A Paradox about the Distributions of Likelihood Ratios?

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Abstract

We consider whether the asymptotic distributions for the log-likelihood ratio test statistic are expected to be Gaussian or $\chi^2$. Two straightforward examples provide insight on the difference.

1 Introduction

In analysing data, the likelihood function provides a very useful method of determining free parameters, and also their uncertainties, in any model that is fitted to the data. The input to a likelihood calculation can be individual observations (unbinned likelihood), or histograms (binned likelihood); it is the former that we largely consider here. Likelihoods are also used as part of the procedure to determine the Bayesian posterior probability.

Likelihood ratios (i.e. the ratio of the likelihood for two possible models) are used very much in Hypothesis Testing, where we compare how well the two different hypotheses fit the data. In assessing their numerical values for a particular data set, is useful to know what are their expected asymptotic distributions for a specific hypothesis.

The Central Limit Theorem (CLT) can be used for this. It states that, if we take a linear combination of enough independent random variables $r_i$, the distribution of this sum tends to a Gaussian. The $r_i$ can be from a single distribution, or from several different distributions, provided there are enough samples from each distribution. The variances of each of these distributions must be finite.

The relevance of the CLT is as follows. To construct a likelihood function, we first need the probability density function (pdf) $p(x|\mu)$ for obtaining data $x_i$ for a given value of the theoretical parameter $\mu$. Here $x_i$ denotes a series of independent and identically distributed measurements of a single physical quantity $x$. Then the likelihood $L(\mu)$ is given by

$$L(\mu) = \prod p(x_i|\mu),$$  \hspace{1cm} (1)

where the product extends over the different and independent $x_i$. Its logarithm is

$$\ln L = \Sigma \ln p(x_i|\mu)$$  \hspace{1cm} (2)

\footnote{Both $x$ and $\mu$ can be multi-dimensional.}
It thus appears that the CLT applies to $\ln L$, and similarly to the logarithm of a likelihood ratio (LLR), and so their distributions should be Gaussian.

In contrast, a mathematical $\chi^2$ distribution is obtained for a variable

$$ S = \Sigma q_i^2 $$

where each of the $q_i$ is randomly and independently Gaussian distributed with zero mean and unit variance. If there are $K$ terms in the summation, $S$ will have a $\chi^2$ distribution with $K$ degrees of freedom.

Wilks’ Theorem\(^1\) (see Section 2) states that, provided certain conditions are satisfied, $-2\cdot$LLR has a $\chi^2$ distribution; this appears to contradict our previous conclusion about the distributions of the logarithm of a likelihood or likelihood ratio being Gaussian. Do we have a paradox?\(^2\)

Section 2 contains some background information on different types of hypotheses and on various likelihood ratios. Likelihoods and likelihood ratios for the easily understood exponential distribution are examined in Section 3 where the paradox is resolved. The relationship between the locations and the widths of the pdf’s of the LLR is also discussed in Section 3. A similar analysis for a Gaussian distribution is presented in Section 4. Finally the issue of whether unbinned likelihood provides information on Goodness of Fit is recalled in Section 5.

2 Aside on Hypotheses and Likelihood Ratios

Statisticians divide hypotheses into those in which there are no free parameters, and those where there are; they are called Simple and Composite respectively. An example of the former would be that the spin of the Higgs boson is zero,\(^3\) while the possible existence of a heavy neutrino with any mass would be composite. For comparing two simple hypotheses, the Neyman-Pearson Lemma\(^2\) says that the likelihood ratio (LR) provides the best way of distinguishing the hypotheses.

Even when the hypotheses are composite, the LR may provide a reasonable way of assessing how two different hypotheses compare in describing the data. In that case, however, theorems about the distribution of a test statistic for simple hypotheses may not apply, and distributions then have to be determined by simulation.

A special case of a composite hypothesis occurs when Wilks’ Theorem applies (see Section 2 above). It says that $-2\cdot$LLR for two hypotheses has a $\chi^2$ distribution provided:

- The null hypothesis is true.
- The hypotheses are nested. i.e. By a special choice of parameter values for the larger hypothesis $H1$, it can be reduced to the smaller hypothesis $H0$. This automatically requires $H1$ to be composite.
- The extra parameters in $H1$ that are required to reduce it to $H0$ are all uniquely defined, and are not at the extreme end of their allowed ranges.
- There are enough data for asymptotic approximations to apply.

\(^2\)Given that the $\chi^2$ distribution is asymptotically Gaussian, it might be thought that the different expectations of Gaussian or $\chi^2$ for the LLR are compatible asymptotically. This is incorrect: in the statement about $\chi^2$ becoming Gaussian, ‘asymptotically’ refers to the number of degrees of freedom for the $\chi^2$ being large, and does not refer to the number of observations.

\(^3\)In practice, hypotheses in Particle Physics are rarely simple. Even if there are no extra physics parameters involved, there are almost always systematic nuisance parameters of an experimental nature (e.g. energy calibrations, electron identification efficiency, etc.) However, if these systematic effects have only a small effect on the analysis, it may be an adequate approximation to treat the hypothesis as simple.
The number of degrees of freedom of the $\chi^2$ distribution is equal to the number of extra free parameters in $H_1$.

There are several different sorts of LRs that are used in Particle Physics, and so it is important to specify which we are discussing at any time. Here we consider $\mathcal{L}(x|H_0)/\mathcal{L}(x|H_1)$ where the hypothesis $H_0$ may or may not involve free parameter(s), and $H_1$ does. Variants of this LR are discussed in [3].

The expected asymptotic distributions of various LLRs are discussed in [4].

3 Examples with an exponential distribution

We resolve the paradox with a straightforward example where the pdf is an exponential distribution

$$p(t|\tau) = \frac{1}{\tau} \exp(-t/\tau)$$

with parameter $\tau$ and observation $t$. This could be for the decay time $t$ of a radioactive system with mean life parameter $\tau$. Then, with a set of $t_i$ observed decay times, the likelihood is

$$\mathcal{L}(\tau) = \prod [(1/\tau) \exp(-t_i/\tau)]$$

where the product is over the $N$ observations. Then its logarithm is

$$\ln \mathcal{L}(\tau) = \Sigma \left[ -\ln \tau - t_i/\tau \right]$$

where $\bar{t}$ is the mean of the observed decay times $t_i$.

3.1 One simple hypothesis: $\tau = \tau_1$

First we consider the simple hypothesis, where $\tau$ has a fixed value $\tau_1$. By the CLT, $\bar{t}$ is asymptotically Gaussian. Since the mean and variance of the exponential distribution of eqn. 4 are $\tau$ and $\tau^2$, respectively, the mean of the Gaussian for $\bar{t}$ is $\tau$ and its variance is $\tau^2/N$.

For fixed $\tau_1$, $\ln \mathcal{L}$ of eqn. 6 is a linear function of the single variable $\bar{t}$, and so it too will be Gaussian.

3.2 One composite hypothesis: variable $\tau$

Now we consider a composite hypothesis, with $\tau$ varied to find $\tau_{best}$ that maximises $\ln \mathcal{L}$. This yields

$$\tau_{best} = \bar{t}$$

Inserting this in eqn. 6 gives

$$\ln \mathcal{L}(\tau_{best}) = \Sigma \left[ -\ln \tau_{best} - t_i/\tau_{best} \right]$$

$$= -N \ln \bar{t} - N$$

4 In realistic situations, decay time distributions are more complicated than this. Thus background, time resolution, acceptance cuts, etc. would need to be taken into account. We deal with the idealised case as it is amenable to analytic solution, and hence is useful for obtaining insights.

5 It is important not to be confused between (a) the likelihood as a function of its parameter for a single data set, which often is asymptotically Gaussian; and (b) the distribution of the logarithm of the likelihood for a repeated set of experiments, which is also Gaussian if the CLT applies. The former involves plotting $\mathcal{L}(\mu)$ against $\mu$, while the second is a histogram of the LLR.

6 Equation 7 looks trivially true as it can casually be read as “The average lifetime is the average lifetime”. However it does have real content, as the more accurate description is “Our best estimate of the parameter $\tau$ of the exponential function fitted to the data is given by the mean of the $N$ observed decay times.”
Asymptotically $\bar{t}$ is still Gaussian but $\ln \mathcal{L}$ involves $\ln \bar{t}$. However, the distribution of a variable $\ln z$ is related to the distribution in $z$ simply by a factor $z$. Since for large $N$, the expected width of the $\bar{t}$ distribution becomes narrow, the extra factor of $\bar{t}$ will not vary too much over the main part of the $\bar{t}$ distribution, and so we expect that asymptotically $\ln \bar{t}$ will also be Gaussian.

Thus for variable $\tau$, $\ln \mathcal{L}(\tau_{\text{best}})$ is a linear function of the single variable $\ln \bar{t}$, and so it too asymptotically will be Gaussian.

### 3.3 Two simple hypotheses: $\tau = \tau_1$ and $\tau_2$

Similarly for the logarithm of the ratio of the likelihoods for two different assumed lifetimes $\tau_1$ and $\tau_2$ is

$$\ln(\mathcal{L}(\tau_1)/\mathcal{L}(\tau_2)) = -N * \ln(\tau_1/\tau_2) - N * \bar{t} * (1/\tau_1 - 1/\tau_2)$$

The LLR for these two simple hypotheses is also linearly dependent on $\bar{t}$, and hence the distribution of $\ln(\mathcal{L}(\tau_1)/\mathcal{L}(\tau_2))$ is again asymptotically Gaussian. We expect $\bar{t} = \tau_1(1+g/\sqrt{N})$ if $\tau = \tau_1$, or $\tau_2(1+h/\sqrt{N})$ if $\tau = \tau_2$, where $g$ and $h$ are standard Gaussians of mean zero and unit variance.

Writing $\tau_1 = (1+k)\tau_2$, where $k$ is small if $\tau_1 \sim \tau_2$, we obtain for the expected values of the likelihood ratio, assuming that $\tau_1$ is the true value

$$\langle \ln(\mathcal{L}(\tau_1)/\mathcal{L}(\tau_2)) \rangle_{\tau_1} = -N \ln(1+k) - N(1 + g/\sqrt{N})(1 - (1+k))$$

$$\sim -N[(k-k^2/2 + k^3/3 + ... ) - k] + Nkg/\sqrt{N}$$

$$\sim [Nk^2(1/2 - k/3 + ...)] + [\sqrt{N}kg]$$

Alternatively, if $\tau_2$ is the true value

$$\langle \ln(\mathcal{L}(\tau_1)/\mathcal{L}(\tau_2)) \rangle_{\tau_2} = -N \ln(1+k) - N(1 + h/\sqrt{N})(1/(1+k) - 1)$$

$$\sim -N[(k-k^2/2 + k^3/3 + ... ) + (1-k+k^2 - k^3,...) - 1] + N(k-k^2...h/\sqrt{N}$$

$$\sim [-Nk^2(1/2 - 2k/3 + ...)] + [\sqrt{N}hk(1-k+...)]$$

Because $g$ and $h$ are standard Gaussians, the first term on the right hand side of eqns 10 and 11 gives the location of the peak, and the second term determines its width. Thus for the two similar pdfs (exponentials with $\tau_1 \sim \tau_2$), $k$ is small and the distributions of the LLR for the two hypotheses peak at symmetric values $\pm T_E$ of the LLR, equidistant from zero, and their widths $w_E$ are equal. Furthermore with close values of $\tau$, the widths and locations of the LLR distributions for the two hypotheses are related by

$$w_E = \sqrt{2T_E}$$

This result is reminiscent of the situation of trying to distinguish the two hypotheses of normal and inverted hierarchies for the masses of neutrinos of different flavour which result in small differences of observed neutrino spectra. The claim there is that the LLR distributions for these two hypotheses tend to be Gaussians with locations $\pm T$ and widths given by eqn 12.

When the pdf’s are more different, the higher order terms of the expansions of eqns 10 and 11 are relevant, and the symmetry of locations and equality of widths no longer holds. (Compare, for example, the case of trying to distinguish spin-parity $0^+$ from $1^+$ for the Higgs boson - see fig. 5 of ref. [7]).

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7It might be thought that rather larger values of $N$ are required for this approximation to be good, than for $\bar{t}$ itself; this is plausible but incorrect. It turns out that for our exponential example the Gaussian approximation is better for $\ln \bar{t}$ than for $\bar{t}$.

8Sometimes the distributions of $-2\ln \mathcal{L}$ are considered. In that case, the locations $\pm T^*$ and widths $w^*$ are related by $w^* = 2\sqrt{T^*}$.

9In the neutrino mass hierarchy situation, the data pdf’s for the two hypotheses have different functional forms. This is not so in our simple example where both $H_0$ and $H_1$ correspond to exponential distributions (with different values of $\tau$).
Another interesting result is that, for small \( k \) (i.e. \( \tau_1 \sim \tau_2 \)),
\[
2T_{E_i}/w_E \sim \sqrt{N} \tau = \sqrt{N} (\tau_2 - \tau_1)/\tau_1
\] (13)
That is, the separation of the peaks of the distributions of the LLR for the two hypotheses is approximately equal to the difference in the mean lifetimes, divided by the uncertainty \( \tau/\sqrt{N} \) in determining a lifetime from \( N \) events.

3.4 Nested hypotheses and Wilks’ Theorem for Exponentials

Wilks’ Theorem applies to the situation where \( H_0 \) (e.g. \( \tau = \tau_{gen} \)) is true, and \( H_1 \) is just an extended version of \( H_0 \) with extra parameter(s) - see Section 2 in our exponential example, \( \tau \) is allowed to vary. Then \( H_1 \)'s likelihood must be at least as large (as good) as that for \( H_0 \), but if \( H_0 \) is true, the freedom due to the extra parameter(s) of \( H_1 \) is not required, and we expect \(-2 \times \ln(L_0/L_1)\) to be small. Wilks’ Theorem gives us a way of quantifying this. In contrast, if \( H_0 \) is not true, \(-2*LLR\) can be large.

Here we look at \( \Delta \ln L = \ln L(\tau_{test}) - \ln L(\tau_{best}) \), where the data consist of decay times generated according to an exponential distribution with \( \tau = \tau_{gen} \), and the two likelihoods are respectively for specific tested values and for its best value \( \tau_{best} \) for that data set.

If we set \( \tau_{test} = \tau_{gen} \), we expect \(-2\Delta \ln L\) to have a small positive (or zero) value. In fact, asymptotically the conditions for Wilks’ Theorem are satisfied, in which case its expected distribution is \( \chi^2 \) with one degree of freedom.

We can verify this because from equations 6 and 8 we obtain
\[
\Delta \ln L = (-N \ln \tau_{test} - N\bar{I}/\tau_{test}) - (-N \ln \bar{I} - N)
= N(\ln \bar{I}/\tau_{test} - (\bar{I}/\tau_{test} - 1))
\] (14)
We expect \( \bar{I} = \tau_{best} \) to be Gaussian distributed about \( \tau_{gen} \) with width \( \tau_{gen}/\sqrt{N} \) (see first paragraph of section 3.3) i.e.
\[
\tau_{best} = \tau_{gen}(1 + g/\sqrt{N})
\] (15)
where \( g \) is a standard Gaussian random variable, and so
\[
\Delta \ln L = N(\ln(1 + g/\sqrt{N}) - g/\sqrt{N})
\] (16)
For large \( N \) we can expand \( \Delta \ln L \) in powers of \( g/\sqrt{N} \), to obtain
\[
\Delta \ln L = N(-g^2/2N + \ldots)
\] (17)
The leading term in \( g/\sqrt{N} \) vanishes, and so asymptotically \(-2\Delta \ln L = g^2 \), the square of a standard Gaussian variable, and hence its expected distribution is indeed \( \chi^2 \) with one degree of freedom. It is the cancellation of the leading term in \( g/\sqrt{N} \) which results in the LLR not having a Gaussian distribution in this case.

Not specifically related to the ‘Gaussian or \( \chi^2 \)’ paradox, but interesting in its own right is the fact that when we obtain the likelihood function for the exponential’s parameter \( \tau \) from \( N \) observed decay times, the difference \( \Delta \ln L \) between the likelihood and its best value is a universal function of \( \tau/\tau_{best} = \lambda \). From equation 8, we obtain
\[
\Delta \ln L = \ln L(\tau) - \ln L(\tau_{best})
= N(\ln \bar{I}/\tau + 1 - \bar{I}/\tau)
= N(1 - 1/\lambda - \ln \lambda)
\] (18)
thus demonstrating the assertion. This implies that the uncertainty on \( \tau/\tau_{best} \) is independent of \( \tau_{best} \) and of the individual data values (apart from their average \( \bar{I} \)), and depends only on \( N \). For example, if the uncertainty on \( \tau \) is estimated as \((-d^2 \ln L/d\tau^2)^{-1/2} \), we obtain \( \sigma_{\tau} = \tau/\sqrt{N} \).
4 Examples with Gaussian distribution

Here we follow the same situations as for Section 3, but this time using a Gaussian pdf

\[ p(x|\mu) = \frac{1}{\sqrt{2\pi\sigma}}\exp(-0.5 \times (x - \mu)^2/\sigma^2) \]  

(19)

i.e. The pdf for the data \( x \) is a Gaussian centred at \( \mu \) and with fixed width \( \sigma \). Then for a set of \( N \) observations \( x_i \), the log-likelihood is

\[ \ln L(\mu) = -\Sigma(0.5(x_i - \mu)^2/\sigma^2) + C \]

\[ = -0.5N(\bar{x} - \mu)^2/\sigma^2 + C \]  

(20)

where the constant \( C = -N \ln(\sqrt{2\pi}\sigma) \). Thus, as in the exponential case, the log-likelihood depends on the data only though its mean \( \bar{x} = \Sigma x_i/N \).

4.1 One simple hypothesis: \( \mu = \mu_1 \)

For fixed \( \mu_1 \), the log-likelihood is thus given by

\[ \ln L(\mu_1) = -\Sigma(0.5(x_i - \mu_1)^2/\sigma^2) + C \]

(21)

Since with \( x \) having a Gaussian distribution, that for \( (x - \mu)^2 \) is specified, and so by the CLT, \( \ln L \) will have a Gaussian distribution asymptotically.

An alternative derivation uses the fact that each \( x_i \) is independently Gaussian distributed with mean \( \mu_1 \) and variance \( \sigma^2 \). Thus each \( (x_i - \mu_1)/\sigma \) is distributed as a standard Gaussian, with zero mean and unit variance. Then, apart from the constant \( C \), \( -2\ln L(\mu_1) \) is distributed as \( \chi^2 \) with \( N \) degrees of freedom. Since asymptotically (i.e. large \( N \)), \( \chi^2 \) tends to a Gaussian distribution, this also applies to the log-likelihood.

4.2 One composite hypothesis: variable \( \mu \)

We now consider a composite hypothesis, with \( \mu \) varied to find \( \mu_{\text{best}} \) that maximises \( \ln L \). As with the exponential case, the best value of the parameter is equal to the mean of the data, i.e. \( \mu_{\text{best}} = \bar{x} \). Inserting this into eqn. 21 yields

\[ \ln L(\mu_{\text{best}}) = -0.5\Sigma(x_i - \bar{x})^2/\sigma^2 + C \]  

(22)

4.3 Two simple hypotheses: \( \mu = \mu_1 \) and \( \mu_2 \)

Similarly the LLRs for two different assumed central values \( \mu_1 \) and \( \mu_2 \) is

\[ \ln(\mathcal{L}(\mu_1)/\mathcal{L}(\mu_2)) = -\frac{1}{2\sigma^2}[2\Sigma x_i\mu_1 + 2\Sigma x_i\mu_2 + \mu_1^2 - \mu_2^2] \]

\[ = -\frac{N(\mu_2 - \mu_1)}{\sigma^2}[\bar{x} - (\mu_1 + \mu_2)/2] \]  

(23)

where the terms quadratic in \( x_i \) and the constant \( C \) have cancelled between the two log-likelihoods. The LLR for these two simple hypotheses is linearly dependent on \( \bar{x} \), and hence the distribution of \( \ln(\mathcal{L}(\mu_1)/\mathcal{L}(\mu_2)) \) is again Gaussian. But here there is no need to invoke the CLT, since the sum of any number of random variables drawn from identical Gaussians (i.e. equal widths and equal central values)
has a Gaussian distribution. We expect $\bar{x} = \mu_1 + g\sigma/\sqrt{N}$ if $\mu = \mu_1$, or $\mu_2 + h\sigma/\sqrt{N}$ for $\mu_2$, where $g$ and $h$ are standard Gaussians of mean zero and unit variance.

Assuming that $\mu_1$ is the true value

$$[\ln(\mathcal{L}(\mu_1)/\mathcal{L}(\mu_2))]_{\mu_1} = -\frac{N(\mu_2 - \mu_1)}{\sigma^2}[(\mu_1 + g\sigma/\sqrt{N}) - (\mu_1 + \mu_2)/2]$$

(24)

Because $g$ is a standard Gaussian, the first term above gives the location $T_G$ of the peak of the LLR distribution, while the coefficient of $g$ in the second term gives its width $w_G$ i.e.

$$T_G = \frac{N}{\sigma^2} (\mu_2 - \mu_1)^2 / 2; \quad w_G = \sqrt{N}|\mu_2 - \mu_1|/\sigma$$

(25)

Alternatively, if $\mu_2$ is the true value, the peak is at $-T_G$, and the width is as in eqn 25.

Thus for the two Gaussian pdfs the distributions of the LLR for the two hypotheses peak at symmetric values $\pm T_G$, equidistant from zero, and their widths $w_G$ are equal. Furthermore, the widths and locations of the LLR distributions for the two hypotheses are related by

$$w_G = \sqrt{2T_G}$$

(26)

as in the case of two exponentials (but there the values of $\tau_1$ and $\tau_2$ need to be close and we require asymptotic data for the relationships concerning the distributions’ locations and widths to apply). Equations 25 and 26 are true for any values of the parameters $\mu_1$ and $\mu_2$, and do not require asymptotic data.

It is also worth noting that

$$2T_G/w_G = |\mu_2 - \mu_1|\sqrt{N}/\sigma$$

(27)

i.e. the separation of the peaks of the LLR distributions, divided by their width, is equal to the separation of the original Gaussian pdfs, divided by the uncertainty $\sigma/\sqrt{N}$ in their experimental location (cf. eqn. 13).

### 4.4 Nested hypotheses and Wilks’ Theorem for Gaussians

Here we look at $\Delta \ln \mathcal{L} = \ln \mathcal{L}(\mu_{\text{test}}) - \ln \mathcal{L}(\mu_{\text{best}})$, where the data $x$ are generated according to a Gaussian distribution with $\mu = \mu_{\text{gen}}$, and the two likelihoods are respectively for the specific tested value and for its best value $\mu_{\text{best}}$ for that data set.

If we set $\mu_{\text{test}} = \mu_{\text{gen}}$, we expect $-2\Delta \ln \mathcal{L}$ to have a small positive (or zero) value. The conditions for Wilks’ Theorem are satisfied, in which case its expected distribution is $\chi^2$ with one degree of freedom.

We can verify this because from equation 28

$$\Delta \ln \mathcal{L} = \ln \mathcal{L}(\mu_{\text{gen}}) - \ln \mathcal{L}(\mu_{\text{best}})$$

$$= -\frac{N}{\sigma^2}(\mu_{\text{best}} - \mu_{\text{gen}})(\bar{x} - (\mu_{\text{best}} + \mu_{\text{gen}})/2)$$

(28)

We expect $\bar{x} = \mu_{\text{best}}$ to be Gaussian distributed about $\mu_{\text{gen}}$ with width $\sigma/\sqrt{N}$ i.e.

$$\mu_{\text{best}} = \mu_{\text{gen}} + l\sigma/\sqrt{N}$$

(29)

where $l$ is a standard Gaussian random variable, and so

$$\Delta \ln \mathcal{L} = -\frac{N}{\sigma^2} \sqrt{N} [0.5(\mu_{\text{gen}} + l\sigma/\sqrt{N}) - 0.5\mu_{\text{gen}}]$$

$$= -l^2/2$$

(30)
Thus $-2\Delta \ln L = l^2$, the square of a standard Gaussian variable, and hence its expected distribution is indeed $\chi^2$ with one degree of freedom. Again this result involves neither approximation nor the need for asymptotic data.

5 Unbinned likelihoods and Goodness of Fit

While considering likelihood functions for exponentials and for Gaussians, we discuss an interesting property.

The likelihood method asserts that the best value of a parameter is obtained by maximising the likelihood with respect to the parameter. It thus might be thought that large likelihood values are better than smaller ones, and hence that large likelihood values are indicative of a better goodness of fit between data and the chosen parametric form.

For unbinned likelihoods, this is incorrect. The likelihood is a measure of the probability density for obtaining the given data set, which is **fixed**; it uses these probabilities as the parameter is varied. In contrast, Goodness of Fit involves the probabilities of **different** data sets, for a fixed value of the parameter.

The inability of the unbinned maximum likelihood to distinguish between data which does have the expected distribution and data which does not is illustrated for the exponential example by eqn 8. This shows that $L(\tau_{\text{best}})$ depends on the data only through the average of their decay times $\bar{t}$. Thus any sets of $N$ observations which happen to have the same value of $\bar{t}$ will have the identical value of the maximum likelihood; these data sets could be distributed as expected for an exponential distribution, or one where all the decays occurred at the identical time. Thus the value of $L(\tau_{\text{best}})$ is incapable of distinguishing between an acceptable data set, and one which is very strongly in disagreement with the exponential decay hypothesis (see also ref. [8]).

The Gaussian case provides an even stronger example. We want to test goodness of fit of the Gaussian distribution of eqn. 19 with fixed width with two data sets: the first has the individual unbinned $x_i$ distributed as expected for eqn. 19 while the second has all the data $x_i$ equal to $\mu$. This second set is not compatible with our chosen fixed width Gaussian, but clearly results in a larger value for the unbinned likelihood than the first data set. The data which is less compatible with the hypothesis gives a larger likelihood. The value of the unbinned likelihood is clearly not a good measure of Goodness of Fit.

Baker and Cousins[9] provide a prescription for obtaining Goodness of Fit information for a likelihood approach to a histogram, i.e. for a binned likelihood approach[10]. But even here, the likelihood alone cannot be used. A reason for this is that histogram bins with $n_{\text{obs}}$ observed and $\lambda_{\text{pred}}$ predicted events being 1 and 1.0 repectively, or with $n_{\text{obs}} = 100$ and $\lambda_{\text{pred}} = 100.0$, both have perfect agreement for data and prediction. However, because the Poisson distribution
\[
p(n|\lambda) = e^{-\lambda}\lambda^n/n!
\]

is much wider for $\lambda = 100.0$ than for $\lambda = 1.0$, the likelihoods are very different (0.37 for $\lambda = 1.0$, but only 0.04 for $\lambda = 100.0$). Baker and Cousins overcome the problem by considering instead the likelihood ratio $L(\lambda|n)/L(n|n)$, where $L(n|n)$ is the likelihood for the ‘saturated’ model i.e. where $\lambda$ is chosen as the value which maximises $L(\lambda|n)$ for the observed $n$. See [9] for further details.

6 Conclusion

The Table summarises the various results for the exponential and for the Gaussian pdf’s.

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[9] In contrast, the likelihood-ratio Wilks’ Theorem can use unbinned data.
Table 1: Summary of examples with exponential or Gaussian pdfs.

|                      | Exponential                  | Gaussian                     |
|----------------------|------------------------------|-----------------------------|
| pdf                  | $p(t|\tau) = (1/\tau) \exp(-t/\tau)$ | $p(x|\mu) = \frac{1}{\sqrt{2\pi}\sigma}\exp(-0.5*(x-\mu)^2/\sigma^2)$ |
| Best value of param  | $\tau = \bar{t}$            | $\mu = \bar{x}$             |
| $\ln L(\tau$ or $\mu)$ | $\ln L(\tau) = -N \ln \tau - N * \bar{t}/\tau$ | $\ln L(\mu) = -0.5N(\bar{x} - \mu)^2/\sigma^2 - N \ln(\sqrt{2\pi}\sigma)$ |
|                      | i.e. linear in $\bar{t}$    | i.e. linear in $(\bar{x} - \mu)^2$ |
| $\ln L(\tau_{\text{best}}$ or $\mu_{\text{best}})$ | $\ln L(\tau_{\text{best}}) = -N * \ln N$ | $\ln L(\mu_{\text{best}}) = -0.5\Sigma(x_i - \bar{x})^2/N - N \ln(\sqrt{2\pi}\sigma)$ |
|                      | i.e linear in $\ln \bar{t}$ | i.e. linear in $\Sigma(x_i - \bar{x})^2$ |
| LLR for 2 simple hyps | For $\tau_1 \sim \tau_2$ | For any $\mu_1$ and $\mu_2$ |
|                      | peaks at $\pm T_E$, equal widths $w_E$ | peaks at $\pm T_G$, equal widths $w_G$ |
|                      | $w_E^2 = 2T_E$ | $w_G^2 = 2T_G$ |
|                      | $2T_E/w_E \sim |\tau_1 - \tau_2|/(\tau_1/\sqrt{N})$ | $2T_G/w_G = |\mu_1 - \mu_2|/(\sigma/\sqrt{N})$ |
| $-2 \ln(L(\tau$ or $\mu)/L_{\text{best}})$ | Asymptotically $\chi^2$ | Always $\chi^2$ |

The straightforward example of an exponential distribution for the pdf illustrates that the logarithm of the likelihood will asymptotically be Gaussian. This is also true for the logarithm of the likelihood ratio for two simple hypotheses each with a fixed value of $\tau$. If the values of $\tau$ for the two hypotheses are close to each other, the peaks of the Gaussian distributions of the LLR for the two hypotheses will be symmetrically located at $\pm T$ and with widths equal to $\sqrt{2T}$.

However, for the LLR in the case of nested hypotheses where Wilks Theorem applies and assuming that the smaller hypothesis is true, it is a cancellation between the leading term in each of the individual likelihoods which results in $-2\times$LLR being distributed as a $\chi^2$, rather than Gaussian. There is thus no paradox.

The above results are also true for Gaussian pdf’s, but the results are exact and no approximation is necessary.

It is interesting to speculate whether the above results about the positions and widths of the LLR distributions have a wider applicability than for just exponential and Gaussian pdf’s.

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