 where we show the error intervals for a measurement of the decay parameter $\gamma = 1$ obtained from the observations of ten and two decays, respectively. In the figure equal tail is synonymous with central, short indicates that the interval has minimum length. There are considerable differences for small event numbers. In the case of ten events the differences between various definitions are already negligible.

The Bureau International de Poids et Mesures (BIPM) and the International Organization for Standardization (ISO) have issued some recommendations on how to define the error bars. In our context the least squares estimate is equivalent.
define errors. After having distributed a questionnaire among a large number of scientists BIPM and ISO have essentially adopted a Bayesian inspired method. They recommend to quantify the uncertainty by the variance and not by a classical confidence interval or a likelihood ratio interval.

6.5.2 Error propagation in general. To conserve the confidence level or the probability, all methods call for an explicit transformation following generalized Eqs. (19). The multivariate problem $Y_k = Y_k(X_1, X_2, ... X_N)$ involves a variable transformation plus the elimination of nuisance parameters. Here again, classical methods fail. Only the Bayesian way permits a consistent solution of the problem.

Transformations conserving probability often produce strong biases and very asymmetric error bounds in the new variables. Following the ISO recommendations one has to accept a certain violation of probability conservation and work with the moments of the Bayesian distributions or the asymmetric likelihood errors.

A reasonable approximation is obtained inserting the moments of the probability densities of the variates $X_i$ into the Taylor expansions of $Y_k$.

6.5.3 Systematic errors.

Example 33 Variations in the response of a calorimeter introduce a systematic uncertainty in the measurement of some particle mass. Calibration runs are performed at the beginning and the end of the experiment to obtain the energy scale. The systematic r.m.s. uncertainty is estimated to be half the difference of the observed variation. This estimate is rather crude and very little is known about the corresponding probability density. We would certainly hesitate to believe in a Gaussian three standard deviation probability derived from it. If in our experiment calibration runs were performed with high frequency we could get a rather precise knowledge of the fluctuations and derive a statistical calibration error.

Usually, errors are called systematic if the are independent of the number of observations, typically when they cannot be derived from Poisson or multinomial distributions. However, the separation of statistical and systematic errors often is rather artificial and often systematic errors can be reduced with higher statistics. A wider definition includes all kind of errors where the pdf is badly known.

A crudely known systematic error can be modelled by a pdf with long tails.

The combination of many different systematic error distributions with similar variance, according to the Central Limit Theorem, can be approximated by a Gaussian with variance equal to the sum of the individual variances. Then non-Gaussian tails can be neglected.

It is useful to state statistical and systematic errors separately. For example, when we observe a five standard deviation effect, we would like to know whether the error is dominated by systematics or whether it is purely statistical. Sometimes we have to combine the two kind of errors, when results from different experiments are summarized or when a hypothesis is to be tested. Then we should add the errors in quadrature. When a single systematic error has similar size as the statistical error, we better use a conservative estimate of the systematic error before combining the two.

It is not clear how to incorporate the frequentist notion of coverage in the definition of systematic errors.
6.6 Combining data

One of the simpler aspects of error propagation is the computation of an average from individual measurements of the same quantity.

Increasing precision by combining data from different experiments contributes to a continuous progress of knowledge in science.

Following the LP we conclude:

*The only way to combine measurements without loss of information is to add their log-likelihood functions.*

This step does not require a definition of the error.

*Frequentist methods* cannot compute confidence limits from the likelihood function. Thus they have to invent other prescriptions to combine data. No generally accepted method is known to me. Especially in unified approaches additional information to the error limits is necessary to perform sensible combinations. Complicated procedures have been invented to combine upper limits [74].

The usual averaging procedure, weighting the individual measurement with \( \delta^{-2} \), the inverse of the error squared, assumes that the errors are proportional to the standard deviation of a probability density of the measured quantity and that the measurement itself corresponds to its expectation value. Coverage properties are not considered.

The PDG [75] uses the following recipe for the combination of measurements with asymmetric errors: The mean value is computed iteratively, weighting the individual measurements with the inverse of the error squared. The error is a function of the resulting mean value. When the mean value is located inside the error interval a linear interpolation between the lower and upper side errors is used. When the mean value is outside the interval, the corresponding lower or upper error is chosen.

In principle, it would be more consistent to apply the linear error function also outside the interval. Let us call this method *PDG extended*. On the other hand the pragmatic procedure of the PDG has the advantage to be less sensitive to tails in the distributions.

Applying the usual prescriptions to add measurements with error intervals as described in the PDG book i) certainly will not conserve coverage and ii) the result will depend on the chosen scheme of defining the bounds.

For asymmetric likelihood ratio errors, the standard averaging procedure where the inverse of the full width is used as a weighting factor is only approximately correct. Better results are obtained with the PDG prescription. Alternatively, one could construct approximate log-likelihood functions of parabolic shape from the maximum likelihood estimate and the asymmetric errors and then add the approximated log-likelihoods.

**Example 34** We assume that an infinite number of identical experiments determine the mean lifetime of a particle with true mean lifetime \( \tau_0 \) from the observation of two decay times. The time distribution is exponential. The results \( \tau_i \) of the estimates from the individual experiments are averaged. Table 3 summarize the results of different averaging procedures. The first column presents the results when the procedure is applied to the lifetime estimates \( \tau_i \), the second column contains the results when the averaging starts from the estimates of the decay constants \( \gamma_i = 1/\tau_i \). There is no unique prescription for averaging classical intervals. To compute the classical value given in the table, the maximum likelihood estimate and central intervals were used.
In this special example a consistent result is obtained in the Bayesian method with uniform prior for the decay constant. This indicates how critical the choice of the parameter is in the Bayesian approach. It is also clear that an educated choice is also important for the pragmatic procedures. From the discussion of Example 22 it should be clear that the decay constant is the better parameter. Methods approximating the likelihood function provide reasonable results unless the likelihood function is very asymmetric. The conservative weighting procedure of the PDG is inferior to the extended scheme (which may be dangerous in other cases). The simple classical average is the least precise of all. As is well known, the combination of likelihood functions is optimum.

### 6.7 Bias

Most of the text books on statistics and also the PDG claim that parameter estimates should be unbiased\(^{28}\), and when they are not, we are advised to correct for the biases. One argument for preferring unbiased estimators is the property of the maximum likelihood estimate to be efficient (most precise) when unbiased. Estimates from small samples often are biased.

Since both properties, efficiency and bias, are not invariant under change of parameter, the requirement that estimated parameters should be unbiased is not so obvious. The situation is more tricky than it appears at first sight. What should we conclude from the fact that the maximum likelihood estimate \(\hat{\gamma}\) of the decay constant from an exponential decay distribution is biased but \(\hat{\tau} = 1/\hat{\gamma}\) is not? Is the result \(\hat{\tau}\) more precise than \(\hat{\gamma}\) and should we correct \(\hat{\gamma}\) for its bias?

A bias in itself is not necessarily a bad property. What really matters is a bias of the estimator weighted with its inverse error squared, the quantity which is used for averaging data. When we compute an average of several unbiased measurements the result may very well be biased and the average of a large number of biased estimates may be unbiased.

An average of unbiased measurements with errors proportional to the parameter value will be systematically too small. We have demonstrated this in the previous section (see Table 3). The unbiased lifetime estimate produces a strongly biased average and the biased decay parameter estimate gives an unbiased result.

The correct procedure is obviously to combine the log-likelihoods. A bias in the maximum likelihood estimate present in the individual experiments asymptotically disappears with increasing number of data. The PDG prescription, when using the asymmetric likelihood ratio errors is an approximation of the exact method, namely, adding the log-likelihoods.

---

\(^{28}\)The expectation value of an unbiased estimator of a parameter is equal to the parameter.
Biases usually are correlated with small event numbers and large errors which require a cautious treatment also in the context of error propagation. A non-linear function $y(x_{ub})$ with $x_{ub}$ unbiased and large uncertainty will give a biassed result $y$. The bias corrected estimators $x_{ub}$, $y_{ub}$ would not follow the same function, i.e. $y_{ub}(x_{ub}) \neq y(x_{ub})$ and consequently confidence limits which are invariant under the variable transformation $y(x)$ would not be invariant under $y_{ub}(x_{ub})$ and thus not be relevant for the estimate $y_{ub}$.

We will have to be very careful in the treatment of biases.

Not much can be said about the bias observed in classical methods. There are too many ways to define the limits and also a clear prescription of combining measurements is missing.

### 6.8 Subjectivity

In the field of statistics the word *subjective* usually is associated to probabilities not definable through frequencies and also as a somewhat negative label for the Bayesian school. Here, we will use it in its common meaning. In experimental design and data analysis many decisions have to be made which are not obvious and consequently depend on personal judgements. However, these decisions should be concerned merely with the quality (precision) of the result and avoid as much as possible to introduce biases. Where this is unavoidable, the procedure has to be documented and allow to the reader of a publication to use the results without adopting the personal judgements of the publishing group. To be more precise, we would like the results to be as much as possible independent of event selection criteria, stopping rules, Monte Carlo parameters, fitting procedures, etc..

Bayesian methods often are accused of being subjective and sometimes they really are. However, the Bayesian confidence intervals as defined in this article obviously contain no subjective elements except for the choice of the parameter which is documented. Transformations to other parameters are possible with the published results, of course with limited precision.

Likelihood ratio intervals are rather insensitive to subjective decisions.

On the other hand it is very difficult to avoid subjective elements in a classical confidence level analysis: Consider two identical experiments looking for a rare event to be identified in a mass plot. In the first experiment within a range corresponding to 3 st. dev. of the mass resolution no event is observed at the expected mass and a 90% upper limit for the occurrence is computed. In the second experiment there are a few events in the region of interest but these events are compatible with background. Usually the experimentalist would try to reduce the background by applying some clever cuts and if this is not successful he would estimate the background probability and include it in the computation of the limit. He also might decide not to publish, because his colleague of the first experiment has obtained a more restrictive limit. These subjective decisions completely ruin the classical probability interpretation which is only valid if the scientist decides when to stop an experiment, how to treat the data and whether to publish before he looks at the data - not a very realistic scenario.

A blind analysis avoids some of these subjective elements and in some situations it is quite sensible independent of the statistical procedure used. Adopted as a general principle it would inhibit discoveries and delay the progress in science.
6.9 Universality

As has been shown in our examples, the classical scheme has a limited range of applications: There are problems with physical bounds and discrete samples (digital measurements). It produces useless intervals in other cases and so far there is no general method to eliminate nuisance parameters. Especially in Poisson processes with background and uncertainty on the background mean there are unsolved problems. The unified approach in the version proposed by Feldman and Cousins improves the situation of some problems but reduces the applicability of the method to others. There remains the problem of interpretation and application: Are the classical bounds useful measures of the uncertainty of measurements and how should we use them in error handling and testing of parameter predictions?

The use of simple likelihood ratio intervals is subject to similar restrictions as the classical confidence intervals. When there is no smooth likelihood function with a maximum in the physical region, the standard limits do not indicate the same precision as in the standard case. For this reason, upper limits deduced from the likelihood ratio should not be transformed into confidence statements. Likelihood ratio intervals are more general than classical limits in some respects: They are able to handle a discrete sample space and there is a logical transition from continuous parameter problems to discrete hypothesis evaluation. They have a clear and simple interpretation, the interval is linked to the maximum likelihood estimate and combination of errors is straightforward.

The Bayesian method is the most general approach. It is able to cope with all the difficulties mentioned above.

6.10 Simplicity

Simplicity is an important aspect for the judgement not only for physical theories but also for statistical methods.

While methods based on the likelihood function are fairly simple both in the conception and their application, the classical approaches are complicated. This is the main reason why the latter are not used for standard interval estimation. Hardly any physicist knows the different ways to define the probability intervals. Thus, for standard applications in physics, classical methods are mainly of academic interest.

The newly proposed unified approaches for the computation of upper limits are even more complicated. Even specialists have difficulties to understand the details. I am convinced that only a fraction of the authors of the recent papers on neutrino oscillations is familiar with the underlying calculation of the limits and able to interpret them correctly. The variety of different classical approaches to Poisson upper limits adds to the confusion. Practical applications will in some situations require considerable computing time. While combining results based on the likelihood function is transparent and simple in most cases, the combination of classical limits, if possible at all, is a quite tricky task.

7 Summary and proposed conventions

There is no common agreement on how to define the error of an estimated parameter, but obviously we would like our error interval to include the true value with high probability,
to be well defined, and to be as small as possible. Of course, as discussed above, there are other features which are important when we compare different methods: A procedure should be simple, robust, cover all standard cases and it should enable us to combine results from different experiments. Parameter and interval estimation is used in very different applications, such as simple few parameter estimates, upper limit computation, unfolding and image reconstruction. It is not obvious that one single method would be optimum for all these situations.

In the standard situation with high event numbers the likelihood can be approximated by a Gaussian and all methods give the same results within an adequate precision.

7.1 Classical procedure

The evaluation of classical approaches is problematic: There is no prescription how to use the limits.

The essential principle of classical confidence bounds is coverage. Knowing that a certain fraction of published measurements cover within their error limits the true parameter value is an attractive property at first sight but unfortunately it is not very useful in practice. After all, experimental results should be used to make decisions but even frequentists admit that classical bounds are not well suited for this purpose.

The main difficulties of the standard classical approaches are.

- Occasionally, they produce inconsistent results (see Sect. 6.2).
- Their range of applicability is restricted.
  - Discrete variates can only be treated by relaxing the requirement of exact coverage. Digital measurements cannot be treated.
  - Parameters defined in a restricted region may lead to empty or unphysical intervals.
- The results in many cases do not represent the precision of the measurement.
- The requirement of pre-experimental fixing of the whole analysis method is very unrealistic as a general scheme and would, if followed, in many cases prevent the scientist from extracting the full information from the data and inhibit discoveries.
- Error intervals depend on the choice of the sample variable. An exception are one-dimensional central intervals and unified likelihood ratio ordered intervals.
- A prescription how to combine frequentist intervals from different experiments is missing. Biasses are not discussed.
- Nuisance parameters (background with uncertainty in the mean) often cannot be handled satisfactorily. Estimating them out produces undercoverage in some cases.

The unified classical approach provides the required coverage (approximate in the Poisson case) but shares most of the other difficulties mentioned above and adds new ones. It is applicable only under special conditions and it introduces artificial correlations between independent parameters when the parameters are near physical boundaries.
If I had to choose a frequentist method, I would select the likelihood ratio ordering for standard problems. In situations with physical boundaries, I would follow Bouchet and ignore those. The corresponding limits would represent a reasonable documentation of the experimental result and make the combination of experimental results easier. I would relax the coverage requirement which is anyhow violated at many occasions, not follow the unification concept and treat Poisson limits as exposed in [29].

7.2 Likelihood and Bayesian methods

The log-likelihood function contains the full experimental information. It measures the relative support of different hypothesis or parameter values by the data. It fulfills transitivity, it is additive and it is invariant against transformations of the parameters or the data. Thus it provides a sound basis for all kind of parameter and interval inferences.

Likelihood ratio limits parametrize the experimental observations in a sensible way. They allow the combination of data, error propagation and provide a useful measure of the uncertainty. The use of likelihood ratio errors (without integration) has some restrictions:

- The likelihood function has to be smooth.
- Digital measurements cannot be treated.
- Likelihood ratio limits deduced from likelihood functions that are very different from Gaussians (Upper Poisson limits) have to be interpreted with care.

A fully Bayesian treatment with a free choice of the prior parameter density is not advisable and is not considered further. Fixing the prior density to be uniform retains the mathematical simplicity and thus is very attractive but also has disadvantages.

- The choice of the parameter is rather arbitrary.
- It is less directly related to the data than the likelihood function.

Bayesian methods have been criticized, because they do not provide goodness-of-fit tests. This is correct, but misleading in the present context. Goodness-of-fit tests are irrelevant for parameter interval estimation which relies on a correct description of the data by the parametrization, whereas the tests question the parametrization. Also frequentist intervals do not depend on the quality of the fit.

7.3 Comparison

Obviously all methods have advantages and disadvantages as summarized in Table 4 where we compare the conventional classical, the unified classical, the likelihood and the Bayesian methods with uniform and arbitrary prior densities. The distribution of the plus and minus signs indicate the author’s personal conclusion. The attributes have to be weighted with the importance of the evaluated property.
Table 4. Comparison of different approaches to define error intervals, see text

| method:            | classical | unified | likelihood | Bayesian u.p. | Bayesian a.p. |
|-------------------|-----------|---------|------------|----------------|---------------|
| consistency       | -         | -       | ++         | +              | +             |
| precision         | -         | -       | +          | +              | +             |
| universality      | -         | -       | -          | +              | ++            |
| simplicity        | -         | -       | +          | +              | +             |
| variable transform | -         | ++      | ++         | -              | -             |
| nuisance parameter| -         | -       | -          | +              | +             |
| error propagation | -         | -       | +          | +              | +             |
| combining data    | -         | -       | ++         | +              | -             |
| coverage          | +         | ++      | -          | -              | -             |
| objectivity       | -         | -       | ++         | +              | -             |
| discrete hypothesis| -        | -       | +          | +              | +             |

7.4 Proposed Conventions

There are two correlated principles which I am not ready to give up:

1. **Methods have to be consistent.** (see Sect. 6.2)

2. **Since all relevant information for parameter inference is contained in the likelihood function, error intervals and limits should be based on the likelihood function only.**

These principles exclude the use of classical limits.

All further conventions are debatable. I propose the following guidelines which present my personal view and may serve as a basis for a wider discussion.

1. Whenever possible the full likelihood function should be published. It contains the full experimental information and permits to combine the results of different experiments in an optimum way. This is especially important when the likelihood is strongly non-Gaussian (strongly asymmetric, cut by external bounds, has several maxima etc.) A sensible way to present the likelihood function is to plot it in log-scale and normalized to its maximum. A similar proposal has been made by D’Agostini [48]. This facilitates the reading of likelihood ratios. Also in two dimensions the likelihood contour plots give an instructive presentation of the data. Isn’t the two-dimensional likelihood representation of Fig. 9 more illuminating than drawing confidence contours supplemented by sensitivity curves?

2. Data are combined by adding the log-likelihoods. When not known, parametrization are used to approximate it.

3. If the likelihood is smooth and has a single maximum the likelihood ratio limits should be used to define the error interval. These limits are invariant under parameter transformation. For the measurement of the parameter the value maximizing the likelihood function is chosen. No correction for biased likelihood estimators is applied. The errors are usually asymmetric. These limits can also be interpreted as Bayesian one standard deviation errors for the specific choice of the parameter variable where the likelihood of the parameter has a Gaussian shape.
4. Nuisance parameters are eliminated by integrating them out using a uniform prior. Correlation coefficients should be computed. Alternatively, the nuisance parameters are estimated out. Then it is mandatory to document their values, errors and correlation coefficients.

5. For digital measurements the Bayesian mean and r.m.s. should be used.

6. In cases where the likelihood function is restricted by physical or mathematical bounds and where there are no good reasons to reject a uniform prior the measurement and its errors defined as the mean and r.m.s should be computed in the Bayesian way.

7. Upper and lower limits are computed from the tails of the Bayesian probability distributions. An even better alternative are the likelihood ratio limits. They have the disadvantage of being less popular.

8. Non-uniform prior densities should not be used.

9. It is the scientist’s choice whether to present an error interval or a one-sided limit.

10. If measurements depending significantly on systematic errors are used to establish new physics, conservative error estimates should be used.

11. In any case the applied procedure has to be documented.

These recipes contain no subjective element and more or less reflect our everyday practice. An exception are Poisson limits where for strange reasons the coverage principle - though only approximately realized - has gained preference.

Frequentists will object to these propositions. They are invited in turn to present their solutions to the many examples presented in this article, to define precisely error limits and to explain how to use them for error propagation, combination of results and hypothesis exclusion. If they accept the LP, they will have to explain why the likelihood function or its parametrization is not sufficient to compute confidence limits.

It is obvious from the discussion of the treatment of errors in the preceding section that statistical framework is lacking. Even in the pure Bayesian approach it is not clear whether to choose moments or probability intervals to characterize the errors. In any case, compared to frequentist methods, likelihood based methods are better suited for error calculations. This does not mean that classical methods in general are useless and that only Bayesian recipes should be adopted.

For checking statistical methods, frequentist arguments may be useful. Bayesian confidence intervals with low coverage could be suspicious but they are not necessarily unrealistic.

An example of a bad use of the Bayesian freedom are some unfolding methods. In some cases the regularization reduces the error below the purely statistical one and results are obtained which are more precise than they would have been in an experiment with no smearing where unfolding would not have been necessary.
7.5 Summary of the summary

Frequentist intervals depends on the probability of observations which are not there and on the choice of the probability interval in the sample space. The Bayesian approach requires a prior density or a choice of the variable space. Only the likelihood function is free of arbitrariness. It is the natural link between the observation and the parameter. We have to parameterize it in a sensible way such that the resulting parameters represent the accuracy of the measurement. If this is not possible, we should provide the full function.

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Appendix A: A short remark on probability

In Kendall and Buckland’s *Dictionary of Statistical Terms* we find: “probability

A basic concept which may be taken either as undefinable, expressing ‘degree of belief’, or as the limiting frequency in an infinite random series. Both approaches have their difficulties and the most convenient axiomatization of probability theory is a matter of personal taste. Fortunately both lead to much the same calculus of probabilities.”

This statement is a bit too short to be of much help in concrete statistical applications and it is not entirely correct. Let us be more explicit.

Probability must satisfy Kolmogorov’s axioms and these theorems define the calculus of probability. This is not a matter of taste.

Probability statements are based on partial information. They should include the whole of the available information. Otherwise contradictions may result between procedures using different bits of information.

The essential problem is to relate probability to the real world. We need a concept which allows us to handle and to document in a well defined way partially uncertain results.

Most people accept the frequency concept of probability. Assuming that an experiment can be repeated under identical situations, the frequency of a certain outcome in the limit of an infinite number of trials is the probability to be associated to the outcome. One may question both the idea of infinite repeatability and the idea of identical conditions since in reality the conditions will never be exactly the same in two experiments. We should ignore this kind of destructive objections. We have to use idealizations. It would be stupid to reject the theory of special relativity because it is impossible to realize constant velocity. I see no difficulty with probabilities based on the frequency concept.

In our every day life we have to base decisions on probabilities which we cannot relate easily to well defined repeatable situations: Will it be raining today? Will my daughter get sick? Will the stock values raise?
Also in science we find difficulties to incorporate uncertainties in our knowledge into a strict frequency concept. Are we allowed to talk about the probability that the Higgs mass is located between 100 and 200 GeV? How likely is it that the calibration constant of a certain device was within certain limits? Can we associate probabilities to something that has happened in the past but is not known to us?

In the mathematical description of a deterministic world there is no substantial difference between future and past. It is quite natural to attribute probabilities to something fixed but where we have only partial information. Probability here refers to our knowledge and not to the facts. The probability that a fair coin thrown yesterday gave head is one half.

What about constants like particle masses? Can we incorporate all probabilities in a frequency scheme?

Well, we can imagine a huge number of worlds, all with different Higgs masses distributed according to a certain probability distribution. Similarly, we can easily imagine that similar weather, health or economic conditions occur repeatedly. Considering different alternative states, one of which is realized but unknown to us, with some partial knowledge we can attribute probabilities to them. In our life we will encounter many such situations, and we hope that the probabilities on average will correspond to the frequencies with which we are right. I believe that probability always can be understood in terms of limiting frequency. It does not matter that situations often cannot be reproduced in reality, it is enough that it can be done in our imagination.

Is then the debate between frequentists and Bayesians about probability just a useless academic game? The answer is No!

Bayesians associate prior probabilities to parameters which are to be measured in an experiment and they produce updated probabilities for the parameters after the measurement\[29\]. There, the real problem is not that we cannot define the notion of prior probability but that we do not know its pdf. In fact, we know the prior to some extent, we have a crude idea of it, otherwise it would be impossible to design the experiment. But we cannot, prior to an experiment, associate to the Higgs mass a well known pdf like we do for the lifetime of an unstable particle.

In physics, usually there is a quite clean distinction between exactly known pdfs (sometimes up to parameters) and hardly known pdfs. In sciences like biology or economics often empirical pdfs have to be used, hence there is a continuous transition between the two extremes. Also in our discipline, we are sometimes forced to use empirical, badly known pdfs, for example when we discuss systematic errors or when we apply a least square fit to observations without knowing the distribution of the fluctuations.

The inclusion of partially known pdfs considerably widens the range of applications of statistical inference, and we should profit from the corresponding tools, but it also introduces problems. The modern Bayesian school has tried to solve some of them. A scheme has been developed by De Finetti and Savage to associate pdfs to the “personal probabilities” as they are called by Savage but their method is not relevant for typical physics situations.

When we use prior probabilities or empirical pdfs, we should state them and the results of the analysis partially depend on the validity of our assumptions. In many

\[29\] Of course, we cannot produce a distribution of a parameter like a particle mass but a probability distribution of the parameter. The parameter has a fixed value but our knowledge is incomplete.
cases the dependence is weak.

**Appendix B: Shortest classical confidence interval for a lifetime measurement**

In some cases we can find a *pivotal quantity* $Q(X, \theta)$ of a variate $X$ and a parameter $\theta$. A pivot has a probability density which is independent of the parameter $\theta$ (like $X - \theta$ for a Gaussian with mean $\theta$) and consequently its probability limits $Q_1, Q_2$ of $Q$ are also independent of $\theta$:

$$P(Q_1 < Q(X, \theta) < Q_2) = \alpha$$ (20)

By solving the inequality for $\theta$ we find:

$$P(\theta_1(Q_1, X) < \theta < \theta_2(Q_2, X)) = \alpha$$ (21)

Equation (21) relates $Q_1$ and $Q_2(Q_1, \alpha)$. The remaining free parameter $Q_1$ is used to minimize $|\theta_2 - \theta_1|$.

We look at the example of a lifetime observation $x$. The width of a confidence interval $[\gamma_1, \gamma_2]$ of the decay constant $\gamma$ is minimized. Here $Q = \gamma X$ is a pivotal quantity.

$$f(X) = \gamma e^{-\gamma X}$$
$$Q = \gamma X$$
$$g(Q) = e^{-Q}$$

For a given confidence level $\alpha$ the two limits depend on each other: $Q_2(\alpha, Q_1)$. The limits transform to limits on the parameter $\theta$: $[\theta(Q_1), \theta(Q_2)]$ Then $|\theta(Q_2(\alpha, Q_1)) - \theta(Q_1)|$ is minimized:

$$e^{-Q_1} - e^{-Q_2} = \alpha$$
$$Q_2 = -\ln(-\alpha + e^{-Q_1})$$
$$Q_1 < \gamma X < Q_2 = -\ln(-\alpha + e^{-Q_1})$$
$$\frac{Q_1}{X} < \gamma < -\ln(-\alpha + e^{-Q_1})$$

Minimizing the interval length is equivalent to minimizing

$$\ln \left( \frac{e^{-Q_1}}{-\alpha + e^{-Q_1}} \right)$$

Taking into account the boundary condition $Q_1 > 0$, we find $Q_1 = 0, Q_2 = -\ln(1 - \alpha)$ and

$$\gamma_1 = 0$$
$$\gamma_2 = -\frac{1}{X} \ln(1 - \alpha)$$

For $\alpha = 0.6826$, and an observation $x = 1$ we find $\gamma_1 = 0, \gamma_2 = 1.15$. (The likelihood ratio limits are $\gamma_1 = 0.30, \gamma_2 = 2.36$)
When we play the same game with the parameter \( \tau = 1/\gamma \) and the same pivot we obtain

\[
\frac{x}{\tau} < Q_1' < \frac{x}{\tau} = -\ln(-\alpha + e^{-Q_1'})
\]

Minimizing

\[
\frac{1}{Q_1'} + \frac{1}{\ln(-\alpha + e^{-Q_1'})}
\]

we find \( \tau_1 = 0.17 , \tau_2 = 2.65 \) (The likelihood ratio limits are invariant \( \tau_1 = 0.42 , \tau_2 = 3.31 \))

The pivotal limits obviously depend, as expected, on the choice of the parameter.

**Appendix C: Objective prior density for an exponential decay**

In the literature we find arguments for *objective priors*. A nice example which illustrates the methods used, is the derivation of the decay constant for particle decays.

Two different particles with exponential decays have the probability densities of the decay time \( T \) and decay constant \( \lambda \)

\[
f(T, \lambda) = f(T|\lambda)\pi(\lambda) \\
f'(T', \lambda') = f(T'|\lambda')\pi(\lambda')
\]

where \( \pi(\lambda) \) is the prior density and \( f(T|\lambda) = \lambda \exp(-\lambda T) \). The decay constants \( \lambda \) and \( \lambda' \) are related by \( \lambda' = \alpha \lambda \). This fixes \( \alpha \). Then for times \( t' = t/\alpha \) we have the transformation

\[
f(T, \lambda)dTd\lambda = f'(T', \lambda')dT'd\lambda'
\]

from where we obtain

\[
\alpha \pi(\alpha \lambda) = \pi(\lambda)
\]

This relation is satisfied by

\[
\pi(\lambda) = \frac{\text{const.}}{\lambda}
\]

The prior density is inversely proportional to the decay constant. The flaw of the argument is easily identified: Why should there be a universal prior density \( \pi(\lambda) \) for all particles? There is no reason for this assumption which was used when we tacitly substituted \( \pi'(\lambda') \) with \( \pi(\lambda') \).

We can also argue in a slightly different way: Two physicists measure the lifetime of the same particle in different time units, \( T \) in seconds and \( T' \) in minutes. The numerical values are then related by \( T' = T/\alpha \) and \( \lambda' = \alpha \lambda \) as above with \( \alpha = 60 \). The prior densities have to fulfill

\[
\pi(\lambda)d\lambda = \pi'(\lambda')d\lambda'
\]
Now the two physicists choose the same functional form of the prior density. Thus we get

\[ \pi(\lambda) d\lambda = \pi(\lambda') d\lambda' \]
\[ \pi(\lambda) d\lambda = \pi(\alpha \lambda) \alpha d\lambda \]
\[ \pi(\lambda) = \frac{\text{const.}}{\lambda} \quad (22) \]

The resulting prior densities are not normalizable, a fact which already indicates that the result cannot be correct. Again there is no compelling reason why \( \pi \) should be equal to \( \pi' \). It is also easily seen that prior densities different from (22) do not lead to contradictions. For example a uniform prior in the interval \( 0 < T < 1 \) sec would produce \( \pi(T) = 1 \) and \( \pi'(T') = 1/60 \).

Similar plausibility arguments as used above are applied for the derivation of the a priori density for the Poisson parameter. They are in no way convincing.

It is impossible to determine prior densities from scaling laws or symmetries alone. We can use non-uniform prior densities when they are explicitly given as in Example 19.

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