Implementation of upper limit calculation for a Poisson variable by Bayesian approach*

ZHU Yong-Sheng(朱永生)[1)]

(Institute of High Energy Physics, CAS, Beijing 100049, China)

Abstract The calculation of Bayesian confidence upper limit for a Poisson variable including both signal and background with and without systematic uncertainties has been formulated. A Fortran 77 routine, BPULE, has been developed to implement the calculation. The routine can account for systematic uncertainties in the background expectation and signal efficiency. The systematic uncertainties may be separately parameterized by a Gaussian, Log-Gaussian or flat probability density function (pdf). Some technical details of BPULE have been discussed.

Key words upper limit, systematic uncertainties, Poisson distribution, Bayesian statistics

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1 Introduction

A group of particle physics experiments involves the search for new signal or measuring small signal at the circumstance with significant background. A limit on, or a measurement of, a physical quantity at a given confidence level is usually set by comparing a number of detected events with the expected number of background events in the "signal" window where the signal events (if exist) shall reside. How well this comparison can be made for the observed events and the expected background depends strongly on the systematic uncertainties existing in the measurement. Therefore, systematic uncertainties must be taken into consideration in the limit or confidence belt calculation.

Conrad et al.[1] reviewed the methods of confidence belt construction in the frame of frequentist statistics, and developed a FORTRAN program, POLE[2], to calculate the confidence intervals for a maximum of the observed events of 100 and a maximum signal expectation of 50. The ordering schemes for frequentist construction supported are the Neyman method[3], likelihood ratio ordering[4] and improved likelihood ratio ordering[5]. The systematic uncertainties in both the signal and background efficiencies as well as systematic uncertainty of background expectation have been taken into account in the confidence belt construction by assuming a probability density function (pdf) which parameterizes our knowledge on the uncertainties and integrating over this pdf. This method, combining classical and Bayesian elements, is referred to as semi-Bayesian approach.

In the frame of Bayesian statistics[6], Narsky[7, 8] depicted the estimation of upper limits for Poisson statistic with the known background expectation. Treatment of background uncertainty is discussed with the flat prior for simplified cases of background expectation distributions in Refs. [9, 10]. Inclusion of systematic uncertainties in both the signal efficiency and background expectation in the upper limit calculation via Bayesian approach has been recently discussed by Yongsheng ZHU[11].

In this paper, we describe the implementation of Bayesian confidence upper limit calculation for a Poisson variable including both signal and background with and without systematic uncertainties and its relevant FORTRAN program BPULE[12].

2 Formulation for Bayesian upper limit calculation

For the detailed discussion on the Bayesian confi-

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1) E-mail: zhuys@ihep.ac.cn

dence upper limit calculation for a Poisson process with and without systematic uncertainties, please refer to Ref. [11]. Here, we only list the necessary formulae used in the calculation. Throughout this paper we assume that in the signal window, where the signal events (if exist) shall reside, the number of signal events is a Poisson variable with unknown expectation s to be inferred, and the number of background events is a Poisson variable with known expectation b, and the conditional pdf of observing n total events in the window is represented by $q(n|s)_b$, which will be discussed below in this section.

The upper limit of the expected number of signal events at given confidence level CL=$1-\alpha$, S_{UP}, is given by:

$$1-\alpha=\int_0^{S_{\mathrm{UP}}} h(s|n)\mathrm{d}s\,, \tag{1}$$

where $h(s|n)$ is the posterior pdf, and can be expressed as

$$h(s|n)=\frac{q(n|s)_b\pi(s)}{\displaystyle\int_0^\infty q(n|s)_b\pi(s)\mathrm{d}s}\,. \tag{2}$$

$\pi(s)$ is the non-informative prior:

$$\pi(s)\propto\frac{1}{(s+b)^m},\quad s\geqslant 0,\quad b\geqslant 0,\quad 0\leqslant m\leqslant 1, \tag{3}$$

where m=0 corresponds to Bayes prior, m=0.5 to $1/\sqrt{s+b}$ prior, and m=1 to $1/(s+b)$ prior. The statistical bases on these three priors are referred to Refs. [13—16]. One can choose m value as he/she thinks appropriate, however, it should always be kept in mind that different m values will give different answers for the upper limit. The expected coverage and length of confidence intervals constructed with these three priors and with the Neyman construction[3] and unified approach[4] can be found in Ref. [8]. It has been shown that the $1/\sqrt{s+b}$ prior is the most versatile choice among the Bayesian methods, it provides a reasonable mean coverage for the confidence interval and upper limit for Poisson observable.

2.1 Upper limit without inclusion of systematic uncertainties

In the case that the systematic uncertainties of the signal efficiency and background expectation can be neglected, the signal expectation s is an unknown constant and the background expectation b is a known value. In this case, $q(n|s)_b$ in Eq. (2) is simply equal to the usual Poisson probability $p(n|s)_b$

$$p(n|s)_b=\mathrm{e}^{-(s+b)}\frac{(s+b)^n}{n!}\,, \tag{4}$$

and the posterior pdf is then given by

$$h(s|n)=\frac{(s+b)^{n-m}\mathrm{e}^{-(s+b)}}{\Gamma(n-m+1,b)}\,, \tag{5}$$

where

$$\Gamma(x,b)=\int_b^\infty s^{x-1}\mathrm{e}^{-s}\mathrm{d}s\,,\quad x>0,b>0 \tag{6}$$

is an incomplete gamma function. Substituting this posterior pdf into Eq. (1) we obtain

$$\alpha=\frac{\Gamma(n-m+1,S_{\mathrm{UP}}+b)}{\Gamma(n-m+1,b)}\,. \tag{7}$$

If the flat prior (m=0) is used, Eq. (7) turns into

$$\alpha=\mathrm{e}^{-S_{\mathrm{UP}}}\cdot\frac{\sum_{k=0}^n\frac{(S_{\mathrm{UP}}+b)^k}{k!}}{\sum_{k=0}^n\frac{b^k}{k!}}\,. \tag{8}$$

The upper limit S_{UP} at a given confidence level CL=1–α can be acquired by solving Eq. (7) or Eq. (8) numerically from the measured values of n and b.

2.2 Upper limit with inclusion of systematic uncertainties

Now we turn to the question of inclusion of systematic uncertainties. In this case, both the signal expectation and background expectation are not the constants, but the variables; they have respective distributions.

First we consider only the uncertainty of background expectation is present, and the distribution of the background expectation is represented by a pdf $f_{b'}(b,\sigma_b)$ with the mean b and standard deviation σ_b. The conditional pdf is expressed as

$$q(n|s)_b=\int_0^\infty p(n|s)_{b'}\cdot f_{b'}(b,\sigma_b)\mathrm{d}b'\,, \tag{9}$$

where $p(n|s)_{b'}$ has the same expression in Eq. (4) with b replaced by b'.

Next we take into account the uncertainties of the signal efficiency and background expectation simultaneously, and assume they are independent of each other. The distribution of the relative signal efficiency ε (with respect to the predicted value of the signal detection efficiency η) is described by a pdf $f_\varepsilon(1,\sigma_\varepsilon)$ with the mean 1 and standard deviation σ_ε. The conditional pdf now is

$$q(n|s)_b=\int_0^\infty\int_0^\infty p(n|s\varepsilon)_{b'}f_{b'}(b,\sigma_b)f_\varepsilon(1,\sigma_\varepsilon)\mathrm{d}b'\mathrm{d}\varepsilon\,, \tag{10}$$

where $p(n|s\varepsilon)_{b'}$ represents that in Eq. (4), b is replaced by b', and s by $s\varepsilon$. One notices that the lower limits of integrals in Eqs. (9), (10) are all zeros, which are the possible minimum value of any efficiencies and number of background events. One can then calculate the upper limit S_{UP} on s at any given confidence level with inclusion of systematic uncertainties in terms of Eqs. (1), (2).

3 BPULE: an algorithm for calculating Bayesian upper limit

We have developed an algorithm for calculating the upper limit (UL) on Poisson observables for any given confidence level with or without inclusion of systematic uncertainties in background expectation and signal efficiency. It has been implemented as a FORTRAN program, BPULE (Bayesian Poissonian Upper Limit Estimator)[12], where an iterative procedure is carried out by minimizing the difference between the given confidence level and the calculated value in terms of Eqs. (1), (2) until a convergence is reached. Some technical issues of BPULE are described below.

3.1 Upper limit without inclusion of systematic uncertainties

To determine the upper limit without inclusion of systematic uncertainties, we need to solve Eq. (7) numerically. Given the initial value for $S_{\rm UP}$ first, we calculate the corresponding α value by calling the subroutine GAMDIS from CERN Program Library (G106)[17]. It can be easily shown from Eq. (7) that

$$\alpha=\frac{1-GAMDIS(S_{\rm UP}+b,n-m+1)}{1-GAMDIS(b,n-m+1)}\,. \qquad (11)$$

By minimizing the object function $F{=}(CL-CL_0)^2$, with CL and CL_0 being the calculated and given confidence level, respectively, we obtain the desired solution $S_{\rm UP}$.

3.2 Upper limit with inclusion of systematic uncertainties

To determine the upper limit with inclusion of systematic uncertainties, we need to solve Eq. (1) numerically together with Eqs. (2), (9), (10). The denominator of $h(s|n)$ shown in Eq. (2) is an integral over s with the upper bound of infinity, which makes the numerical calculation difficult. To ease the calculation, we use a variable transformation of s to z with $z{=}\exp(-s)$, then the lower and upper bounds for s, $(0,\infty)$, transformed to (0,1) for z:

$$\int_0^\infty g(s){\rm d}s=\int_0^1\frac{1}{z}g(s(z)){\rm d}z\,. \qquad (12)$$

Then, Eq. (1) can be rewritten as

$$1-\alpha=\frac{\displaystyle\int_0^{S_{\rm UP}}q(n|s)_b\pi(s){\rm d}s}{\displaystyle\int_0^\infty q(n|s)_b\pi(s){\rm d}s}=\frac{\displaystyle\int_{z_{\rm UP}}^1\frac{1}{z}q(n|s(z))_b\pi(s(z)){\rm d}z}{\displaystyle\int_0^1\frac{1}{z}q(n|s(z))_b\pi(s(z)){\rm d}z}, \qquad (13)$$

where $z_{\rm UP}{=}\exp(-S_{\rm UP})$. Notice that $q(n|s)_b$ now is an one-fold or a two-fold integral, therefore, both the denominator and numerator of Eq. (13) are two-fold or three-fold integrals, which we calculate by using the subroutine DGMLTN from CERN Program Library (D110).

3.3 Input of BPULE

To run the BPULE, the following valuables are required to input:

ID, IBK, IE, N, B, SIGBK, SIGE, ETA, CL, AM.

Their meanings are listed in Table 1.

Table 1. Input variables of BPULE and their meanings.

notation	meaning
ID	flag to select the type of the upper limit to be calculated.
IBK	flag to select the distribution for bkgd expectation.
IE	flag to select the distribution for signal detection efficiency.
N	number of total events observed in signal window,n.
B	predicted bkgd expectation in signal window,b.
SIGBK	standard deviation of the distribution for relative bkgd expectation,σ_b/b.
SIGE	standard deviation of the distribution for relative signal efficiency,σ_ε .
ETA	predicted signal detection efficiency,η.
CL	confidence level, $CL=1-\alpha$.
AM	prior selection. $AM{=}m$, prior is $1/(s+b)^m$, $0\leqslant m\leqslant 1$.

Flag ID can take four values with the following assignment: 1—UL without considering any systematic uncertainties; 2—UL incorporating systematic uncertainty of bkgd expectation; 3—UL incorporating systematic uncertainty of signal efficiency; 4—UL incorporating systematic uncertainties of bkgd expectation and signal efficiency simultaneously, and they are assumed to be independent of each other.

For the distribution of relative signal efficiency (signal efficiency divided by η) or relative background expectation (background expectation divided by b), three types of functions with the mean 1 and standard deviation σ are supported: Gaussian, Log-Gaussian and flat distributions. They correspond to flag value of IBK or IE of 1, 2, 3, respectively. For the Gaussian distribution, the pdf is

$$f_x(1,\sigma)=\frac{1}{\sqrt{2\pi}\sigma}{\rm e}^{-\frac{(x-1)^2}{2\sigma^2}}\,,\quad x\in(-\infty,\infty). \qquad (14)$$

For the Log-Gaussian distribution, the pdf is

$$f_x(1,\sigma)=\frac{1}{\sqrt{2\pi}\sigma_x x}{\rm e}^{-\frac{(\ln x-\mu)^2}{2\sigma_x^2}}\,,\quad x\in(0,\infty), \qquad (15)$$

where $\mu=-\ln(1+\sigma^2)/2$, $\sigma_x=\sqrt{\ln(1+\sigma^2)}$. For the flat distribution, the pdf is

$$f_x(1,\sigma)=\frac{1}{x_{\max}-x_{\min}},\quad x\in[x_{\min},x_{\max}], \qquad (16)$$

where $x_{\min}=1-\sqrt{3}\sigma$, $x_{\max}=1+\sqrt{3}\sigma$.

3.4 Bounds of the integral of Eqs. (9), (10)

Although the bounds of the integral of Eqs. (9), (10) are written as $(0,\infty)$, however, in the numerical calculation, the integral over 0 to ∞ is difficult to implement. Instead, we use different lower and upper bounds for different functions shown in Eqs. (14)—(16). For the Gaussian pdf, the lower and upper bounds, $x_{\rm min}$ and $x_{\rm max}$, are set to 0 and $1+4\sigma$, respectively. In the region of $x > x_{\rm max}$, the integrated probability is less then 3.2×10^{-5}, which is negligible. One must be aware that, Gaussian pdf spans from $-\infty$ to $+\infty$, the program user must consider if the Gaussian pdf is an appropriate description for the distribution of relative signal efficiency or relative background expectation. In the case of $\sigma < 1/3$, the cut-off effect below $x=0$ is negligible, therefore, the use of Gaussian pdf has practically no problem. For the Log-Gaussian pdf, $x_{\rm min}$ and $x_{\rm max}$ are set to 0 and $e^{\mu+4\sigma_x}$, respectively, over which the cumulative probability is larger than 0.99997. For the flat distribution, $x_{\rm min}$ and $x_{\rm max}$ are given in Eq. (16), which is determined by the requirements of mean value being 1 and standard deviation being σ. Besides, there are common constraints for $x_{\rm min}$ and $x_{\rm max}$: if the $x_{\rm min}$ determined above is less then zero, then the $x_{\rm min}$ is set to zero; if the $x_{\rm max}$ for relative signal detection efficiency is larger than $1/\eta$, then the $x_{\rm max}$ is set to $1/\eta$, to ensure the signal detection efficiency not larger than 1.

3.5 Run the BPULE

The algorithm BPULE contains two executable files: BPULE.exe for calculating single upper limit while BPULE_batch.exe for a batch of upper limits. They can be downloaded from Ref. [12]. Type "BPULE.exe" to run the program, the prompt is as follows:

"(notice types of variables)
Input ID, IBK, IE, N, B, SIGBK, SIGE, ETA, CL, AM".

Then you type in the corresponding values, for example,

4 1 1 10 7. 0.1 0.08 0.15 0.9 0.

The program will automatically generate an output file "BPULE.out", which gives, in addition to the input values, two numbers:

$S_{\rm UP}$—the upper limit of s with given confidence level,
FCN—$0.001\sqrt{FCN} = |CL(\text{calculated})\text{-}CL(\text{given})|/\ CL(\text{given})$.

To run the BPULE_batch.exe, an input file, BPULE_batch.int, must be prepared beforehand, which should contain the following information:

k (number of upper limits to be calculated)
ID IBK IE N B SIGBK SIGE ETA CL AM (1)
ID IBK IE N B SIGBK SIGE ETA CL AM (2)
....
ID IBK IE N B SIGBK SIGE ETA CL AM (k).

The program will automatically generate an output file "BPULE_batch.out", which gives, in addition to the input values, k corresponding upper limits.

4 Summary

We have formulated the upper limit calculation at any given confidence level in the line of Bayesian approach for the Poisson observable incorporating systematic uncertainties in both the signal efficiency and background expectation prediction. A FORTRAN program, BPULE, has been developed to implement the upper limit calculation. Some technical details have been described. The typical results acquired by BPULE are referred to Ref. [11].

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