Signal Significance in the Presence of Systematic and Statistical Uncertainties

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Abstract
The incorporation of uncertainties to calculations of signal significance in planned experiments is an actual task. Several approaches to this problem are discussed. We present a procedure for taking into account the systematic uncertainty related to nonexact knowledge of signal and background cross sections. A method for account of statistical uncertainties in determination of mean numbers of signal and background events is proposed. The law of conservation of unit and zero in plane “number of events versus parameter of Poisson distribution” is formulated.

1. INTRODUCTION
One of the common goals in the forthcoming experiments is the search for new phenomena. In estimation of the discovery potential of the planned experiments the background cross section (for example, the Standard Model cross section) is calculated and, for the given integrated luminosity \( L \), the average number of background events is \( n_b = \sigma_b \cdot L \). Suppose the existence of a new physics leads to additional nonzero signal cross section \( \sigma_s \) with the same signature as for the background cross section that results in the prediction of the additional average number of signal events \( n_s = \sigma_s \cdot L \) for the integrated luminosity \( L \). The total average number of the events is \( <n> = n_s + n_b = (\sigma_s + \sigma_b) \cdot L \). So, as a result of new physics existence, we expect an excess of the average number of events. The probability of the realization of \( n \) events in experiment is described by Poisson distribution [1, 2]

\[
f(n; \lambda) = \frac{\lambda^n}{n!} e^{-\lambda}.
\]

In the report the approach to determination of the “significance” of predicted signal on new physics in concern to the predicted background is considered. This approach is based on the analysis of uncertainty [3, 4], which will take place under the future hypotheses testing about the existence of a new phenomenon in Nature. We consider a simple statistical hypothesis \( H_0 \): new physics is present in Nature (i.e. \( \lambda = n_s + n_b \)) against a simple alternative hypothesis \( H_1 \): new physics is absent (\( \lambda = n_b \)). The value of uncertainty is defined by the choosing of the critical value \( n_0 \), i.e. by Type I error \( \alpha \) and Type II error \( \beta \). The concept of the “statistical significance” of an observation is reviewed in ref. [5].

2. “SIGNIFICANCE” IN PLANNED EXPERIMENT [6]
“Common practice is to express the significance of an enhancement by quoting the number of standard deviations” [7]. In the most of proposals of the experiments the following “significances” are used for testing the possibility to discover new physics:

(a) “significance” \( S_1 = \frac{n_s}{\sqrt{n_b}} \) [8, 9],

(b) “significance” \( S_2 = \frac{n_s}{\sqrt{n_s + n_b}} \) [10],

(c) “significance” \( 2 \cdot S_{12} = 2(\sqrt{n_s + n_b} - \sqrt{n_b}) \) [11, 3].
As shown [4, 12] the “significance” $2 \cdot S_{12}$ more proper in planned experiments. Note, all these “significances” assume a 50% acceptance for positive decision about new physics observation.

If we define the “signal significance” according to ref. [13] as “effective significance” $s$

\[
\frac{1}{\sqrt{2\pi}} \int_{s}^{\infty} \exp(-x^2/2)dx = \sum_{k=n_0}^{\infty} f(k; n_b),
\]

(2)

where $n_0$ is the critical value for hypotheses testing, the system

\[
\beta = \sum_{n=n_0+1}^{\infty} f(n; n_b) \leq \Delta
\]

(3)

\[
1 - \alpha = \sum_{n=n_0+1}^{\infty} f(n; n_s + n_b)
\]

(4)

allows us to construct dependences $n_s$ versus $n_b$ on given value of Type II error $\beta \leq \Delta$ and given acceptance $1 - \alpha$. If $\Delta = 2.85 \cdot 10^{-7}$ ($s \geq 5$, i.e. the value $n_0$ has $5\sigma$ deviation from average background $n_b$), the corresponding acceptance can be named the probability of discovery and the dependence of $n_s$ versus $n_b$ - the $5\sigma$ discovery curve; if $\Delta = 0.0014$ ($s \geq 3$), the acceptance is the probability of strong evidence, and, if $\Delta = 0.028$ ($s \geq 2$), the acceptance is the probability of weak evidence. The case of weak evidence for 50% acceptance ($s = S_1 = 2$) is shown in Fig.1. The $5\sigma$ discovery, $3\sigma$ strong evidence, and $2\sigma$ weak evidence curves for 90% acceptance are presented in Fig.2.

For the estimation of “effective significance” $s$ with given acceptance $1 - \alpha$ approximate formulae can be used:

\[
s(\alpha) = S_1 - k(\alpha)\sqrt{1 + \frac{n_s}{n_b}}
\]

(5)

or

\[
s(\alpha) = 2 \cdot S_{12} - k(\alpha).
\]

(6)

where $k(\alpha)$: $k(0.5) = 0; k(0.25) = 0.66; k(0.1) = 1.28; k(0.05) = 1.64$ (for instance, Tab.28.1 [1]).

3. AN ACCOUNT OF SYSTEMATIC UNCERTAINTY RELATED TO NONEXACT KNOWLEDGE OF BACKGROUND AND SIGNAL CROSS SECTIONS [3]

In ref. [14], for instance, the systematic uncertainty is the uncertainty in the sensitivity factor. This uncertainty has statistical properties which can be measured or estimated. Model [15] estimates the uncertainty by repeating the calculation of the model with several sets of randomly selected input parameters, each drawn from a Gaussian distribution defined by the experimental value and error for the input parameter. In ref. [17] says that input parameters should have been drawn from uniform distributions. The systematic effects in ref. [16] as supposed have stochastic behaviour too. The account for statistical uncertainties due to statistical errors in determination of values $n_b$ and $n_s$ [12] implies the existence of conditional probability for parameter of Poisson distribution.

We consider here forthcoming experiments to search for new physics. In this case we must take into account the systematic uncertainty which have theoretical origin without any statistical properties. For example, two loop corrections for most reactions at present are not known. In principal, it is “reproducible inaccuracy introduced by faulty technique” [18] and according to [19] it contains the sense of “incompetence”. It means that we can only estimate the scale of influence of background uncertainty on
Fig. 1: The case $n_b \gg 1$. Poisson distributions with parameters $\lambda = 1000$ (left) and $\lambda = 1064$ (right). Here $1 - \alpha = 0.5$ and $\beta = 0.02275$ (i.e. $s = S_1 = 2$).

Fig. 2: Dependences $n_a$ versus $n_b$ for $1 - \alpha = 0.9$ and for different values of $\beta$. 
the observability of signal, i.e. we can point the admissible level of uncertainty in theoretical calculations for given experiment proposal.

Suppose uncertainty in the calculation of exact background cross section is determined by parameter $\delta$, i.e. the exact cross section lies in the interval $(\sigma_b, \sigma_b(1+\delta))$ and the exact value of average number of background events lies in the interval $(n_b, n_b(1+\delta))$. Let us suppose $n_b \gg n_s$. In this instance the discovery potential is the most sensitive to the systematic uncertainties. As we know nothing about possible values of average number of background events, we consider the worst case [3]. Taking into account formulae (3) and (4) we have the formulae

$$
\beta = \sum_{n=n_0+1}^{\infty} f(n; n_b(1+\delta)) \leq \Delta \tag{7}
$$

$$
1 - \alpha = \sum_{n=n_0+1}^{\infty} f(n; n_b + n_s) \tag{8}
$$

The example of using these formulae (7, 8) is shown in Fig. 3. We see the sample of 100 signal and 100 background events will be enough to reach 90% probability of discovery with 25% systematic uncertainty of theoretical estimation of background.

4. AN ACCOUNT OF STATISTICAL UNCERTAINTY IN THE DETERMINATION OF $n_s$ AND $n_b$.

If the probability of true value of parameter of Poisson distribution to be equal to any value of $\lambda \geq 0$ in the case of one measurement $n_b = \hat{n}$ or $n_s + n_b = \hat{n}$ is known we have to take into account the statistical uncertainties in the determination of these values.

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1Formulae (8, 9) realize the worst case when the background cross section $\sigma_b(1+\delta)$ is the maximal one, but we think that both the signal and the background cross sections are minimal.
Let us write down the density of Gamma distribution \( \Gamma_{a,n+1} \) as

\[
g_n(a, \lambda) = \frac{a^{n+1}}{\Gamma(n+1)} e^{-a\lambda} \lambda^n,
\]

where \( a \) is a scale parameter, \( n + 1 > 0 \) is a shape parameter, \( \lambda > 0 \) is a random variable, and \( \Gamma(n + 1) \) is a Gamma function. Since the \( n \) is integer, then \( n! = \Gamma(n + 1) \).

Let us set \( a = 1 \), then for each \( n \) a continuous function

\[
g_n(\lambda) = \frac{\lambda^n}{n!} e^{-\lambda}, \ \lambda > 0, \ n > -1
\]

is the density of Gamma distribution \( \Gamma_{1,n+1} \) with the scale parameter \( a = 1 \) (see Fig.4). The mean, mode, and variance of this distribution are given by \( n + 1 \), \( n \), and \( n + 1 \), respectively.

As it follows from the article [20] and is clearly seen from the identity [21] (Fig.5)

\[
\sum_{n=\hat{n}+1}^{\infty} f(n; \lambda_1) + \int_{\lambda_1}^{\lambda_2} g_{\hat{n}}(\lambda)d\lambda + \sum_{n=0}^{n_0} f(n; \lambda_2) = 1, \ \text{i.e.}
\]

\[
\sum_{n=\hat{n}+1}^{\infty} \frac{\lambda_1^n e^{-\lambda_1}}{n!} + \int_{\lambda_1}^{\lambda_2} \frac{\lambda_{\hat{n}} e^{-\lambda_1}}{\hat{n}!} d\lambda + \sum_{n=0}^{\hat{n}} \frac{\lambda_{\hat{n}}^n e^{-\lambda_2}}{n!} = 1
\]

for any \( \lambda_1 \geq 0 \) and \( \lambda_2 \geq 0 \), the probability of true value of parameter of Poisson distribution to be equal to the value of \( \lambda \) in the case of one measurement \( \hat{n} \) has probability density of Gamma distribution \( \Gamma_{1,1+n} \).

This allows to transform the probability distributions \( f(n; n_s + n_b) \) and \( f(n; n_b) \) accordingly to calculate the probability of discovery [12]

\[
1 - \alpha = 1 - \int_{0}^{\infty} g_{n_s+n_b} (\lambda) \sum_{n=0}^{n_0} f(n; \lambda) d\lambda = 1 - \sum_{n=0}^{n_0} \frac{C_{n_s+n_b+n}^n}{n_s+n_b+n+1},
\]

where the critical value \( n_0 \) under the future hypotheses testing about the observability is chosen so that the Type II error

\[
\beta = \int_{0}^{\infty} g_{n_b} (\lambda) \sum_{n=n_0+1}^{\infty} f(n; \lambda) d\lambda = \sum_{n=n_0+1}^{\infty} \frac{C_{n_b+n}^n}{2n_b+n+1}
\]

(13)

could be less or equal to \( 2.85 \cdot 10^{-7} \). Here \( C_{m}^{k} \) is \( \frac{m!}{k!(m-k)!} \).

The Poisson distributed random values have a property: if \( \xi \sim Pois(\lambda_1) \) and \( \eta \sim Pois(\lambda_2) \) then \( \xi + \eta \sim Pois(\lambda_1 + \lambda_2) \). It means that if we have two measurements \( \hat{n}_1 \) and \( \hat{n}_2 \) of the same random value \( \xi \sim Pois(\lambda) \), we can consider these measurements as one measurement \( \hat{n}_1 + \hat{n}_2 \) of the random value \( 2 \cdot \xi \sim Pois(2 \cdot \lambda) \).

Correspondingly, in the case of \( m \) measurements \( \hat{n}_1, \hat{n}_2, \ldots, \hat{n}_m \) of the random values \( \xi_1, \xi_2, \ldots, \xi_m \), where \( \xi_i \sim Pois(\lambda) \) for \( i = 1, 2, \ldots, m \), the probability of true value of parameter of Poisson distribution to be equal to the value of \( \lambda \) has probability density of Gamma distribution \( \Gamma_{m,1+m} \), i.e.

\[
g(\sum_{i=1}^{m} \hat{n}_i) (m, \lambda) = \frac{m^{1+m} \lambda^{1+m} \hat{n}_i}{(\sum_{i=1}^{m} \hat{n}_i)!} e^{-m\lambda} \lambda^{\sum_{i=1}^{m} \hat{n}_i}. \]

(14)
Fig. 4: The behaviour of the probability density of the true value of parameter $\lambda$ for the Poisson distribution in case of $n$ observed events versus $\lambda$ and $n$. Here $f(n; \lambda) = g_n(\lambda) = \frac{\lambda^n}{n!} e^{-\lambda}$ is both the Poisson distribution with the parameter $\lambda$ along the axis $n$ and the Gamma distribution with a shape parameter $n + 1$ and a scale parameter 1 along the axis $\lambda$.

Fig. 5: The Poisson distributions $f(n, \lambda)$ for $\lambda$’s determined by the confidence limits $\hat{\lambda}_1 = 1.51$ and $\hat{\lambda}_2 = 8.36$ in case of the observed number of events $\hat{n} = 4$ are shown. The probability density of Gamma distribution with a scale parameter $a = 1$ and a shape parameter $n + 1 = \hat{n} + 1 = 5$ is shown within this confidence interval.
5. CONCLUSIONS

In this paper we have described a method to estimate the discovery potential on new physics in planned experiments where only the average number of background \( n_b \) and signal events \( n_s \) is known. The “effective significance” \( s \) of signal for given probability of observation is discussed. We also estimate the influence of systematic uncertainty related to nonexact knowledge of signal and background cross sections on the probability to discover new physics in planned experiments. An account of such kind of systematics is very essential in the search for supersymmetry and leads to an essential decrease in the probability to discover new physics in future experiments. The texts of programs can be found in http://home.cern.ch/bityukov. A method for account of statistical uncertainties in determination of mean numbers of signal and background events is proposed. The law of conservation of unit and zero in plane “number of events versus parameter of Poisson distribution” is formulated in Appendix I. The approach for estimation of exclusion limits on new physics is described in Appendix II.

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References


APPENDIX I: THE LAW OF CONSERVATION OF UNIT AND ZERO

The identity (11) (Fig.5)

\[ \sum_{n=n+1}^{\infty} f(n; \lambda_1) + \int_{\lambda_1}^{\lambda_2} g_n(\lambda)d\lambda + \sum_{n=0}^{\hat{n}} f(n; \lambda_2) = 1 , \]

can be easily generalized, as an example, to

\[ \sum_{n=k_{m+1}}^{\infty} f(n; \lambda_1) + \sum_{i=1}^{m} \left[ \int_{\lambda_i}^{\lambda_{i+1}} g_{k_{m+1-i}}(\lambda)d\lambda + \sum_{n=k_{m-i+1}}^{k_{m+1-i}} f(n; \lambda_{i+1}) \right] \]

\[ + f(k_0; \lambda_{m+1}) = 1 \]

for any real \( \lambda_i \geq 0, i \in [1, m + 1], \) integer \( m > 0, k_l > k_{l-1} \geq 0, l \in [1, m], k_0 = 0. \)

As a result of such type generalizations we have got

\[ \int_{\lambda_1}^{\lambda_2} g_m(\lambda)d\lambda + \sum_{i=n+1}^{m} f(i; \lambda_2) + \int_{\lambda_1}^{\lambda_2} g_n(\lambda)d\lambda - \sum_{i=n+1}^{m} f(i; \lambda_1) = 0 , \]

i.e.

\[ \int_{\lambda_1}^{\lambda_2} \frac{\lambda^m e^{-\lambda}}{m!} d\lambda + \sum_{i=n+1}^{m} \frac{\lambda_i^i e^{-\lambda_i}}{i!} + \int_{\lambda_1}^{\lambda_2} \frac{\lambda^n e^{-\lambda}}{n!} d\lambda - \sum_{i=n+1}^{m} \frac{\lambda_i^i e^{-\lambda_i}}{i!} = 0 , \]

for any real \( \lambda_1 \geq 0, \lambda_2 \geq 0, \) and integer \( m > n \geq 0. \)

APPENDIX II: EXCLUSION LIMITS [3, 4]

It is important to know the range in which a planned experiment can exclude presence of signal at given confidence level \((1 - \epsilon)\). It means that we will have uncertainty in future hypotheses testing about non-observation of signal which equals to or less than \(\epsilon\). In refs.[22, 23] different methods to derive exclusion limits in prospective studies have been suggested.

We propose to use the relative uncertainty

\[ \tilde{\kappa} = \frac{\alpha + \beta}{2 - (\alpha + \beta)} \]  

which will take place under hypotheses testing \( H_0 \) versus \( H_1 \). It is a probability of wrong decision. This probability \( \tilde{\kappa} \) in case of applying the equal-probability test [4] is a minimal relative value of the number of wrong decisions in the future hypotheses testing for Poisson distributions. It is the uncertainty in the observability of the new phenomenon. Note that the probability of correct decision \( 1 - \tilde{\kappa} \) (the relative number of correct decisions) may be considered as a distance between two distributions (the measure of distinguishability of two Poisson processes) in frequentist sense.