A Note on $\Delta \ln L = -\frac{1}{2}$ Errors

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Abstract

The points at which the log likelihood falls by $\frac{1}{2}$ from its maximum value are often used to give the ‘errors’ on a result, i.e. the 68% central confidence interval. The validity of this is examined for two simple cases: a lifetime measurement and a Poisson measurement. Results are compared with the exact Neyman construction and with the simple Bartlett approximation. It is shown that the accuracy of the log likelihood method is poor, and the Bartlett construction explains why it is flawed.
1. Introduction

In the limit where the number of measurements $N$ is large, the variance of the maximum likelihood estimator $\hat{a}$ of a parameter $a$ is given by

$$V(\hat{a}) = \left( -\frac{d^2 \ln L}{da^2} \right)^{-1}$$

(1)

and the quoted error $\sigma_\hat{a} = \sqrt{V(\hat{a})}$ can be read off the parabolic likelihood curve from the points at which the likelihood $L(a)$ falls by $\frac{1}{2}$ from its peak value $L(\hat{a})$: $\Delta \ln L = -\frac{1}{2}$.

For experiments with finite $N$ a similar procedure is in general use: the values $a_\pm$ below and above $\hat{a}$ for which $\Delta \ln L = \ln L(a_\pm) - \ln L(\hat{a}) = -\frac{1}{2}$ are found, and the 68% central confidence interval quoted as $[a_-, a_+]$ or $[\hat{a} - \sigma_-, \hat{a} + \sigma_+]$.

This is given a somewhat non-rigorous justification [1,2,3]: even though the log likelihood curve for $a$ may not be a parabola, the parameter $a$ could be converted to some $a'$ for which the log likelihood curve is parabolic; symmetric errors $\sigma_a'$ could be read off in the standard way, and the $a'$ interval converted back to the corresponding interval for $a$. The invariance of the maximum likelihood formalism then ensures that this interval is just the $\Delta \ln L = -\frac{1}{2}$ interval for $a$.

This practice is now being questioned [4,5,6] and an examination of how well it actually works in practice is needed to inform this discussion. In this note we consider two typical cases where Maximum Likelihood estimation is used: the determination of the lifetime of an unstable state decaying according to the radioactive decay law, and the determination of the number of events produced by a Poisson process. In these we can determine the interval produced by the $\Delta \ln L = -\frac{1}{2}$ recipe and contrast them with the exact Neyman interval. This is found [2,7] from the values satisfying:

$$\int_0^{\hat{a}} P(\hat{a}' ; a_+) d\hat{a}' = 0.16$$

$$\int_\hat{a}^\infty P(\hat{a}' ; a_-) d\hat{a}' = 0.16$$

(2)

where $P(\hat{a}; a)$ is the probability density for a true value $a$ giving an estimate $\hat{a}$. These equations define the confidence belt such that the probability of a measurement lying within the region is, by construction, 68%.

An alternative approximation technique is that of Bartlett [1,7,8]. For any $N$ the quantity $\frac{d \ln L}{da}$ is distributed with mean zero and variance $-\left\langle \frac{d^2 \ln L}{da^2} \right\rangle$. For large $N$ the Central Limit Theorem prescribes that $\frac{d \ln L}{da} = \sum_1^N \frac{d \ln P(x_i; a)}{da}$, the sum of $N$ random quantities, is Gaussian. If this quantity can be expressed in terms of $\hat{a} - \langle \hat{a} \rangle$ this can be used to give confidence regions for $\hat{a}$. Further refinements can be used to correct for the non-Gaussian finite $N$ behaviour, but these lie beyond the scope of this work.

This note uses the 68% central confidence region for illustration, but the techniques can be applied to central or one-sided regions with any probability content.

Bayesian statistics can also be used to give confidence intervals. This is an entirely different technique, and is not considered here. This study compares the exact Neyman confidence intervals with two methods which claim to approximate to them.
2. Lifetime Measurements

The probability for a state with mean lifetime $\tau$ to decay after an observed time $t$ is given by

$$P(t; \tau) = \frac{1}{\tau} e^{-t/\tau}. \quad (3)$$

The log likelihood for $N$ measurements $t_1 \ldots t_N$ is

$$lnL = -N\frac{\overline{t}}{\tau} - N\ln\tau \quad (4)$$

where $\overline{t} = \frac{1}{N} \sum t_i$. Differentiation to find the maximum immediately gives $\hat{\tau} = \overline{t}$ and $lnL(\hat{\tau}) = -N(1 + \ln \overline{t})$. The problem scales with $\tau/\overline{t}$, and without loss of generality we can take $\overline{t} = 1$. We consider the 68% confidence region for various values of $N$.

The probability of obtaining a particular value of $\overline{t}$ contains a term $e^{-N\overline{t}/\tau}$ from equation 3, and a factor $\overline{t}^{N-1}$ from the convolution. Normalisation gives (see [5], Equation 4)

$$P(\overline{t}; \tau) = \frac{N^N\overline{t}^{N-1}}{\tau^N(N-1)!} e^{-N\overline{t}/\tau}. \quad (5)$$

For the exact Neyman region we require the integral of this quantity from zero to the measured value, which is to be 16% for the upper limit $\tau_+ = \overline{t} + \sigma_+$ and 84% for the lower limit $\tau_- = \overline{t} - \sigma_-$. This is given by

$$\int_0^{\overline{t}} P(\overline{t}'; \tau) \, d\overline{t}' = 1 - e^{-N\overline{t}/\tau} \sum_{r=0}^{N-1} \frac{\overline{t}^r N^r}{r!\tau^r}. \quad (6)$$

The region thus obtained, expressed as differences from the measured $\overline{t}$ of 1, is shown in the columns 2 and 3 of Table 1, for values between $N = 1$ to $N = 25$.

| N  | Exact | $\Delta \ln L = -\frac{1}{2}$ | Bartlett |
|----|-------|-----------------------------|----------|
|    | $\sigma_-$ | $\sigma_+$ | $\sigma_-$ | $\sigma_+$ | $\sigma_-$ | $\sigma_+$ |
| 1  | 0.457  | 4.787                     | 0.576    | 2.314    | 0.500    | $\infty$ |
| 2  | 0.394  | 1.824                     | 0.469    | 1.228    | 0.414    | 2.414    |
| 3  | 0.353  | 1.194                     | 0.410    | 0.894    | 0.366    | 1.366    |
| 4  | 0.324  | 0.918                     | 0.370    | 0.725    | 0.333    | 1.000    |
| 5  | 0.302  | 0.760                     | 0.340    | 0.621    | 0.309    | 0.809    |
| 6  | 0.284  | 0.657                     | 0.318    | 0.550    | 0.290    | 0.690    |
| 7  | 0.270  | 0.584                     | 0.299    | 0.497    | 0.274    | 0.608    |
| 8  | 0.257  | 0.529                     | 0.284    | 0.456    | 0.261    | 0.547    |
| 9  | 0.247  | 0.486                     | 0.271    | 0.423    | 0.250    | 0.500    |
| 10 | 0.237  | 0.451                     | 0.260    | 0.396    | 0.240    | 0.463    |
| 15 | 0.203  | 0.343                     | 0.219    | 0.310    | 0.205    | 0.348    |
| 20 | 0.182  | 0.285                     | 0.194    | 0.261    | 0.183    | 0.288    |
| 25 | 0.166  | 0.248                     | 0.176    | 0.230    | 0.167    | 0.250    |

Table 1: 68% Confidence regions obtained by the 3 methods for a lifetime measurement.
The $\Delta \ln L = -\frac{1}{2}$ points can be found numerically from Equation 4. These are shown in columns 4 and 5 of Table 1.

For the Bartlett approximation, the differential of Equation 4 gives $\frac{N}{\tau}(\bar{t} - \tau)$, and the expectation value of the second differential gives the variance of this as $\frac{N}{\tau^2}$. Thus for a given $\tau$ the probability distribution for $\bar{t}$ has mean $\tau$ and standard deviation $\tau/\sqrt{N}$. This is exact. We then – this is the approximation – take this as being Gaussian and use it in the Neyman prescription, accordingly requiring that $\bar{t}$ lie one standard deviation above $\tau_+ = \tau + \sigma_+$ and one standard deviation below $\tau_- = \bar{t} - \sigma_-$. Thus

$$\bar{t} = \tau_- + \frac{\tau_-}{\sqrt{N}} \quad \bar{t} = \tau_+ - \frac{\tau_+}{\sqrt{N}}$$

(7)

i.e. $\sigma_- = \frac{\bar{t}}{\sqrt{N+1}}$ and $\sigma_+ = \frac{\bar{t}}{\sqrt{N-1}}$. These are shown in the final two columns of Table 1. The results are also presented graphically in Figure 1.

![Graph](image)

Figure 1: Upper and lower limits on the 68% central confidence interval for a lifetime measurement showing the exact construction (red), the Bartlett approximation (blue) and the $\Delta \ln L$ approximation (green)

Two points emerge, from both Table 1 and Plot 1. One is that the Bartlett approximation does surprisingly well (except at very small $N$, of order 1). The second is that the Log likelihood approximation does surprisingly badly. For $N \sim 10$ the differences are of order 10%. The convergence towards agreement is clearly slow.
3. Poisson Measurements

If $N$ events are seen from a Poisson process, Equation 2 gives the upper and lower limits of the 68% central region as

$$ \sum_{0}^{n} e^{-\lambda} \frac{\lambda^N}{N!} = 0.16 \quad \sum_{0}^{n-1} e^{-\lambda} \frac{\lambda^N}{N!} = 0.84. \quad (8) $$

These are shown in columns 2 and 3 of Table 2 for a range of values of $N$. The $\Delta \ln L = -\frac{1}{2}$ errors are read off $N - \lambda + N\ln(\lambda/N)$. These are shown in columns 4 and 5 of Table 2.

| N | Exact $\sigma_-$ | Exact $\sigma_+$ | $\Delta \ln L = -\frac{1}{2}$ Bartlett $\sigma_-$ | Bartlett $\sigma_+$ |
|---|-----------------|-----------------|-----------------|-----------------|
| 1 | 0.827           | 2.299           | 0.698           | 1.358           |
| 2 | 1.292           | 2.637           | 1.102           | 2.291           |
| 3 | 1.633           | 2.918           | 1.416           | 2.803           |
| 4 | 1.914           | 3.162           | 1.682           | 3.062           |
| 5 | 2.159           | 3.382           | 1.916           | 3.291           |
| 6 | 2.380           | 3.583           | 2.128           | 3.500           |
| 7 | 2.581           | 3.770           | 2.323           | 3.693           |
| 8 | 2.768           | 3.944           | 2.505           | 3.872           |
| 9 | 2.943           | 4.110           | 2.676           | 4.041           |
|10 | 3.108           | 4.266           | 2.838           | 4.202           |
|15 | 3.829           | 4.958           | 3.547           | 4.905           |
|20 | 4.434           | 5.546           | 4.145           | 5.500           |
|25 | 4.966           | 6.066           | 4.672           | 6.025           |

Table 2: 68% Confidence regions obtained by the 3 methods for a Poisson measurement

The Bartlett method gives the familiar fact that the variance of $n - \lambda$ is just $\lambda$. This suggests that

$$ n - \lambda_- = \sqrt{\lambda_-} \quad \lambda_+ - n = \sqrt{\lambda_+}. $$

However $P(n; \lambda)$ is defined for integer $n$ only. To make this set of discrete spikes look like a Gaussian requires us to replace it by a histogram where the value is defined as $\exp^{-\lambda} \frac{\lambda^n}{n!}$ for values of the continuous abscissa variable between $n - \frac{1}{2}$ and $n + \frac{1}{2}$. This requires us to add $\frac{1}{2}$ to each of the ranges, giving

$$ \sigma_- = \sqrt{n + \frac{1}{4}} \quad \sigma_+ = \sqrt{n + \frac{1}{4} + 1} \quad (9) $$

These are shown in columns 6 and 7 of Table 2. The data are shown graphically in Figure 2.
Figure 2: Upper and lower limits on the 68% central confidence interval for a Poisson measurement, showing the exact construction (red), the Bartlett approximation (blue) and the $\Delta \ln L$ approximation (green)

Again, the Bartlett approximation does surprisingly well, and the $\ln L$ approximation surprisingly badly. Furthermore, in this case it underestimates both errors, which will inevitably lead to a smaller than desired coverage. (This could be remedied by adding 0.5 to each limit, to account for the discrete binning, though this is still worse than the Bartlett approximation, as can be seen from Table 2.)

4. Summary

The poor behaviour of the log likelihood error approximation can be understood within the Bartlett approximation. The distribution for $\frac{d \ln L}{da}$ is re-expressed in terms of a distribution for $a - \hat{a}$ which is assumed to be Gaussian

$$p(\hat{a}; a) = \frac{1}{\sqrt{2\pi \sigma(a)}} e^{-(a-\hat{a})^2/2\sigma(a)^2}$$

(10)

where the notation $\sigma(a)$ makes the point that the variance of this Gaussian depends on $a$.

The 68% limits are given by finding the $a$ for which $\hat{a} - a = \pm \sigma(a)$. These do indeed correspond to a fall of $\frac{1}{2}$ in the log likelihood from the exponential. However the total log likelihood also changes with $a$ due to the $-\ln \sigma(a)$ from the denominator. The simple $\Delta \ln L = -\frac{1}{2}$ method considers all factors together, and thus wrongly includes this term.
The inaccuracy of the logarithmic method is appreciable. For reasonable values of \( N \) it is generally wrong in the second significant figure, and often pretty grossly wrong. That this occurs for both cases examined suggests that this is true in general. And yet values obtained by this method are frequently quoted to considerable precision by experiments.

In the complicated likelihood functions used in real experimental results, a simple Bartlett approach may not be possible. However the logarithmic approximation clearly does not provide the accuracy with which experiments wish to report their results. An alternative, available today but not in the 1950’s when these techniques were developed, is to use the known Likelihood function to perform the Neyman construction using Monte Carlo integration (the so-called ‘toy Monte Carlo’). This should be strongly recommended.

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