Limits, discovery and cut optimization for a Poisson process with uncertainty in background and signal efficiency: TRolke 2.0

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Abstract

A C++ class was written for the calculation of frequentist confidence intervals using the profile likelihood method. Seven combinations of Binomial, Gaussian, Poissonian and Binomial uncertainties are implemented. The package provides routines for the calculation of upper and lower limits, sensitivity and related properties. It also supports hypothesis tests which take uncertainties into account. It can be used in compiled C++ code, in Python or interactively via the ROOT analysis framework.

Key words: Confidence intervals, Hypothesis tests, systematic uncertainties, Poisson statistics

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• **Title of Program:** TRolke version 2.0

• **Program available from:** CPC Program Library, ...

• **Licensing provisions:** MIT License

• **Computer for which the program is designed:** Unix, GNU/Linux, Mac

• **Operating Systems under which the program has been tested:** Linux 2.6 (Scientific Linux 4 and 5, Ubuntu 8.10), Darwin 9.0 (Mac-OS X 10.5.8)

• **Programming Language used:** ISO C++

• **Memory required to execute with typical data:** $\sim 20$ MB,

• **No. of bytes in distributed program, including initialization file, etc..** 1 MB

• **Distribution Format:** tar file

• **Keywords:** confidence interval calculation, systematic uncertainties, profile likelihood

• **Nature of the Physical Problem:** The problem is to calculate a frequentist confidence interval on the parameter of a Poisson process with statistical or systematic uncertainties in signal efficiency or background.

• **Method of solution:** Profile likelihood method, Analytical

• **Typical Running Time:** $< 10^{-4}$ seconds per extracted limit.
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1 Introduction and scope

Routines were written for the calculation of frequentist confidence intervals using the profile likelihood method. The package provides routines for the calculation of upper and lower limits, average limits (sensitivity) and related properties, taking uncertainties in background estimate and signal efficiency into account. The implementation considers seven different statistical models with different combinations of Binomial, Gaussian, Poissonian or no uncertainties. For example in the Gaussian background case, our package derives upper and lower limits on the signal strength for a Poisson process with Gaussian background expectation $b \pm \delta b$. It is also possible to construct hypothesis tests which take uncertainties into account. The statistical problems are treated using the Profile Likelihood method.

The package provides a C++ class with accompanying examples. It can be used in compiled code, interactively via the ROOT [1] analysis framework, and from Python. This is TRolke version 2.0. It adds to version 1 (implemented in Fortran and in C++): hypothesis tests, a reworked user interface, documentation, examples and python support.

This paper is organized as follows. First, the profile likelihood methods is summarized, section 2; second, it is shown how our routines can be used for optimization of statistical discovery or limit setting power, section 3. The means for specification of the statistical model, and in general the class interface are described in section 4.
2 The profile likelihood method

Frequentist limits are constructed from data such that when repeated with new data the limits cover the fixed but unknown parameter value $\pi$ with a frequency which converges to the requested probability, the confidence level $1 - \alpha$. Limit calculation methods are often based on the inversion of an hypothesis test, as described in e.g. [2][3][4], and we follow the same scheme. Classical hypothesis tests investigate the validity of a default hypothesis, the null hypothesis $\mathcal{H}_0$; that an examined sample of data is compatible with background and we call the complementary hypothesis $\mathcal{H}_1$ a discovery. The profile likelihood method is based on the likelihood ratio tests statistic now described. For some observable $X$, let us assume a probability density function $f(X_i|\pi, b)$ depending on $k$ parameters $\pi = \{\pi_1, \ldots, \pi_k\}$ of interest to the researcher (such as the strengths of different signal sources), and $l$ additional nuisance parameters $b = \{b_1, \ldots, b_l\}$ (such as the strengths of different background sources). For a set of $n$ independent observations $X = \{X_1, \ldots, X_n\}$ the likelihood is

$$L(\pi, b|X) = \prod_{i=1}^{n} f(X_i|\pi, b).$$

The likelihood ratio test statistic is defined as

$$\lambda(\pi_0|X) = \frac{\sup\{L(\pi, b|X); \pi = \pi_0, b\}}{\sup\{L(\pi, b|X); \pi, b\}},$$

where the denominator is the likelihood maximized over the whole $\{\pi, b\}$ space, while the nominator is maximized over the more restrictive null hypothesis space $\{\pi = \pi_0, b\}$. The likelihood ratio $\lambda$ is also known as the profile likelihood and is a stochastic function explicitly depending on the data (and the null hypothesis) but not the nuisance parameters.
In general the inversion of a test to find the confidence region requires scanning over all possible signals, as described for example in [2]. Our routines instead make use of a very powerful result from mathematical statistics, that under some general conditions the distribution of $-2 \log \lambda$ converges to a chi-square distribution with $k$ degrees of freedom. Although these conditions are not satisfied in the problem considered here it has been shown that its performance is surprisingly good, especially when, as here, nuisance parameters are included. The statistical performance of the Profile likelihood method is studied in Ref.[5].

3 Analysis optimization for optimal limits or discovery power

In this section we describe how our routines are used for optimization of analysis cuts, with the figure of merit being either stringent limits (in case the signal is expected to be weak), or probability for discovery (if the signal is expected to be strong).

3.1 Analysis optimization for stringent limits in case of vanishing signal

When a signal is expected to be weak enough so that significant discovery is unlikely, it is relevant to optimize the analysis for optimal limit setting power. This can be done by assuming no signal and minimizing the so-called sensitivity. For example with a 90% confidence level (that is, $\alpha=10\%$), let us denote a calculated upper limit $s_{90}$. The sensitivity of the experiment is
defined as the average upper limit in case of vanishing signal;

\[ s_{90}(b) = \sum_{x=0}^{\infty} P(x, b)s_{90}(x, b), \quad (1) \]

where \( P(x, b) \) is the Poisson probability of observing \( x \) events for background expectation \( b \), in absence of signal. For finding the optimal analysis cut we can assume without loss of generality that the background and signal expectations are monotonically decreasing functions of a cut \( c \): \( s(c) = \mu_s \epsilon_s(c) \), and \( b(c) \). The constant \( \mu_s \) is the assumed normalisation of the signal at some arbitrary "no cut" level so that all uncertainties in the signal rate expectation are attributed to the signal detection efficiency \( \epsilon_s \).

As an example, let’s consider an energy dependent spectrum of particles probed by a particle detector. For the physical test spectrum

\[ \frac{d\Phi_{\text{test}}(E)}{dE} = a_{\text{test}} \frac{d\phi(E)}{dE}, \quad (2) \]

the expected number of observed signal events is

\[ s_{\text{test}} = a_{\text{test}} \cdot T \int d\Omega \int \frac{d\phi(E)}{dE} \sigma(E) dE. \quad (3) \]

The cross section \( \sigma \) determines the detection efficiency which is now a function of the energy \( E \), and \( T \) is the exposure time. For the observation of \( x \) events the model rejection factor \( \xi(x) \) is defined as

\[ \xi(x) = s_{90}(x_0, b)/s_{\text{test}}. \quad (4) \]

The upper limit can be written in terms of the test signal

\[ \frac{d\Phi_{90}(E)}{dE} = \xi(x) \cdot \frac{d\Phi_{\text{test}}(E)}{dE}, \quad (5) \]
and the average limit on the signal strength, set by repeated independent experiments in case of vanishing signal is
\[
\frac{d\Phi_{90}(E)}{dE} = \xi \cdot \frac{d\Phi_{\text{test}}(E)}{dE},
\]
where \(\xi = \frac{s_{90}(b)}{s_{\text{test}}}\) is called the model rejection potential.

Our package provides \(s_{90}\) through the method `GetSensitivity(D & s_L, D & s_U)`, and the upper limit \(s_{90}\) (and the lower limits) through `GetLimits(D & s_L, D & s_U)`, where \(D\) indicates a double precision value.

### 3.2 Hypothesis testing with uncertainties

In order to reject \(H_0\) with significance \(\alpha\), the number of observed events \(x_0\) must be equal to or higher than a critical number \(x_C(b)\), where \(b\) is the background expectation. The significance \(\alpha\) is the probability of observing \(x_C\) or more events from a stochastic background with mean \(b\) assuming vanishing signal.

The part of sample space rejecting \(H_0\) is called the critical region, while its complement is called the acceptance region. In the constructed test the critical region is completely defined by \(x_C\). If the background expectation \(b\) was completely known, we could find \(x_C\) by solving
\[
P(n \geq x_C|b) = \sum_{n=x_C}^{\infty} P(n|b) \leq \alpha,
\]
where \(P(n|b)\) is the Poisson distribution, but in general the background expectation is unknown and so we find the critical value by inverting the profile likelihood method. Remembering that confidence regions are constructed such
that the true but unknown signal strength $S$ is outside the confidence region with probability $\alpha$ for any fixed $S$ we assume the hypothesis $\mathcal{H}_0$ which means $S = 0$. The critical region is therefore defined as the subset of values $x$ which gives rise to limits not covering $S = 0$. That is, $\mathcal{H}_0$ is rejected for observations that lead to lower limits $s_L$ larger than zero. The limits are monotonic in $x$, so the hypothesis test is completely characterised by a critical number $x_c$, and written $x \geq x_c$. This critical number algorithm is implemented as the method GetCriticalNumber(int& $n_c$).

3.3 Analysis optimization for signal discovery

Assuming a specific signal strength $s = S$, it is relevant to consider the probability of making a discovery. This is given by the power of the hypothesis test, $F_\beta \equiv 1 - \beta$. A signal hypothesis $\mathcal{H}_{\text{th}}$ is said to be at the visibility threshold if it leads to a discovery with a pre-specified probability $F_\beta$, for example 50%. Discovery is claimed when $x_0 \geq x_c$, so in order to minimise the visibility threshold, signal is added to the (background) expectation until the probability for $x \geq x_c$ is at least $F_\beta$.

For the case of vanishing uncertainties, the visibility threshold can be directly calculated from the Poisson distribution by finding the smallest signal $s_{\text{thP}}$ fulfilling

$$P(n \geq x_{\text{cP}}|b + s_{\text{thP}}) \geq F_\beta$$

or equivalently $P(n < x_{\text{cP}}|b + s_{\text{thP}}) < \beta$, where the critical value $x_{\text{cP}}$ is that found using equation $7$. The quantity $s_{\text{thP}}$ is the visibility threshold for the signal expectation in case of vanishing uncertainties. The construction is
shown in figure 1. Uncertainties are accounted for through the critical number $x_c$ as function of significance and expectation number. A method similar to this has previously been described by Punzi[7]. As in equation 8, signal is added to the (background) expectation until the probability for rejection of $H_0$ is at least $F_\beta$. This means

$$x_c \left( F_\beta, b + s, \Delta_{b+s} \right) \geq x_c \left( \alpha, b, \Delta_b \right)$$

where $\Delta_b$ and $\Delta_{b+s}$ represent the total uncertainties of background, and background plus signal respectively. Equation 9 is solved numerically by finding the smallest allowed signal expectation $s$ and the solution is called $s_{th}$. Since the tested hypothesis $H_0$ assumes exactly $S = 0$, we do not include any uncertainty in the signal efficiency, while here the background estimate is assumed Gaussian. The described procedure for finding the critical number in the presence of uncertainties is thus a function on the form $x_c(\alpha, b, \Delta_b)$, where $\Delta_b$ is
the background uncertainty.

Assuming that the uncertainties of signal efficiency and the background estimate are sufficiently uncorrelated and Gaussian (or exact), equation 9 becomes

\[ x_c \left( F_\beta, b(c) + s(c), \sqrt{\Delta_b(c)^2 + \Delta_s(c)^2} \right) \geq x_c (\alpha, b(c), \Delta_b(c)) . \]  

(10)

For the observation of \( x \) events the model rejection factor \( \xi(x) \) is defined as

\[ \xi(x) = \frac{s_{90}(x_0, b)}{s_{\text{test}}} , \]

(11)

where \( s_{\text{test}} \) is, as in section 3.3, the expectation number of signal events for an assumed test signal. The optimal cut \( c \) and the corresponding critical number \( x_c \) is found by minimising the signal strength \( \mu_{s_{\text{th}}} \) as function of the cut \( c \).

The visibility threshold for the expected number of observed signal events for a fixed cut \( c \) is

\[ s_{\text{th}} = \mu_{s_{\text{th}}} \epsilon_s(c) . \]

(12)

The physical threshold signal strength is found in terms of the test spectrum (in analogy with equation 6) by \( a_{\text{th}} = a_{\text{test}} \cdot s_{\text{th}} / s_{\text{test}} \), or equivalently

\[ \frac{d\Phi_{\text{th}}(E)}{dE} = \eta \cdot \frac{d\Phi_{\text{test}}(E)}{dE} , \]

(13)

where \( \eta = s_{\text{th}} / s_{\text{test}} \) is the model detection potential. Minimizing \( \eta \) optimizes the analysis such that the signal strength required for detection (with at least probability \( F_\beta = 1 - \beta \)) is minimized. Our code provides the critical number and the \( s_{\text{th}} \) through \texttt{GetCriticalNumber(int& nc)} and \texttt{bool TRolke2::GetLeastDetectableSignal(D& s_{\text{th}}, D \beta)}.
4 Class interface and use

The library allows seven combinations of efficiency and background rate models, each presented here. Once the model and its parameters are specified, the user can obtain limits, critical numbers and so on as explained in the subsequent sections.

4.1 Model Specification methods

4.1.1 \texttt{SetGaussBkgGaussEff}(x, bm, em, sde, sdb)

Background: Gaussian, Efficiency: Gaussian
This model implements the case of Gaussian background with expectation \( bm \) and standard deviation \( sdb \) and Gaussian efficiency with expectation \( em \) and standard deviation \( sde \). The integer \( x \) is the number of observed events.

4.1.2 \texttt{SetGaussBkgKnownEff}(x, bm, sdb, e)

Background: Gaussian, Efficiency: Known
This model implements the case of Gaussian background with expectation \( bm \) and standard deviation \( sdb \) and known efficiency \( e \). The integer \( x \) is the number of observed events.
4.1.3  *SetKnownBkgGaussEff*(\(x, em, sde, b\))

Background: Known, Efficiency: Gaussian

This model implements the case of Gaussian efficiency with expectation \(em\) and standard deviation \(sde\) and known background \(b\). The integer \(x\) is the number of observed events.

4.1.4  *SetKnownBkgBinomEff*(\(x, z, b, m\))

Background: Known, Efficiency: Binomial

This model implements the case of known background expectation \(b\) and Binomial signal efficiency. The integer \(z\) is the number of observed events (in the signal region) out of the \(m\) evaluated signal (Monte Carlo) events. The integer \(x\) is the number of observed events.
4.1.5  \textit{SetPoissonBkgKnownEff}(x, y, \tau, e)

Background: Poisson, Efficiency: Known
The background is either measured simultaneously with signal, from side-bands, or with separate background Monte Carlo. The real value $\tau$ is the size of the background region in terms of the size of the background regions. It can be used in two ways - Either it's the ratio between the size of the background and the signal regions in case background is observed (from sidebands), or in case background is determined from simulations; the ratio between simulated and observed exposure time. The background in the signal region is estimated from $\tau$ and the integer $y$, the number of observed events in background region. The integer $x$ is the number of observed events; as always in the signal region.

4.1.6  \textit{SetPoissonBkgBinomEff}(x, y, z, \tau, m)

Background: Poisson, Efficiency: Binomial
This model implements the case of Binomial signal efficiency and Poissonian background estimate. For an explanation of Binomial efficiencies, please refer to section 4.1.4 and for Poissonian backgrounds to section 4.1.5. The integer $x$ is the number of observed events.
4.1.7 SetPoissonBkgGaussEff\((x, y, em, sde, \tau)\)

Background: Poisson, Efficiency: Gaussian

This model implements the case of Gaussian signal efficiency and Poissonian background estimate. For an explanation of Binomial efficiency, please refer to 4.1.6, and for Poissonian backgrounds to section 4.1.4. The integer \(x\) is the number of observed events.

4.2 Configuration methods and constructor

The confidence level (CL) is set either at object construction via an optional argument or with either of the SetCL or SetCLSigmas methods.

Two options are offered to deal with cases where the maximum likelihood estimate (MLE) is not in the physical region. Bounding is controled with the SetBounding method. The “bounded likelihood” option corresponds to the “bounds for the physical region” option in MINUIT/MINOS[8][9]. Unbounded likelihood allows the maximum likelihood estimate to be in the unphysical region. It has better coverage[5] and is used by default.

4.3 Limit calculation methods

The calculation of limits for the model and parameters as specified, is performed with the any of the following methods;
4.3.1 bool GetLimits(D & s_L, D & s_U)

This method calculates and returns the upper and lower limits for the pre-
specified model, confidence level and model parameters.

4.3.2 bool GetSensitivity(D & s_L, D & s_U)

This method returns the average upper and average lower limits assuming
vanishing signal. The summation is a Poisson sum over the background
expectation. This can be used for cut optimization as described in sectioin
3.1.

4.3.3 bool GetLimitsQuantile(D & s_L, D & s_U, int & out_x, D q = 0.5)

This method returns the upper and lower limits for the outcome correspond-
ing to a given quantile q assuming vanishing signal and a simple Poisson
summation using the background expectation. As a default, the quantile
value 0.5 is used, corresponding to median limits. The quantile and median
method has the advantage over the sensitivity that it is independent of the
signal parameter metric. The quantile x value is returned as out_x.

4.3.4 bool GetLimitsML(D & s_L, D & s_U, int & out_x)

This method provides the upper and lower limits for the most likely outcome
(out_x), assuming vanishing signal.
4.4 Hypothesis test methods

These two methods are used for hypothesis testing as described in section 3.3.

4.4.1 bool GetCriticalNumber(int& nC)

Get the smallest number of observed events $x$, corresponding to rejection of the null hypothesis.

4.4.2 bool TRolke2::GetLeastDetectableSignal($D & s_{th}, D \beta$)

Get the smallest signal strength leading to rejection of the null hypothesis with probability $\beta$ as described in section 3.2. Currently Gaussian as well as vanishing uncertainties are supported.

4.5 Availability and prerequisites

The latest versions of the code, its documentation and examples are freely available[10]. The class makes use of a number of ROOT [11] routines for standard mathematical functions, the interactive interface and bindings which makes it easy to use our methods in Python. Examples of all functionality of the C++ class are included in our code and demonstrate its use with Python, as interactive C++, and as a compiled example program.
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