OPTHyLiC: an Optimised Tool for Hybrid Limits Computation

E. Busato, D. Calvet and T. Theveneaux-Pelzer

LPC Clermont-Ferrand, CNRS/IN2P3, Université Blaise Pascal, France

February 10, 2015

Abstract

A software tool, computing observed and expected upper limits on poissonian process rates using a hybrid frequentist-bayesian $CL_s$ method, is presented. This tool, optimised for counting experiments combining several channels, takes into account statistical and systematic uncertainties, as well as correlations of systematic uncertainties between channels. It has been validated against other software tools or analytical calculations, in several cases.

Contents

1 Introduction 2

2 Notations 2

3 Method description 2

3.1 Statistical model ........................................ 3
3.2 Treatment of statistical uncertainties .................. 3
3.3 Treatment of systematic uncertainties ................ 5
3.4 Inference of observed upper limit $\mu_{up}$ ............... 9
3.5 Computation of expected limits ....................... 10

4 Software description 10

4.1 Structure and prerequisites ............................. 10
4.2 Installation and examples ............................... 11
4.3 Input file format ....................................... 11
4.4 Running the software ................................... 14

5 Software validation 17

5.1 Validation of calculations without uncertainties .......... 17
5.2 Validation of calculations with statistical and systematic uncertainties ............ 19

6 Conclusion 22

Acknowledgements 22

References 22
1 Introduction

In a physics experiment, the result must sometimes be interpreted in term of upper limits on the rate of a particular physical process of interest, dubbed signal. The most simple situation is the co-called counting experiment, in which the upper limit is inferred from the total number of observed events (the outcome of the experiment), using an estimation of the expected number of signal events and of the expected number of events due to other physical processes – the backgrounds.

OpTHyLiC offers an easy-to-use hybrid frequentist-bayesian solution to the counting experiment problem for an arbitrary number of channels and backgrounds, using the CLs method. Statistical and systematic uncertainties are taken into account in a bayesian way, and correlations of systematic uncertainties across backgrounds and channels are properly accounted for. OpTHyLiC can be downloaded from [1].

Other tools such as MCLIMIT [2] or RooStats [3] provide the ability to compute limits using the same method. However, OpTHyLiC was specifically optimized for counting experiments. It is light, simple and fast. Furthermore, it provides several options to configure the treatment of statistical and systematic uncertainties.

The document is organized as follows. The notations used in this paper are introduced in Sec. 2. The statistical method implemented in OpTHyLiC is described in Sec. 3. The software is described in Sec. 4 and its validation in Sec. 5.

2 Notations

The following notations will be used throughout the document:

- $\mu$: signal strength, defined as the actual signal rate divided by a fixed reference signal rate value (such as obtained from a theoretical prediction);
- $\mu_{\text{up}}$: upper limit on the signal strength;
- $n$: number of channels for the counting experiment;
- $s_c$: event yield for signal process in channel $c$ ($c \in [1,n]$);
- $s_{c}\text{\text{om}}$: nominal event yield for signal process in channel $c$;
- $\sigma_c$: absolute statistical uncertainty for signal process in channel $c$;
- $b_{ci}$: event yield for type $i$ background process in channel $c$;
- $b_{c}\text{\text{om}}$: nominal event yield for type $i$ background process in channel $c$;
- $b_{c}\text{\text{om}} = \sum_{i \in \text{backgrounds}} b_{ci}\text{\text{om}}$: total nominal yield for background processes in channel $c$;
- $\sigma_{ci}$: absolute statistical uncertainty for type $i$ background process in channel $c$;
- $N_c$: event yield in channel $c$;
- $N_{c}\text{\text{obs}}$: event yield actually observed in the data or the pseudo-data in channel $c$.

3 Method description

OpTHyLiC implements the frequentist $CL_s$ method [4]. Pseudo-experiments are generated and the distribution of a test statistic is determined under both signal plus background and background only hypotheses. From these distributions, $CL_s$ is computed and the upper signal strength $\mu_{\text{up}}$ is found by solving the equation

$$CL_s(\mu) = \alpha,$$

(1)
for a fixed value of $\alpha$ which is set depending on the chosen confidence level $1 - \alpha$. For 95% confidence level upper limits, $\alpha = 0.05$. The test statistic used is the ratio of likelihoods under signal plus background and background only hypotheses:

$$q_\mu = -2 \ln \frac{\mathcal{L}(\mu)}{\mathcal{L}(\mu = 0)}.$$  \hspace{1cm} (2)

The general form of the likelihood is discussed in Sec. 3.1. The statistical and systematic uncertainties are included by the use of nuisance parameters, as detailed in Sec. 3.2 and 3.3, respectively. These uncertainties are accounted for in a bayesian way: the inference of the observed upper limit is performed from pseudo-experiments using the likelihood marginalised over the nuisance parameters, as explained in Sec. 3.4. The procedure for calculating the expected limits is summarised in Sec. 3.5.

### 3.1 Statistical model

The full likelihood, including all nuisance parameters, is given by:

$$\mathcal{L}(\mu, \{s'_c, b'_ci, \eta_j\}) = \prod_c \left[ \frac{(\mu s_c + b_c)^N_c}{N_c!} e^{-(\mu s_c + b_c)} \right] f(s'_c; s'^{\text{nom}}_c, \sigma_c) \prod_i f(b'_ci; b'^{\text{nom}}_ci, \sigma_{ci}) \prod_j g(\eta_j),$$  \hspace{1cm} (3)

where:

- the index $c$ runs over the channels;
- the index $i$ runs over the backgrounds;
- the index $j$ runs over the systematic uncertainties;
- $s_c = s'_c \times k^{\text{syst}}_c(\{\eta_j\})$;
- $b_c = \sum_{i \in \text{backgrounds}} b_{ci} = \sum_{i \in \text{backgrounds}} b'^{\text{syst}}_{ci}(\{\eta_j\})$.

The set of nuisance parameters $\{s'_c, b'_ci, \eta_j\}$ can be divided into two categories. The first ones, $\{s'_c, b'_ci\}$, account for the statistical uncertainties, arising from the finite size of samples used to estimate the signal and background nominal yields $s'^{\text{nom}}_c$ and $b'^{\text{nom}}_ci$, respectively, are constrained by the functions $f$. The second ones, $\{\eta_j\}$, account for the systematic uncertainties, and are constrained by the functions $g$. The variation of the signal and background yields under the effect of the systematic uncertainties are described by the functions $k^{\text{syst}}_c(\{\eta_j\})$ and $k^{\text{syst}}_{ci}(\{\eta_j\})$, respectively.

### 3.2 Treatment of statistical uncertainties

The nuisance parameters $s'_c$ and $b'_ci$, accounting for the statistical uncertainties on the nominal signal and background yields, are constrained by probability density functions (p. d. f.) $f$ of the form:

$$f(y; y^{\text{nom}}, \sigma),$$  \hspace{1cm} (4)

where $y$ is the nuisance parameter, $y^{\text{nom}}$ the nominal yield and $\sigma$ the statistical uncertainty, which can be the square root of summed squared weights (e.g. when $y^{\text{nom}}$ is estimated from a mixture of normalised simulated samples).

In OpTHyLiC, five different p. d. f. can be used as constraints: a normal distribution, a log-normal distribution, or three different types of gamma distributions.

#### 3.2.1 Normal and log-normal constraints

The parameters of the normal and log-normal p. d. f. are chosen so that the average and the standard deviation of these distributions are equal to $y^{\text{nom}}$ and $\sigma$, respectively. The normal distribution has the form:

$$f_N(y; y^{\text{nom}}, \sigma) = \frac{1}{\sigma \sqrt{2\pi}} \exp \left( -\frac{(y - y^{\text{nom}})^2}{2\sigma^2} \right),$$  \hspace{1cm} (5)
and the log-normal distribution has the form:

\[ f_L(y; y^{\text{nom}}, \sigma) = \frac{1}{y b \sqrt{2\pi}} \exp\left(-\frac{(\ln y - a)^2}{2b^2}\right). \]  

(6)

with

\[ a = \ln \left(\frac{(y^{\text{nom}})^2}{\sqrt{(y^{\text{nom}})^2 + \sigma^2}}\right) \quad \text{and} \quad b = \sqrt{\ln \left(1 + \frac{\sigma^2}{(y^{\text{nom}})^2}\right)}. \]

(7)

The normal distribution can be defined for any real \( y \) values, including non-physical negative event yields. On the contrary, the log-normal distribution is defined only for \( y > 0 \).

### 3.2.2 Gamma constraints

The three gamma p. d. f. have the general form:

\[ f_G(y; a, b) = \frac{a (ay)^{b-1} e^{-ay}}{\Gamma(b)}, \]

(8)

where \( a \) and \( b \) are the rate and shape parameters respectively. As for the log-normal, the gamma distributions are defined for any strictly positive value or \( y \).

This p. d. f. can be seen as the posterior distribution obtained from an auxiliary measurement accounting for the poissonian nature of the statistical uncertainty. Accounting for this nature is not straightforward since events are in general weighted. A popular approach (used for example in HistFactory [5]) is to consider an imaginary auxiliary measurement in which all events have unit weight (which can therefore be described by a Poisson distribution) and in which the relative statistical uncertainty is equal to that used in the main measurement \( (\sigma/y^{\text{nom}}) \).

Let \( N_{\text{aux}} \) be the number of events observed in this auxiliary measurement. The auxiliary measurement likelihood is:

\[ P(N_{\text{aux}}; \lambda) = \frac{\lambda^{N_{\text{aux}}}}{\Gamma(N_{\text{aux}} + 1)} e^{-\lambda}, \]

(9)

where \( \lambda \) is the (unknown) nuisance parameter. It can be written as:

\[ \lambda = \gamma N_{\text{aux}}^{\text{nom}}, \]

(10)

where \( N_{\text{aux}}^{\text{nom}} \) is the nominal value of \( N_{\text{aux}} \) and \( \gamma \) the nuisance parameter affecting the yield in the main measurement – the product of Poisson terms in Eq. 3 – in a multiplicative way: \( y = \gamma y^{\text{nom}} \). \( N_{\text{aux}}^{\text{nom}} \) is found by imposing that the relative statistical uncertainty is the same in the auxiliary and main measurements:

\[ N_{\text{aux}}^{\text{nom}} = \left(\frac{y^{\text{nom}}}{\sigma}\right)^2. \]

(11)

The auxiliary measurement likelihood can then be written as follows:

\[ P(N_{\text{aux}}; \gamma) = \frac{\left(\gamma (y^{\text{nom}}/\sigma)^2\right)^{N_{\text{aux}}}}{\Gamma(N_{\text{aux}} + 1)} e^{-\gamma (y^{\text{nom}}/\sigma)^2}. \]

(12)

From this likelihood, posterior distributions for \( \gamma \) can be determined for various prior distributions \( \pi(\gamma) \):

\[ g(\gamma) = \frac{P(N_{\text{aux}} = N_{\text{aux}}^{\text{nom}}; \gamma) \pi(\gamma)}{\int P(N_{\text{aux}} = N_{\text{aux}}^{\text{nom}}; \gamma) \pi(\gamma) d\gamma}. \]

(13)

These posterior distributions can then be translated into posterior distributions for the yield \( y \) (hereafter denoted as \( f(y; y^{\text{nom}}, \sigma) \), using the same notation as in Eq. 4).

Three prior distributions are considered; in each case, the posterior distribution for \( y \) is a gamma distribution with the general form given by Eq. 8:
• $\pi(\gamma) \propto 1$ (uniform prior); in this case, the posterior distribution is:

$$f(y; y_{\text{nom}}, \sigma) = f_G\left(y; a = y_{\text{nom}}/\sigma^2, b = (y_{\text{nom}}/\sigma)^2 + 1\right);$$

(14a)

• $\pi(\gamma) \propto 1/\sqrt{\gamma}$ (Jeffreys prior\(^1\)); in this case, the posterior distribution is:

$$f(y; y_{\text{nom}}, \sigma) = f_G\left(y; a = y_{\text{nom}}/\sigma^2, b = (y_{\text{nom}}/\sigma)^2 + 1/2\right);$$

(14b)

• $\pi(\gamma) \propto 1/\gamma$ (hyperbolic prior); in this case, the posterior distribution is:

$$f(y; y_{\text{nom}}, \sigma) = f_G\left(y; a = y_{\text{nom}}/\sigma^2, b = (y_{\text{nom}}/\sigma)^2\right).$$

(14c)

The three gamma constraints available in OpTHyLiC correspond to the three posteriors given in Eq. 14a, 14b and 14c. They are summarized in Tab. 1, where expectation and standard deviation for $y$ are also given (we recall that for the gamma p. d. f. in Eq. 8, one has $\mathbb{E}[y] = b/a$ and $\text{var}[y] = b/a^2$). As can be seen from this table, the expectation and standard deviation are equal to the nominal yield and statistical uncertainty only for the hyperbolic prior $\pi(\gamma) \propto 1/\gamma$, as for the normal and log-normal constraints. For the gamma constraints with the uniform and Jeffreys priors, it is not the case, but the difference vanishes in the asymptotic limit.

| prior | posterior parameters | $\mathbb{E}[y]$ | $\text{var}[y]$ |
|-------|----------------------|-----------------|-----------------|
| $\pi(\gamma) \propto 1$ | $y_{\text{nom}}/\sigma^2$ | $y_{\text{nom}} + \sigma^2/y_{\text{nom}}$ | $\sigma^2 \left(1 + \sigma^2/(y_{\text{nom}})^2\right)$ |
| $\pi(\gamma) \propto 1/\sqrt{\gamma}$ | $y_{\text{nom}}/\sigma^2$ | $y_{\text{nom}} + 1/2\sigma^2/y_{\text{nom}}$ | $\sigma^2 \left(1 + 1/2\sigma^2/(y_{\text{nom}})^2\right)$ |
| $\pi(\gamma) \propto 1/\gamma$ | $y_{\text{nom}}/\sigma^2$ | $y_{\text{nom}}$ | $\sigma^2$ |

Table 1: Summary of the three gamma constraints available in OpTHyLiC. The constants $a$ and $b$ are parameters of the posterior distribution which general form is given in Eq. 8.

### 3.2.3 Comparison of the constraint functions

The five available constraint functions – normal, log-normal and the three gamma distributions – are compared for three different values of $y_{\text{nom}}$ and $\sigma$ in Fig. 1. When $\sigma$ is small with respect to $y_{\text{nom}}$, the distributions are very close to each other. Otherwise, the differences between the distributions can be significant.

Care should be taken when statistical uncertainties are large or when nominal yields are equal to zero. When statistical uncertainties are large, constraint p. d. f. can be truncated at zero in the normal case. In such cases, log-normal and gamma should be preferred. When nominal yields are equal to zero, log-normal and gamma are undefined. In such cases, OpTHyLiC automatically selects a normal constraint truncated at zero.

### 3.3 Treatment of systematic uncertainties

Systematic uncertainties on nominal yields $s_{c_{\text{nom}}}^2$ and $b_{c_{\text{nom}}}^2$ are accounted for by including the set of nuisance parameters $\{\eta\}$. They are assumed to be either 100% correlated or completely uncorrelated. The total number of nuisance parameters is therefore equal to the total number of independent systematic uncertainties, including all channels, backgrounds and signals. The correlation factor between two nuisance

\(^1\)We recall that Jeffreys prior is $\pi(\gamma) \propto \sqrt{I(\gamma)}$, where the Fisher information is $I(\gamma) = \mathbb{E}\left[\left(\frac{\partial \log P(N_{\text{data}}|\gamma)}{\partial \gamma}\right)^2\right]$. Injecting Eq. 12 in this expression leads to $\pi(\gamma) \propto 1/\sqrt{\gamma}$.
parameters $\eta_j$ and $\eta_k$ is given by the Kronecker symbol $\delta_{jk}$. The term constraining nuisance parameters in the likelihood can thus be factorized into the product of individual constraint terms. In Eq. 3, the nuisance parameter for each systematic uncertainty of index $j$ is constrained by a standard normal p. d. f. $g$ of the form:

$$g(\eta_j) = \frac{1}{\sqrt{2\pi}} e^{-\frac{\eta_j^2}{2}}. \quad (15)$$

As stated in Sec. 3.1, the effect of systematic uncertainties on the yield is described by relations of the form:

$$y = y^{\text{nom}} \times k^{\text{syst}}(\{\eta_j\}), \quad (16)$$

where $y$ is the varied yield, $y^{\text{nom}}$ the nominal yield and $k^{\text{syst}}(\{\eta_j\})$ the function describing the variation of the yield with the set of nuisance parameters $\{\eta_j\}$. OpTHyLiC provides two different solutions for combining the effect of multiple nuisance parameters:

- additive:

$$k^{\text{syst}}(\{\eta_j\}) - 1 = \sum_{j \in \text{systematics}} [h_j^{\text{syst}}(\eta_j) - 1]; \quad (17a)$$

- multiplicative:

$$k^{\text{syst}}(\{\eta_j\}) = \prod_{j \in \text{systematics}} h_j^{\text{syst}}(\eta_j). \quad (17b)$$

In Eq. 17a and 17b, $h_j^{\text{syst}}(\eta_j)$ is the function describing the variation of the yield with nuisance parameter $j$. In both cases, when the effect of only one nuisance parameter is considered, $k^{\text{syst}}(\eta_j) = h_j^{\text{syst}}(\eta_j)$ as it should.

For each systematic uncertainty $j$, the corresponding nuisance parameter $\eta_j$ is chosen such that $\eta_j = 0$ corresponds to no variation, $\eta_j = +1$ to a $+1\sigma$ variation, and $\eta_j = -1$ to a $-1\sigma$ variation. The main problematic associated to systematic uncertainties is the choice of the function $h_j^{\text{syst}}(\eta_j)$ that relates the effect of the systematic uncertainty to its associated nuisance parameter. Usually, $h_j^{\text{syst}}$ is known, for each systematic, for $\eta_j = 0$, $-1$ and $+1$. The value for $\eta_j = 0$ is by definition equal to 1: it corresponds to the case $y = y^{\text{nom}}$. Let $h_j^\uparrow (h_j^\downarrow)$ be the relative variation of the yield when systematic $j$ is varied by $+1$ ($-1$) $\sigma$. Thus, for all $j$:

$$h_j^{\text{syst}}(\eta_j = 0) = 1; \quad (18a)$$

$$h_j^\uparrow = h_j^{\text{syst}}(\eta_j = +1) - 1; \quad (18b)$$

$$h_j^\downarrow = h_j^{\text{syst}}(\eta_j = -1) - 1. \quad (18c)$$

The problem consists in finding continuous functions $h_j^{\text{syst}}(\eta_j)$, interpolating for $\eta_j \in [-1,+1]$ and extrapolating for $\eta_j > +1$ and $\eta_j < -1$, and such that equations 18 are satisfied – at least approximately. Four choices are currently available in OpTHyLiC, and are represented in Fig. 2:
• piece-wise linear interpolation and extrapolation, defined in Sec. 3.3.1;
• piece-wise exponential interpolation and extrapolation, defined in Sec. 3.3.2;
• polynomial interpolation and exponential extrapolation, defined in Sec. 3.3.3;
• “McLimit” interpolation and extrapolation, defined in Sec. 3.3.4 and corresponding to the choice followed in the McLimit program.

Figure 2: Illustration of interpolation and extrapolation functions implemented in OpTHyLiC for \( h_j^\downarrow = 0.2 \) and \( h_j^\uparrow = -0.5 \) (bottom right).

### 3.3.1 Piece-wise linear interpolation and extrapolation

The piece-wise linear interpolation and extrapolation is defined as follows:

\[
h_{j}^{\text{syst}}(\eta_j) = \begin{cases} 
1 + \eta_j h_j^\uparrow & \text{if } \eta_j \text{ is positive;} \\
1 - \eta_j h_j^\downarrow & \text{if } \eta_j \text{ is negative.}
\end{cases}
\]

(19)

From this definition, it appears that \( h_{j}^{\text{syst}} \) can be negative if \( h_j^\uparrow \) or \( h_j^\downarrow \) is negative. This unphysical behaviour is dealt with in OpTHyLiC by setting \( h_{j}^{\text{syst}} \) to zero when it occurs.
3.3.2 Piece-wise exponential interpolation and extrapolation

The piece-wise exponential interpolation and extrapolation is defined as follows:

\[
 h_{j}^{\text{syst}}(\eta_j) = \begin{cases} 
 (1 + h_j^+)\eta_j & \text{if } \eta_j \text{ is positive}, \\
 (1 + h_j^-)^{-\eta_j} & \text{if } \eta_j \text{ is negative}.
\end{cases}
\]  

(20)

From this definition, it appears that \( h_{j}^{\text{syst}} \) can be negative if \( h_j^+ \) or \( h_j^- \) is lower than -1. This unphysical behaviour is dealt with in OpTHyLiC by applying a linear interpolation and extrapolation instead (see Sec. 3.3.1) when it occurs. If both \( h_j^+ \) and \( h_j^- \) are greater than -1, \( h_{j}^{\text{syst}} \) is positive for all \( \eta_j \) values.

3.3.3 Polynomial interpolation and exponential extrapolation

The polynomial interpolation and exponential extrapolation is defined as follows:

\[
 h_{j}^{\text{syst}}(\eta_j) = \begin{cases} 
 (1 + h_j^+)\eta_j & \text{if } \eta_j \geq 1, \\
 1 + \sum_{i=1}^{6} a_i \eta_j^i & \text{if } -1 < \eta_j < 1, \\
 (1 + h_j^-)^{-\eta_j} & \text{if } \eta_j \leq -1,
\end{cases}
\]  

(21)

where the coefficients \( a_i \) are chosen such that \( h_{j}^{\text{syst}}(\eta_j) \) and its first and second derivatives are continuous at \( |\eta_j| = 1 \) and \( \eta_j = 0 \).

3.3.4 “McLimit” interpolation and extrapolation

The “McLimit” interpolation and extrapolation is defined as follows:

\[
 h_{j}^{\text{syst}}(\eta_j) = \begin{cases} 
 1 + B & \text{if } B \geq 0, \\
 e^B & \text{if } B < 0,
\end{cases}
\]  

(22)

where

\[
 B = \begin{cases} 
 \eta_j h_j^+ (1 - R) + RQ & \text{if } \eta_j \text{ is positive}, \\
 -\eta_j h_j^- (1 - R) + RQ & \text{if } \eta_j \text{ is negative},
\end{cases}
\]  

(23)

and

\[
 Q = \eta_j \left( h_j^+ - h_j^- \right) + \eta_j^2 \left( h_j^+ + h_j^- \right) \quad \text{and} \quad R = \frac{1}{1 + 3|\eta_j|}.
\]  

(24)

This definition ensures that the first derivative of \( h_{j}^{\text{syst}} \) at \( \eta_j = 0 \) is continuous and that \( h_{j}^{\text{syst}} > 0 \) for all \( \eta_j \) values. It should be noted that equation 18b (18c) is exactly satisfied when \( h_j^+ > 0 \) (\( h_j^- > 0 \)) but only to first order when \( h_j^+ < 0 \) (\( h_j^- < 0 \)). Indeed, the following relations hold:

\[
 h_{j}^{\text{syst}}(\eta_j = +1) = \begin{cases} 
 e^{h_j^+} & \text{if } h_j^+ < 0, \\
 1 + h_j^+ & \text{if } h_j^+ \geq 0,
\end{cases}
\]  

(25)

\[
 h_{j}^{\text{syst}}(\eta_j = -1) = \begin{cases} 
 e^{h_j^-} & \text{if } h_j^- < 0, \\
 1 + h_j^- & \text{if } h_j^- \geq 0.
\end{cases}
\]  

(26)

It should also be noted that, when the effect of the considered uncertainty is symmetric (\( h_j^+ = -h_j^- \)), this interpolation/extrapolation scheme is equivalent to the piece-wise linear one (see Sec. 3.3.1) for \( \eta_j > 0 \) if \( h^+ \geq 0 \) or \( \eta_j < 0 \) if \( h^- \geq 0 \).
3.4 Inference of observed upper limit \( \mu_{\text{up}} \)

The observed upper limit on the signal strength \( \mu_{\text{up}} \) is derived from the \( CL_s \) method using \( q_\mu \) (Eq. 2) as test statistic. \( q_\mu \) is computed using the nominal likelihood:

\[
L(\mu) = L(\mu, \{ s'_c \} = \{ s'^{\text{nom}}_c \}, \{ b'_c \} = \{ b'^{\text{nom}}_c \}, \{ \eta_j \} = 0). \tag{27}
\]

It thus reduces to the following simple form:

\[
q_\mu = \sum_c q^c_\mu, \tag{28}
\]

where \( q^c_\mu \) is the test for channel \( c \) given by:

\[
q^c_\mu = 2 \left( \mu s'^{\text{nom}}_c - N_c \ln \frac{\mu s'^{\text{nom}}_c + b'^{\text{nom}}_c}{b'^{\text{nom}}_c} \right). \tag{29}
\]

The distributions of \( q_\mu \) under signal plus background and background only hypotheses (hereafter denoted as \( p(q_\mu|\mu) \) and \( p(q_\mu|0) \) respectively) are determined by generating pseudo-experiments from the marginal likelihood:

\[
L_m(\mu) = \int L(\mu, \{ s'_c, b'_c, \eta_j \}) \prod_j d\eta_j \prod_c ds'_c \prod_i db'_c. \tag{30}
\]

In practice, this is done by first generating nuisance parameter values from their constraint p. d. f. and by then generating \( N_c \) using the nuisance parameter values obtained in the first step. Typical distributions produced by OpTHyLiC are shown in Fig. 3.

![Figure 3: Example of distributions of \( q_\mu \) under signal+background (\( \mu' = \mu \)) and background only hypotheses (\( \mu' = 0 \)).](image)

Once \( p(q_\mu|\mu) \) and \( p(q_\mu|0) \) have been determined, the \( CL_s \) is computed by using:

\[
CL_s(\mu) = \frac{\sum_{q_\mu = q_{\mu \text{obs}}}^{\infty} p(q_\mu|\mu)}{\sum_{q_\mu = q_{\mu \text{obs}}}^{\infty} p(q_\mu|0)}, \tag{31}
\]

where \( q_{\mu \text{obs}} \) is the observed value of the test \( q_{\mu \text{obs}} = q_\mu \{ N_c \} = \{ N_{\text{obs}} \} \). The upper limit is found by searching \( \mu \) such that \( CL_s(\mu) \) is equal to \( \alpha \) (see Eq. 1).
3.5 Computation of expected limits

OpTHyLiC can also be used to compute expected limits on the signal strength, under background only hypothesis. Five expected limit quantiles are available: median, $-2\sigma$, $-1\sigma$, $+1\sigma$ and $+2\sigma$. The last four ones are defined using the standard normal distribution. Denoting these quantiles by $Z$ and the corresponding probability by $p$, one has:

$$Z = \Phi^{-1}(p),$$

where $\Phi$ is the cumulative distribution function of the standard normal distribution. The values of probabilities for the quantiles available in OpTHyLiC are given in Tab. 2.

| $Z$ | -2  | -1  | 0 (median) | +1  | +2  |
|-----|-----|-----|------------|-----|-----|
| $p$ | 0.0228 | 0.1587 | 0.5 | 0.8413 | 0.9772 |

Table 2: Values of probabilities associated to the quantiles available in OpTHyLiC for the calculation of expected limits.

Two methods are provided to compute expected limits. In the first one, the distribution of $\mu_{up}$ is determined by generating pseudo-experiments under background only hypothesis. Expected limits are then given by the quantiles (as defined above) of this distribution. In the second one, expected limits are calculated in the same way as observed ones (see Sec. 3.4) replacing the observed $CL_s$ by median, $-2\sigma$, $-1\sigma$, $+1\sigma$ and $+2\sigma$ quantiles of the $CL_s$ distribution under background only hypothesis.

Both methods are equivalent from the statistical point of view but different in terms of implementation and computing time. In most cases, the second method performs much faster than the first one and should therefore be preferred. The first method can be used for cross-checks or if the distribution of $\mu_{up}$ is needed.

It should be noted that, when using the second method, quantiles are not computed from a single distribution as in the first method: each quantile is computed in a separate job. Therefore, due to statistical fluctuations, the expected values may not be sorted as they should (for example, the $-2\sigma$ expected value can be higher than the $-1\sigma$ expected value). In such cases it is recommended to increase the number of pseudo-experiments.

4 Software description

4.1 Structure and prerequisites

OpTHyLiC is written in C++ and uses the ROOT library [6]. The code is separated in different classes. Their definitions and implementations are separated into different files which are placed in the main OpTHyLiC directory. Once compiled, the libraries can either be used dynamically by using a macro interpreted with the ROOT interpreter (CINT and CLING for version 5 and 6 of ROOT, respectively), or using a proper C++ program compiled into an executable with a software like gcc. Two simple examples, working for both cases, are available in the examples sub-directory.

As the statistical method relies on pseudo-experiments, pseudo-random number generators are used. ROOT provides in its TRandom3 class an implementation of the MT19937 Mersenne twister [7]. The C++ standard library in its recent C++11 standard [8] also provides various pseudo-random number engines, allowing to generate numbers distributed with the various probability distributions mentioned in this paper. Therefore, if the available compiler or ROOT version makes the use of the C++11 standard possible, the user has the possibility to chose these pseudo-random engines instead of the TRandom3 class. Thanks to relevant preprocessor directives, the portions of the code specific to the C++11 standard are ignored, either by the interpreter or by the compiler, when its use is not possible.

If used as a compiled executable, the examples have been tested to be fully functional with gcc version 4.8.2 (4.3.0) or newer, with ROOT version 5.28/00b, when C++11 features are (are not) used. If used as interpreted macros, the examples have been tested to be fully functional with ROOT versions as old as 6.02/03 (5.28/00b), when C++11 features are (are not) used. Older versions of gcc and ROOT may
also be used but have not been tested. Other compilers than gcc could also have been chosen, but have not been considered in the installation procedure described below.

The usage instructions given below corresponds to version 1.00 of OpTHyLiC.

4.2 Installation and examples

OpTHyLiC is installed in three steps:

1. running the INSTALL script to prepare the compilation by creating a Makefile which structure depends on how OpTHyLiC is intended to be used;
2. running make to compile the shared libraries according to the Makefile;
3. running the setup.[c]sh script created in the first step, to update the LD_LIBRARY_PATH environment variable with the directory where the shared libraries are available.

The INSTALL shell script is in the main directory. Using INSTALL --help (or INSTALL -h) displays an help detailing the different options, which allows the user to configure the Makefile:

- --executable (or -e) to compile executables with gcc; if this option is not used, two ROOT macros, Compile.C and examples/load.C, for the compilation and needed for the compilation and for loading the shared libraries, are created in addition to the Makefile;
- --C++11 (or -C) to enable the C++11 features; in this case, the script checks if the gcc or ROOT versions are recent enough to do so;
- --permissive to override the check of the gcc or ROOT versions when using the previous option.

If no option is used, the libraries will be compiled by ROOT to be used with an interpreted macro, without the C++11 features. Once installed, OpTHyLiC can be used from any location when opening a new shell, by running the script setup.[c]sh.

Two examples of programs using OpTHyLiC, runLimits.C and runSignificance.C, are provided in the examples sub-directory, together with examples of input files "input1.dat" and "input2.dat", the syntax of which is detailed in Sec. 4.3. The example runLimits.C illustrates the calculation of expected and observed limits, while runSignificance.C shows how to plot the $CL_s$ distribution under the background only hypothesis and calculate the p-value for an observed yield value. The syntax of the main functions used in both examples is explained in Sec. 4.4. These example programs can be run from this location using the following syntax:

- root -l load.C 'runLimits.C("input1.dat","input2.dat")' when used as a ROOT macro;
- ./runLimits.exe --files input1.dat input2.dat when used as an executable.

In these examples, preprocessor directives are used to allow their use in both modes, or to enable the C++11 features. In the first mode, these examples can also be run from any location, if the load.C macro written to load the shared libraries is run before. In the second mode, the executable can me moved to any location; furthermore, any program located in the examples sub-directory would be compiled when running the make command, as long as its name is of the form run*.C.

4.3 Input file format

OpTHyLiC takes as input one text file per channel. The general structure of the files is shown if Fig. 4.

The block starting with the +sig tag defines the signal sample. Blocks starting with the +bg tag define the background samples. Finally, the observation is defined with the +data tag. Systematic uncertainties are declared using the .syst tag. Fields <name> define the names for signal, backgrounds and systematic uncertainties. Fields <yield> define the nominal yields for signal and backgrounds and the observed yield for data. Fields <stat> define the absolute statistical uncertainty for signal and backgrounds. Fields <up> and <down> define $h^+$ and $h^-$ for each systematic uncertainty. When systematics for different samples (signal or backgrounds) or different channels have the same name they are supposed 100% correlated.
Figure 4: General structure of OpTHYLiC’s input files.

(i.e. they are described by a unique nuisance parameter $\eta_j$). Otherwise they are treated as uncorrelated. Lines starting with # are not interpreted. The order in which the signal, background and data block appear does not matter.

LaTeX tables summarizing yields and uncertainties can be produced (see Sec. 4.4.2 for instructions on how to do this). By default, the sample and systematic names used in these tables are the ones specified in the input files in the <name> fields. The user can change background sample names by adding .nameLaTeX tags in background sample blocks. Systematic names can be changed by creating a dictionary file mapping names as specified in the <name> fields to names used for LaTeX tables. Channel names used for LaTeX tables can also be specified by adding +nameLaTeX tags in the input files.

Fig. 5 and 6 show an example of what could be the two files in an analysis combining two channels and the dictionary file defining systematic names for LaTeX tables.

Figure 5: Example of input text files for a two channels combination.

Syst1 JES
Syst2 $b$-tagging
Syst3 $E_{T}^{\text{miss}}$
Syst4 norm

Figure 6: Example of dictionary file defining systematic names for LaTeX tables.

In this example, all backgrounds and signals have non-zero statistical uncertainty. The total number of systematic uncertainties (and thus of nuisance parameters $\eta_j$) is 4. The one called Syst1 in the input
files (JES in the LaTeX tables) affects the background yield of the first channel and signal yields of the two channels. LaTeX tables produced by OpTHyLiC for this example are shown in Tab. 3, 4, 5 and 6, including captions that are generated automatically.

| Sample         | eµ        | µµ        |
|----------------|-----------|-----------|
| tt             | 0.80 ± 0.10^{+0.10}_{-0.05} | —         |
| tt + W/Z       | —         | 2.30 ± 0.40^{+0.02}_{-0.00} |
| Total bkg.     | 0.80 ± 0.10^{+0.10}_{-0.05} | 2.30 ± 0.40^{+0.02}_{-0.00} |
| Data           | 1         | 3         |
| Signal         | 2.50 ± 0.60^{+0.53}_{-0.33} | 2.8 ± 1.1^{+0.1}_{-0.4} |

Table 3: Expected and observed yields. The first uncertainty is statistical. The second uncertainty is an approximation of the total systematic uncertainty, not taking into account the correlations between them.

| Sample         | eµ        | µµ        |
|----------------|-----------|-----------|
| tt             | 0.81^{+0.14}_{-0.12} | —         |
| tt + W/Z       | —         | 2.28^{+0.42}_{-0.38} |
| Total bkg.     | 0.81^{+0.14}_{-0.12} | 2.28^{+0.42}_{-0.38} |
| Data           | 1         | 3         |
| Signal         | 2.47^{+0.84}_{-0.63} | 2.4^{+1.2}_{-0.9} |

Table 4: Expected and observed yields. The uncertainty is a combination of the statistical and systematic uncertainties, taking into account the correlations between systematics.

| Uncertainty    | tt   | Signal     |
|----------------|------|------------|
| JES            | −5.00 | +21.00    |
| b-tagging      | ±4.00 | —         |
| $E_T^{miss}$   | —    | —         |
| norm           | —    | —         |
| Total          | +12.65 | +21.00    |
|                | −6.40 | −13.00    |

Table 5: List of relative systematic uncertainties (in %) for channel eµ.

| Uncertainty    | tt + W/Z | Signal     |
|----------------|----------|------------|
| JES            | —        | +5.00      |
| b-tagging      | —        | —          |
| $E_T^{miss}$   | +1.00    | +1.00      |
| norm           | —        | −2.00      |
| Total          | +1.00    | +5.00      |
|                | +0.00    | −15.81     |

Table 6: List of relative systematic uncertainties (in %) for channel µµ.
4.4 Running the software

4.4.1 Configuration

In order to use the software, users need to load the OpTHyLiC library, instantiate an object of type OpTHyLiC and add channels. This can be done interactively in a ROOT session as follows:

```cpp
gSystem->Load("OpTHyLiC_C");
OpTHyLiC oth(OTH::SystMclimit,OTH::StatNormal,OTH::TR3,0,OTH::CombAutomatic);
oth.addChannel("channel 1 name",file1);
oth.addChannel("channel 2 name",file2);
...
```

The constructor requires at least two parameters. The first one is the interpolation/extrapolation method: the possible values are OTH::SystLinear, OTH::SystExpo, OTH::SystPolyexpo, and OTH::SystMclimit, corresponding to the four possibilities described in Sec. 3.3. The second one is the type of constraint for statistical uncertainties: the possible values are OTH::StatNormal, OTH::StatLogN, OTH::StatGammaHyper, OTH::StatGammaUni, and OTH::StatGammaJeffreys, corresponding to the five possibilities described in Sec. 3.2.

In addition, three optional parameters can be provided. The first one is the type of pseudo-random number engine: the possible values are OTH::TR3 (used by default), and, if C++11 features are available, OTH::STD_ followed by the name of one of the nine engines implemented in the C++11 standard library (mt19937, mt19937_64, minstd_rand, minstd_rand0, ranlux24_base, ranlux48_base, ranlux24, ranlux48, knuth_b). The second one is the seed of this engine: the default value 0 has the effect of setting a randomly generated seed. The third one is the chosen solution for the combination of systematic uncertainties, as described in Sec. 3.3: the possible values are OTH::CombAdditive, OTH::CombMultiplicative, or OTH::CombAutomatic (used by default), the latter requesting additive (multiplicative) combination when the OTH::SystLinear or OTH::SystMclimit (OTH::SystExpo or OTH::SystPolyexpo) options are used for the interpolation/extrapolation method.

The addChannel member function takes two parameters of type std::string. The first one is the name of the channel and the second one the name of the input file (see Sec. 4.3).

4.4.2 LaTeX tables production

LaTeX tables are produced as follows:

```cpp
ofstream ofs(filename);
int precision = -1;
int NpseudoExps = 1000000;
oth.createInputYieldTable(ofs,precision);
oth.createGeneratedYieldTable(ofs,precision,NpseudoExps);
oth.createSysteTables(ofs,"systDict.txt",precision);
```

These three methods take as first parameter an output stream, which can be the standard output (std::cout). The functions createInputYieldTable and createGeneratedYieldTable produce tables of expected and observed yields. In the first case, the total uncertainty for each process is evaluated by summing in quadrature all uncertainties without taking into account the correlations, while in the second case the total uncertainty is assessed by using pseudo-experiments (the number of pseudo-experiments is given as the facultative third parameter). An example of such tables are shown in Tab. 3 and 4. The precision of the numbers in these tables can be adjusted to a fixed value (given as the second parameter) or to be automatically adjusted depending on the size of the uncertainties (when the precision parameter is set to -1, which is the default value).

The function createSysteTables creates one table for each channel which summarises all the systematic uncertainties. Examples of such tables are shown in Tab. 5 and 6. The second parameter of createSysteTables is a string specifying the dictionary file. An example of such file is given in Fig. 6.
4.4.3 Observed limit computation

Observed limits are computed as follows:

```c
double cls;
double limit=oth.sigStrengthExclusion(OTH::LimObserved,nbExp,cls);
```

The first parameter of function `sigStrengthExclusion` defines the limit type (here observed). Other types can be used for expected limits (see Sec. 4.4.4). The second parameter (`nbExp`) is the number of pseudo-experiments and the third parameter the final $CL_s$ value (corresponding to the exclusion). By default, the computed limits are for a 95% confidence level. It is possible to modify this confidence level as follows:

```c
oth.setConfLevel(0.9);
```

for example for a 90% confidence level.

4.4.4 Expected limits computation

Two methods are provided to compute expected limits as described in Sec. 3.5.

With the main method, a single expected (median, $-2\sigma$, $-1\sigma$, $+1\sigma$ or $+2\sigma$) limit is computed as the observed one (see Sec. 4.4.3) changing the first parameter to `OTH::LimExpectedM2sig`, `OTH::LimExpectedM1sig`, `OTH::LimExpectedMed`, `OTH::LimExpectedP1sig` or `OTH::LimExpectedP2sig` depending on the limit type. For example, the expected median limit is computed using

```c
double limit=oth.sigStrengthExclusion(OTH::LimExpectedMed,nbExp,cls);
```

With the alternative method, all expected (median, $-2\sigma$, $-1\sigma$, $+1\sigma$ and $+2\sigma$) limits are computed at the same time using:

```c
oth.expectedSigStrengthExclusion(nbMu,nbExp);
```

where `nbMu` and `nbExp` are the number of entries in the $\mu_{up}$ distribution (see Sec. 3.5) and the number of pseudo-experiments, respectively.

4.4.5 Access to histograms

During the limit computation, several histograms are produced. After the computation, some of these histograms are available.

The final $q_{\mu}$ distributions can be accessed using the following commands:

```c
oth.getHisto(OpTHyLiC::hLLRb)->Draw();
oth.getHisto(OpTHyLiC::hLLRsb)->Draw("same");
```

In the case of the alternative expected limit computation, the $q_{\mu}$ distributions are not accessible but two other histograms are available:

```c
oth.getDistrExpMu() -> Draw();
oth.getDistrCLs() -> Draw();
```

where the first one is the expected distribution of $\mu_{up}$ from which the expected limits are derived and the last one is the full distribution of computed $CL_s$ (that should peak at 1-confidence level).

Other interesting distributions are channel dependent, therefore the user must first access a specific channel. There are two ways to do so:

- `oth.getChannel("name")` where `name` is the name of the channel,

- `oth.getChannel(index)` where `index` is the index of the channel returned by the `addChannel` function.

The final $q_{\mu}$ distributions for a single channel can be accessed using the following commands:
oth.getChannel(index)->getHisto(OTH::Channel::hLLRb)->Draw();

as well as the distributions of number of events:

oth.getChannel(index)->getHisto(OTH::Channel::hDistrBg)->Draw();

Other interesting histograms are the distributions of the systematic uncertainties, for example:

oth.getChannel(index)->getSigSystDistr("Syst1")->Draw();

where the last parameter is the name of the systematic uncertainty and the first parameter of the getBkgSystDistr function is the name of the background.

4.4.6 Single channel computations

To compute the limits for a single channel, not combining with the others, the following function is available:

double limit=oth.getChannel(index)->sigStrengthExclusion(OTH::LimObserved,nbExp,cls);

After this call, channel dependent histograms (as described in the previous section) are available.

For the alternative expected limit computation, the following function may be invoked:

double limit=oth.getChannel(index)->expectedSigStrengthExclusion(nMu,nbExp);

In this case, all previous histograms are available as well as a few more:

oth.getChannel(index)->getDistrExpMu()->Draw();

where the second one is the expected \( \mu_{\text{up}} \) as a function of the number of observed events.

It is also possible to study the distribution of the yields after the statistical and systematic variations. In order to generate these distributions, the following function must be called:

oth.getChannel(index)->generateDistrYield(nbExp);

then, the generated distributions are available:

oth.getChannel(index)->getSigYieldDistr()->Draw();

where the first function gives the distribution for the signal, the second one for a single background sample, and the third one is the distribution for the total background. These distributions are also available after a call to createGeneratedYieldTable.

4.4.7 Test statistic distribution and derived quantities

The test statistic distributions under background and signal plus background hypotheses for a desired value of the signal strength \( \mu \) can be computed as follows:

oth.setSigStrength(mu);

where \( \mu \) is the desired \( \mu \) value and \( \text{nbExp} \) is the number of pseudo-experiments. Once this is done, distributions can be accessed as described in Sec. 4.4.5. The p-value of the observation under the background hypothesis and the \( CL_s \) can be computed as follows:
double pvalue = oth.pValueData();
double cls = oth.computeCLsData();

The p-value under the background hypothesis and the CLs for a single channel can be computed using:

double pvalue = oth.getChannel(index)->pValue(nObs);
double cls = oth.getChannel(index)->computeCLs(nObs);

where nObs is the observed yield. For a single channel, the user can also compute the excluded yield for the chosen μ value using:

int yield = oth.getChannel(index)->findObsExclusion();

5 Software validation

The computation of upper limits and observation significances with OpTHyLiC involves many calculations of different types: generation of random numbers, calculation of p-values (CLs+b and CLb), scanning over μ values to solve Eq. 1, combination of channels, interpolation and extrapolation of systematic uncertainties, marginalization of statistical and systematic uncertainties, calculation of quantiles for expected limits, etc. Several studies have been performed in order to validate these calculations. OpTHyLiC is compared either to a theoretical solution in situations where such a solution exists, to bayesian calculations in situations where they are equivalent to the hybrid CLs under interest or to results obtained with the MCLIMIT software which is equivalent to OpTHyLiC when specific choices for the interpolation/extrapolation of systematics and constraints for statistical uncertainties are made. These studies are summarized in the following sections.

5.1 Validation of calculations without uncertainties

OpTHyLiC has first been validated in the simplest situation where signal and background yields have no uncertainties (neither systematic nor statistical), both in the single and multiple channels cases.

In the single channel case, an analytical solution for μup exists. Indeed, CLs+b and CLb are given by

\[
CL_{s+b} = \sum_{N=0}^{N_{\text{obs}}} \frac{(\mu_s^{\text{nom}} + \mu_b^{\text{nom}})^N}{N!} e^{-\left(\mu_s^{\text{nom}} + \mu_b^{\text{nom}}\right)} = 1 - F_{\chi^2} \left(2 \left(\mu_s^{\text{nom}} + \mu_b^{\text{nom}}\right); 2 \left(N_{\text{obs}} + 1\right)\right)
\]

and

\[
CL_b = \sum_{N=0}^{N_{\text{obs}}} \frac{\mu_b^{\text{nom}})^N}{N!} e^{-\mu_b^{\text{nom}}} = 1 - F_{\chi^2} \left(2 \mu_b^{\text{nom}}; 2 \left(N_{\text{obs}} + 1\right)\right)
\]

where \(F_{\chi^2}(x; d)\) is the cumulative distribution function of the chi-squared distribution with \(d\) degrees of freedom at \(x\).

\[
\mu_{up} = \frac{0.5 \times F_{\chi^2}^{-1} \left(1 - \alpha \left[1 - F_{\chi^2} \left(2 \mu_b^{\text{nom}}; 2 \left(N_{\text{obs}} + 1\right)\right)\right] \right) \left(2 \left(N_{\text{obs}} + 1\right)\right) - \mu_b^{\text{nom}}}{s^{\text{nom}}}
\] (33)

Fig. 7 shows a comparison between this analytical result and OpTHyLiC for \(\mu_b^{\text{nom}} = 0.82 \times L\), \(s^{\text{nom}} = 2.49 \times L\) and \(N_{\text{obs}} = 1 \times L\), with \(L = 1, \ldots, 7\). Excellent agreement is found. Other tests have been performed with other values of \(\mu_b^{\text{nom}}, s^{\text{nom}}\) and \(N_{\text{obs}}\), always leading to the same conclusion.

In the multiple channels case, two validations were made. In the first one, upper limits calculated with several channels were compared to upper limits calculated with a single channel in situations where the two are expected to give identical results. Such situations occur when yields in the various channels are related to each other by a simple multiplicative factor. For example, the same limits should be obtained in these two cases:
Figure 7: Upper limit $\mu_{\text{up}}$ as a function of $L$ computed with OpTHyLiC and from the analytical result (Eq. 33) for $b_{\text{nom}}^s = 0.82 \times L$, $s_{\text{nom}}^s = 2.49 \times L$ and $N_{\text{obs}} = 1 \times L$.

- $n$ channels each with
  - background yield $= b_{\text{nom}}^n / n$
  - signal yield $= s_{\text{nom}}^n / n$
  - observed yield $= N_{\text{obs}}^n / n$

- a single channel with
  - background yield $= b_{\text{nom}}$
  - signal yield $= s_{\text{nom}}$
  - observed yield $= N_{\text{obs}}$

It has been checked for several values of $s_{\text{nom}}$, $b_{\text{nom}}$, $N_{\text{obs}}$ and $n$ that OpTHyLiC indeed finds the same limits in both cases. In the second one, the general case where yields in the various channels can’t be related to each other by a simple multiplicative factor has been considered. It can be seen from Eq. 28 and Eq. 29 that the upper limit can be computed using the following test

$$ N_{\text{eff}} = \sum_c N_c \beta_c \text{ with } \beta_c = \ln \frac{\mu s_{\text{nom}}^c + b_{\text{nom}}^c}{b_{\text{nom}}^c} $$

In the asymptotic limit, $N_c$ is normally distributed. Thus

$$ N_{\text{eff}} \sim N \left( \sum_c \beta_c (\mu s_{\text{nom}}^c + b_{\text{nom}}^c), \sum_c \beta_c^2 (\mu s_{\text{nom}}^c + b_{\text{nom}}^c) \right) $$

under the signal plus background hypothesis and

$$ N_{\text{eff}} \sim N \left( \sum_c \beta c^l_{\text{nom}}^s, \sum_c \beta^2 c^l_{\text{nom}}^s \right) $$

under the background only hypothesis ($N (a, b)$ is the normal distribution with mean $a$ and variance $b$). $CL_s$ is therefore given by

$$ CL_s = \frac{\Phi \left( \frac{N_{\text{eff}}^s (\mu) - \sum_c \beta_c (\mu s_{\text{nom}}^c + b_{\text{nom}}^c)}{\sqrt{\sum_c \beta^2 c^l_{\text{nom}}^s}} \right)}{\Phi \left( \frac{N_{\text{eff}}^{b \text{nom}} (\mu) - \sum_c \beta_c b_{\text{nom}}^c}{\sqrt{\sum_c \beta^2 c^l_{\text{nom}}^s}} \right)} $$

(34)
where \( \Phi \) is the cumulative distribution function of the standard normal distribution. Eq. 1 with Eq. 34 can easily be solved by dichotomy. This result has been used to validate the channel combination procedure implemented OpTHyLiC in the asymptotic limit. Fig. 8 shows a comparison of this asymptotic result with OpTHyLiC in the three channels example defined by

- channel 1: \( s^{\text{nom}} = 5.18 \times L, \ b^{\text{nom}} = 2.22 \times L \) and \( N^{\text{obs}} = 3 \times L \)
- channel 2: \( s^{\text{nom}} = 3.05 \times L, \ b^{\text{nom}} = 1.61 \times L \) and \( N^{\text{obs}} = 4 \times L \)
- channel 3: \( s^{\text{nom}} = 4.45 \times L, \ b^{\text{nom}} = 2.95 \times L \) and \( N^{\text{obs}} = 2 \times L \)

Figure 8: Upper limit \( \mu_{up} \) as a function of \( L \) computed with OpTHyLiC and from the asymptotic result (Eq. 34) for the three channels example defined in the text.

As can be seen from Fig. 8, OpTHyLiC converges, as expected, to the asymptotic result as the number of events increases.

5.2 Validation of calculations with statistical and systematic uncertainties

Several other studies have been performed in order to validate the treatment of statistical and systematic uncertainties in OpTHyLiC. As already explained, OpTHyLiC treats uncertainties in a Bayesian way by marginalizing the likelihood. A simple check of the marginalization procedure has been performed in the single channel case by comparing marginal distributions of the yield as computed by OpTHyLiC to analytical distributions in the case where a single background affected by a statistical uncertainty constrained with a gamma p. d. f. contributes to the expected yield. Indeed, it is known that, in this case, that the marginal distribution of the yield, given by the compound of a Poisson and a gamma distribution, is negative binomial:

\[
P(N = n|b^{\text{nom}}, \sigma) = \int_0^{\infty} P(N = n|b) \times f(b; b^{\text{nom}}, \sigma) db = \frac{\Gamma\left(N + \left(\frac{b^{\text{nom}}}{\sigma}\right)^2\right)}{N! \Gamma\left(\left(\frac{b^{\text{nom}}}{\sigma}\right)^2\right)} \left(\frac{b^{\text{nom}}}{b^{\text{nom}} + \sigma^2}\right)^{(b^{\text{nom}}/\sigma)^2} \left(\frac{\sigma^2}{b^{\text{nom}} + \sigma^2}\right)^N \tag{35}\]

where \( N \) is the observed yield, \( b \) is the background yield, \( b^{\text{nom}} \) its nominal value, \( \sigma \) its statistical uncertainty, \( P(N = n|b) \) the Poisson distribution with parameter \( b \), \( f(b; b^{\text{nom}}, \sigma) \) the gamma distribution for \( b \) with mean \( b^{\text{nom}} \) and standard deviation \( \sigma \) (given by Eq. 14c) and \( P(N = n|b^{\text{nom}}, \sigma) \) the marginal (negative binomial) distribution of the yield \( N \). Fig. 9 shows that the agreement between Eq. 35 and marginal distributions calculated by OpTHyLiC is very good. Excellent agreements have also been observed for the two other gamma definitions available in OpTHyLiC (Eq. 14a and 14b).
In order to validate not only the treatment of statistical uncertainties but also that of systematic uncertainties, upper limits calculated with OpTHyLiC have been compared to upper limits calculated using a bayesian method. It can indeed be shown that, in the single channel case, the hybrid $CL_s$ method implemented in OpTHyLiC is equivalent to the bayesian method when a uniform prior on the signal strength $\mu$ is used and when the signal has no uncertainties (neither statistical nor systematic) associated to it [9]. This equivalence holds for any number of background sources, any number of statistical and systematic uncertainties associated to them and any type of correlation between systematic uncertainties across background sources. This result is used to complete the validation of the treatment of statistical uncertainties and to validate the treatment of systematic uncertainties. In order to perform this validation, an independent bayesian software, based on RooStats, has been developed. This software implements exactly the same likelihood as OpTHyLiC and takes as input the same files, hence allowing direct comparison to OpTHyLiC. Several comparisons between OpTHyLiC and bayesian results have been performed by changing the number of background sources and the number of systematic and statistical uncertainties. One such comparison has been performed using the configuration given in Fig. 10, with $L = 1, \ldots, 7$. The result is shown in Fig. 11.

Figure 9: Marginal distribution of the yield under the background only hypothesis in the case where the background has a statistical uncertainty constrained by a gamma p. d. f. with mean $b^{\text{nom}} = 15$ and three different values of standard deviation: $\sigma = 2, 7$ and 14.

Figure 10: One of the examples used to validate the treatment of uncertainties in OpTHyLiC.
Figure 11: Upper limit $\mu_{\text{up}}$ as a function of $L$ without (left) and with (right) statistical and systematic uncertainties. It has been computed using exponential interpolation and extrapolation for systematic uncertainties and normal constraint terms for statistical uncertainty.

This example has been chosen because uncertainties are large and their effect on upper limits is very pronounced (as can be seen by comparing plots on the left and right of Fig. 11). Thus, any mis-treatment of uncertainties in OpTHyLiC should be visible. Very good agreement between OpTHyLiC and the bayesian calculation with uniform prior is found for this example. Similar agreements are found in other cases. Rigorously, these comparisons validate only the treatment of statistical and systematic uncertainties for backgrounds. However, signal uncertainties are treated by the same code as background uncertainties. Signal uncertainties are therefore expected to be treated properly. As will be seen below, the comparison between MC\text{LIMIT} and OpTHyLiC gives confidence that signal uncertainties are indeed treated properly.

The last validation compares observed and expected (-2$\sigma$, -1$\sigma$, median, +1$\sigma$ and +2$\sigma$) upper limits calculated with OpTHyLiC to upper limits calculated with MC\text{LIMIT}. MC\text{LIMIT} is, as OpTHyLiC, a hybrid frequentist-bayesian tool, using the interpolation/extrapolation described in Sec. 3.3.4 and normal constraints for statistical uncertainties. When configured appropriately, OpTHyLiC is therefore expected to give the same upper limits as MC\text{LIMIT}$^2$. For this comparison, typical inputs from high energy physics analysis have been used. Fig. 12 shows a comparison of upper limits as a function of

![Graph showing upper limits as a function of mass](image)

Figure 12: Comparison of observed and expected upper limits calculated with MC\text{LIMIT} and OpTHyLiC in a realistic case (see text).

$^2$Profiling of uncertainties has been turned off in MC\text{LIMIT} so as to allow direct comparison to OpTHyLiC.
the mass of a hypothetical new particle obtained by combining three channels. Six mass points have been considered and seven background processes contribute to the yield in each channel. Signal and background processes are all affected by statistical and systematic uncertainties. For each mass, the total number of nuisance parameters is 51 (27 are associated to systematic uncertainties and 24 to statistical uncertainties). In both cases, 50 000 pseudo-experiments are used. Limits found with OpTHyLiC are in good agreement with those found with McLimit. The main difference between the two softwares is the computing time. For example, on the same computer, it took 25 minutes (8 seconds) to calculate the observed limit for the 1 TeV point with McLimit (OpTHyLiC). The full plot is produced in less that 6 minutes with OpTHyLiC while it takes several hours with McLimit.

6 Conclusion

A tool computing observed and expected limits has been presented. This tool, named OpTHyLiC, is written in C++ and uses the ROOT library. It implements the hybrid frequentist-bayesian $CL_s$ method for hypothesis testing and is optimized for counting experiments. It can be used with an arbitrary number of channels. Statistical and systematic uncertainties are accounted for as well as correlations between systematic uncertainties. Several types of interpolation/extrapolation for systematic uncertainties and constraint terms for statistical uncertainties are provided. OpTHyLiC has been validated by comparing it to known analytical and bayesian results and to McLimit in situations where they are expected to give identical limits. Very good agreement has been found in all cases, hence validating the software.

One of the main advantage of OpTHyLiC is its speed. Even in realistic cases with dozens of nuisance parameters and several channels, limits are typically computed in less than one minute.

Acknowledgements

The authors would like to thank R. Madar and L. Valéry for the fruitful discussions that helped improve the quality of this document. Part of this work was supported by the regional council of Auvergne through the ”nouveau chercheur” research funding program.

References

[1] “OpTHyLiC webpage.” http://opthylic.in2p3.fr.
[2] “McLimit webpage.” http://ww-cdf.fnal.gov/~trj/mclimit/production/mclimit.html.
[3] “RooStats webpage.” http://twiki.cern.ch/twiki/bin/view/RooStats.
[4] A. L. Read, Presentation of search results: The $CL_s$ technique, J. Phys. G 28 (2002) 2693–2704.
[5] ROOT Collaboration, K. Cranmer, G. Lewis, L. Moneta, A. Shibata, and W. Verkerke, HistFactory: A tool for creating statistical models for use with RooFit and RooStats, CERN-OPEN-2012-016. http://cds.cern.ch/record/1456844/.
[6] “ROOT webpage.” http://root.cern.ch.
[7] M. Matsumoto and T. Nishimura, Mersenne Twister: A 623-dimensionally Equidistributed Uniform Pseudo-random Number Generator, ACM Trans. Model. Comput. Simul. 8 no. 1, (1998) 3–30.
[8] B. Stroustrup, The C++ Programming Language, 4th edition. Pearson Education, 2013.
[9] E. Busato, Equivalence between hybrid $CL_s$ and bayesian methods for limit setting. arXiv:1404.1340 [stat.ME].