Confidence level estimation and analysis optimization

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Abstract

This note proposes a method, which can be applied to searches and more in general to any cross section measurement, to maximize the analysis sensitivity.
1 Introduction

During the last years at LEP a new attitude toward searches has developed which tends to separate the actual search for new phenomena from the derivation of an exclusion limit. In this note we would propose a new method of globally optimized analysis which combines the two steps in an optimal and unbiased way by making use of background subtraction.

2 Statistical Issues

Several methods have been proposed at LEP for the extraction of limits on the Higgs boson mass [1–3] and relative selection optimization [4], while for most of other searches the limits are based on the PDG formula [5]. No methods, to our knowledge, have been proposed yet to optimize an analysis aimed at discovery and deriving the related discovery confidence level (CL).

When measuring physical quantities the combination of different results with gaussian errors is straightforward. On the other hand it is usually more complicated to combine different exclusions or discovery CL.

Clearly to derive a discovery CL the background has to be subtracted. Therefore, aiming at a globally optimized analysis capable of discoveries and exclusions at the same time we should definitely consider background subtraction.

To make a CL evaluation there are two possibilities:

• either one has a formula capable of calculating the CL of the outcome of a given experiment

• or one defines an estimator to rank the experiments from the more signal(background)–like to the less signal(background)–like and then, either analytically or by use of Monte Carlo (MC) techniques, evaluates the ranking of the actual experiment.

Some formulae have been proposed for the first case as some CL evaluation methods have been proposed for the second case. We would like to note that in the second case the estimator can be built arbitrarily (provided that it is done a-priori).

In all these approaches the only thing which is used to derive the CL is the signal to background ratio in the points where the candidates are observed.

The formula in [1], derived in the Bayesian approach, is very simple and it naturally includes background subtraction and therefore in the following we will use it. As it has not yet been demonstrated that this formula gives a statistically well defined CL we use its output as an estimator which will then be treated with MC methods. It should be noted at this point that the only difference between the methods is due to the different estimator chosen. Our choice, which is anyway not essential for the results of the method, is due to the simplicity and naturalness of the estimator described in [1] and also to the fact that its output may sometimes be a little conservative but it is a very good approximation of the CL.

The MC method has on the other hand the big advantage that it allows, with virtually no additional effort, to include any sort of statistical and systematic errors on efficiency and background when computing the CL.
3 Confidence Levels

For sake of clarity we try in this section to explain in simple words the definition of confidence level and the different methods used to derive it.

The results of a measurement are compared with a given hypothesis, for instance that the Higgs boson has a given production cross section, and the confidence level associated to the exclusion of our hypothesis gives the probability that the disagreement between the measurement and the given hypothesis is smaller than what actually observed.

As previously stated we can either do an analytical calculation to derive the confidence level for a given experiment, or we can evaluate it with Monte Carlo technique. Unfortunately the first possibility seems not to be viable because it is virtually impossible to obtain an analytical expression to relate any given estimator, that we want to use to rank the experiment in the most effective way, with its probability density function.

The cross check of the analytical calculation of the confidence level can be done by means of Monte Carlo simulations of trial experiments. In practice this means that we perform our measurements many times, introducing each time a number of background and signal events according to a Poisson distribution with mean equal to the sum of the expected background and signal (our hypothesis) levels.

The actual probability associated to the calculated confidence level is then simply given by the rate of simulated measurements in larger disagreement with the given hypothesis than the real one, properly taking into account the fact that the background alone must give a value of the estimator smaller than the observed one. The latter means that the background can not fluctuate over the actual number of events observed in the experiment and that its probability distribution is bound from above. If we do not take into account that, as already reported in Reference [5], we can derive the absurd conclusion that every signal, even with null cross section, can be excluded with extreme over-fluctuation of the background.

It is clear that we can use this Monte Carlo cross check directly as a definition of the confidence level. This turns out to be a powerful tool because we can use what we believe the most sensitive estimator to rank the measurement and then the probability associated to it is simply obtained as previously explained.

4 The Estimator

We would first of all like to stress that the estimator we used [1] is a very simple extension of the PDG prescription to compute $CL$ for experiments with or without background subtraction [5] to the multichannel situation:

$$F(s, b, n) = e^{-(s+b)} \prod_{j=1}^{k} \frac{(s \cdot f_j + b \cdot g_j)^{n_j}}{n_j!}$$

where the index $j$ runs over the different channels and where $f_j$ and $g_j$ are the fraction of all signal events ($s$) and all background events ($b$), which are in the channel $j$. The fraction of the total number of observed candidates $n$, in each channel $j$, is $n_j$. Using the Bayesian approach we can obtain the confidence level for a given number of expected signal events $\sigma$ with the following integrations:

$$P_L = \frac{\int_{\sigma}^{\infty} F(s, b, n)ds}{\int_{0}^{\infty} F(s, b, n)ds} \simeq 1 - CL$$

(1)
$P_L$ is the estimator we use to rank the experiment.

Using it as an estimator, it is straightforward to extend it to be without background subtraction. It is enough to compare the estimator with the distribution of signal-only random experiments.

To get the correct $CL$ we compare the actual value of the estimator to the distribution of trial MC experiments using signal and background. Clearly, given the fact that the experiment excludes the possibility of having a background which gives by itself a larger estimator than the measured one we only consider those MC experiments with the background estimator smaller than the measured estimator. We add to those a random signal, then measure the value of the probability. Usually, as shown below, the true $CL$ is slightly different from the one we can obtain from equation 1. The $CL$ calculated with equation 1, for a small number of events, is always conservative. For a large number of events, it tends to be a correct estimation of the actual $CL$ measured with MC experiments.

5 Analysis Optimization

As said in Section 2 all methods for limits calculation proposed for a single channel are only sensitive to the signal/background ratio in the point or analysis (or whatever) where the data lie.

The new method proposed here is to consider this fact and its direct consequence that an intrinsically optimized analysis can be obtained when for any value of the ratio signal/background we obtain the highest possible overall efficiency.

It is important to understand that the specific power of a subanalysis only depends on the signal to background ratio and not on the absolute amount of the signal selected by the subanalysis. Then the optimization can be achieved including all the available information provided that channels/analyses with different signal/background ratio are not mixed. This means that we have to organize a set of complementary analyses (i.e. each one selects events that no other analysis selects) and then whatever analysis we add the overall sensitivity is improved.

If we are able to devise such an optimal selection, which orders the different subselections in terms of signal to background ratio, whatever estimator we use, the analysis can be optimized by a single cut on the signal to background ratio. The latter in practice is often needed to take into account systematic uncertainties.

To illustrate these concepts, let us consider a simple numerical example. Let us take the usual case of the search for the production of a new particle which can occur in two channels A and B with branching ratios of 20% and 80% respectively. Let us assume that in the two channels we have the same selection efficiency of 50% with a mass resolution for the signal of 0.3 in channel A and 0.1 in channel B, and that we have a flat background of 1 event from −1 to 1 (we take as an example the mass but it can be any other variable). Binning such a distribution in bins of width of 0.1, the result is shown in figure 1-a for channel A and 1-c for channel B.

These two spectra can be rearranged as in figure 1-b for channel A and 1-d for channel B, where the bins of the two analyses are ordered in signal/background ratio. The combination of the first two analyses, shown in figures 1-b and 1-d, is represented by the dots in figure 2.

At this point if we increase the signal efficiency we can improve the overall sensitivity. For instance we take two additional selections, C and D, both with 15% additional efficiency on channel A and B respectively. For simplicity the mass resolution and the background level for
Figure 1: Distributions for signal and background in analyses A (a) B (c) C (e) D (g). Equivalent distributions, analyses A (b) B (d) C (f) D (h), with signal/background ratio ordering.
Figure 2: Combination of analyses A B C D (histogram) and of analyses A and B only (dots). Analysis bins are ordered according to their signal/background ratio.
the new analyses are assumed to be the same as those in the original analyses A and B. The equivalent plots are also shown in figures 1-e-f for analysis C and in figures 1-g-h for analysis D.

From the combination of the four analyses, shown in figure 2, it is apparent that the A-B-C-D analyses combined are better than A-B analyses alone. As it will be explained in more detail in the following it is clear that, depending on the estimator used and on the systematic errors, it may be useful to reject the bins with worse signal/background ratio. In conclusion, to obtain a globally optimized analysis for exclusion and discovery at the same time it is sufficient to have an optimized ordering of the analyses, or of the analysis bins, which can be obtained with the best available variables.

LEP experiments so far for the calculation of Higgs limits have used estimators which evaluate the signal/background ratio by means of the reconstructed Higgs mass. This is not always the best information to discriminate signal from background (for instance in the $H^0qq$ channel the b-tagging is much better) and in any case is not the only one. One possibility, for example, is to use neural network and the neural network output. Another is to use simple selections cuts linked together by means of a global variable as previously shown in [6]. The details of this last technique will be described in a dedicated paper [7].

According to formula [5], where background subtraction is used, adding a new channel, even with very poor signal/background ratio, the average analysis sensitivity does not worsen. This statement implies that all channels should be used because they improve the overall sensitivity, even if very little. Unluckily this is an ideal situation because, as we will see in the following, uncertainties on the background level, both from statistical and systematic sources, do not allow the use of analyses with very poor signal/background ratio. So the optimal analysis should have a cut on the signal/background ratio according to the amplitude of the uncertainties.

In particular as we have already seen it is better not to join in a single analysis channels with different signal/background ratio. Furthermore we split every single channel/analysis into several complementary analyses with different signal/background ratios, and we try to do that in the most effective way. But we would like to warn anyway that one should be cautious with that procedure because it may lead, if we do not take into account uncertainties on the background level, to average and sometimes also actual limit overestimation due to large MC statistical errors in the different bins of the analysis. On the other hand if we take into account properly the uncertainties on the background level and these are too high, we are then obliged to apply a tight cut on the signal/background ratio.

Concluding the definition of the optimal analysis also depends on the amount of MC systematic uncertainties.

To better explain this second important issue of our method, i.e. how many analyses and how much background should be accepted, we will treat in the following section a simple example, rather than describing the application of this method to Higgs searches at LEP 161 ÷ 172 as reported in [8].

6 A Simple Example

Let us now make a simple example, let us consider the case of a binned analysis with different efficiencies and background contaminations. The assumed efficiencies and background are reported in table [1] and the number of expected events for signal and background are shown in figure 3. Each bin can be considered for example as a different decay channel of the same
Figure 3: Number of expected events for signal and background for the different analyses. For the signal we assumed 5 events expected.

Table 1: Efficiency, number of events expected from the background and signal/background ratio for nine different analyses.
First of all we consider the case of background subtraction with no systematic errors to approach the problem only on the statistical side.

We perform a set of MC experiments with the signal and background indicated for each bin, each time adding a new channel. For each experiment we compute $P_L$ as given by equation 1 for the two hypotheses: background only and signal plus background. After correction to have exact probability we get $P_T$, whose definition is described below, and we obtain the results shown in Figures 4 and 5, where we show the distributions for $P_L$ and for $P_T$ for a large number of trial experiments (between 300 thousand and 1 million).

These Figures are ordered in increasing number of included analyses. The value of $P_L$ is directly obtained from equation 1 while the value $P_T$ is obtained with Monte Carlo technique in order to have the exact probability. To obtain the exact probability, from MC experiments, for each value of our estimator $P_L$ we should count the number of experiments ($N_{exp}$) with a $P_L$ for background+signal smaller than $\bar{P}_L$, where $\bar{P}_L$ is the value of the estimator obtained from the measurement. Clearly, to properly take into account the information contained in the experiment under study the background alone should have a $P_L$ smaller than $\bar{P}_L$. We should then divide by the fraction of experiments satisfying this last relation. Consequently we define $P_T$ as:

$$P_T = \frac{\int_{0}^{\bar{P}_L} N_{exp}(P_{L_{\text{sig+back}}}) dP_{L_{\text{sig+back}}}}{\int_{0}^{\bar{P}_L} N_{exp}(P_{L_{\text{back}}}) dP_{L_{\text{back}}}}$$

One indicator of the sensitivity of the experiment is, at this point, the average $P_T$ for experiments without signal, reported in table 2 adding the bins of analysis one by one.

It is apparent that, when dealing only with statistical error and performing background subtraction, the sensitivity of the experiment is never degraded by the addition of additional analyses regardless of the amount of background that they contribute. It can be seen from the average value of $P_L$ and $P_T$ that the gain is remarkable if we include channels with signal/background ratio as low as 0.1, and is almost negligible for channels with signal/background ratio between 0.1 and 0.01.

Table 2: Average $P_L$ and $P_T$ for a large number of trial experiments, in the background only hypothesis. The first row includes only the first analysis, while following rows include every time a new analysis for a total of 9 analyses in the last row.

| Last analysis included | Average $P_L$ | Average $P_T$ |
|-----------------------|--------------|--------------|
| 1                     | 0.2535 ± 0.0001 | 0.2535 ± 0.0001 |
| 2                     | 0.1299 ± 0.0001 | 0.1147 ± 0.0001 |
| 3                     | 0.1119 ± 0.0001 | 0.0877 ± 0.0001 |
| 4                     | 0.1028 ± 0.0001 | 0.0752 ± 0.0001 |
| 5                     | 0.0978 ± 0.0001 | 0.0700 ± 0.0001 |
| 6                     | 0.0956 ± 0.0001 | 0.0686 ± 0.0001 |
| 7                     | 0.0956 ± 0.0001 | 0.0685 ± 0.0001 |
| 8                     | 0.0954 ± 0.0001 | 0.0684 ± 0.0001 |
| 9                     | 0.0955 ± 0.0002 | 0.0676 ± 0.0002 |
Figure 4: Distributions for $P_L$ in the signal + background (a) and background only (b) hypotheses and for $P_T$ in the same hypotheses, (c) and (d), for a large number of trial experiments, starting from analysis 1 alone and adding every time another analysis.
Figure 5: Distributions for $P_L$ in the signal + background (a) and background only (b) hypotheses and for $P_T$ in the same hypotheses, (c) and (d), for a large number of trial experiments, starting from the first five analyses and adding every time another analysis.
| Last analysis included | Average $P_L$  | Average $P_T$  |
|------------------------|---------------|---------------|
| 1                      | 0.2535±.0009  | 0.2880±.0009  |
| 2                      | 0.1296±.0009  | 0.1693±.0009  |
| 3                      | 0.1133±.0009  | 0.1428±.0009  |
| 4                      | 0.1076±.0009  | 0.1307±.0009  |
| 5                      | 0.1081±.0009  | 0.1437±.0009  |
| 6                      | 0.1111±.0009  | 0.1451±.0009  |
| 7                      | 0.1136±.0009  | 0.1614±.0009  |
| 8                      | 0.1182±.0009  | 0.1530±.0009  |
| 9                      | 0.1174±.0009  | 0.1642±.0009  |

Table 3: Average $P_L$ and $P_T$ for 10000 trial experiments, in the background only hypothesis. The first row includes only the first analysis, while following rows include every time a new analysis for a total of 9 analyses in the last row. A systematic uncertainty of 40% both on signal efficiency and on the background level have been introduced.

In this study, even if not unambiguously demonstrated, the value of $P_L$ turned out to be always higher than the value of the true probability; thus it seems impossible that, using $P_L$ as the true confidence level, optimistic limits were obtained.

### 6.2 Statistical and systematic errors

We repeat the same exercise this time taking into account possible systematic errors on the signal efficiency and on the background level and we want to check the stability of the method.

We perform a set of MC experiments with the signal and background indicated for each bin, each time adding a new channel. As before for each experiment we compute $P_L$ for the two hypotheses: background only, signal + background.

Now in addition we introduce a systematic uncertainty of 40% both on signal efficiency and on the background level applied when randomly generating the outcome of the MC experiment. This systematic uncertainty is introduced in each MC experiment according to a gaussian distribution with mean equal to 40%.

A systematic uncertainty of 40% is really an extreme case but is useful to check the results of the method. From Table 3 we realize that starting from the fifth analysis (corresponding to a signal/background ratio of 0.25) the average sensitivity worsens. This is an important result since it clarifies that according to the systematic uncertainty we have to reject analyses with a signal/background ratio lower than a certain value in order to reach the best sensitivity.

In Tables 4 and 5 we show the behaviour of the Average $P_L$ and $P_T$ when a systematic uncertainty of 20% is considered only for signal efficiency (Table 4) or for background level (Table 5).

From Table 4 we can not see any striking worsening of the sensitivity while in Table 5 it is rather significant the worsening starting from the sixth analysis (signal/background ratio equal to 0.1). We can then conclude that systematic errors on the background level are more important than those on the signal efficiency.

In Figure 6 we show the average value of $P_T$ as a function of the number of analyses included. In this Figure we compare the behaviour of $<P_T>$ for different amplitudes of systematic errors. In the same Figure we also show the behaviour of $P_T$ in the case of no background subtraction.
Table 4: Average $P_L$ and $P_T$ for 10000 trial experiments, in the background only hypothesis. The first row includes only the first analysis, while following rows include every time a new analysis for a total of 9 analyses in the last row. A systematic uncertainty of 20% on signal efficiency have been introduced.

| Last analysis included | Average $P_L$   | Average $P_T$   |
|------------------------|----------------|----------------|
| 1          | 0.2535 ± .0009 | 0.2635 ± .0009 |
| 2          | 0.1291 ± .0009 | 0.1261 ± .0009 |
| 3          | 0.1118 ± .0009 | 0.1005 ± .0009 |
| 4          | 0.1039 ± .0009 | 0.0825 ± .0009 |
| 5          | 0.0980 ± .0009 | 0.0829 ± .0009 |
| 6          | 0.0965 ± .0009 | 0.0838 ± .0009 |
| 7          | 0.0970 ± .0009 | 0.0765 ± .0009 |
| 8          | 0.0961 ± .0009 | 0.0809 ± .0009 |
| 9          | 0.0958 ± .0009 | 0.0766 ± .0009 |

Table 5: Average $P_L$ and $P_T$ for 10000 trial experiments, in the background only hypothesis. The first row includes only the first analysis, while following rows include every time a new analysis for a total of 9 analyses in the last row. A systematic uncertainty of 20% on the background level have been introduced.

| Last analysis included | Average $P_L$   | Average $P_T$ |
|------------------------|----------------|--------------|
| 1          | 0.2539 ± .0009 | 0.2597 ± .0009 |
| 2          | 0.1302 ± .0009 | 0.1193 ± .0009 |
| 3          | 0.1130 ± .0009 | 0.0913 ± .0009 |
| 4          | 0.1050 ± .0009 | 0.0716 ± .0009 |
| 5          | 0.0997 ± .0009 | 0.0745 ± .0009 |
| 6          | 0.1006 ± .0009 | 0.0772 ± .0009 |
| 7          | 0.1007 ± .0009 | 0.0773 ± .0009 |
| 8          | 0.1017 ± .0009 | 0.0802 ± .0009 |
| 9          | 0.1017 ± .0009 | 0.0773 ± .0009 |

Table 6: Average $P_L$ and “$P_T$” for 10000 trial experiments, in the background only hypothesis. The first row includes only the first analysis, while following rows include every time a new analysis for a total of 9 analyses in the last row. No background subtraction has been applied to to compute “$P_T$”.

| Last analysis included | Average $P_L$   | Average “$P_T$” |
|------------------------|----------------|----------------|
| 1          | 0.2532 ± .0009 | .2588 ± .0009  |
| 2          | 0.1296 ± .0009 | .1240 ± .0009  |
| 3          | 0.1111 ± .0009 | .1087 ± .0009  |
| 4          | 0.1028 ± .0009 | .1222 ± .0009  |
| 5          | 0.0982 ± .0009 | .1544 ± .0009  |
| 6          | 0.0966 ± .0009 | .2125 ± .0009  |
| 7          | 0.0971 ± .0009 | .2458 ± .0009  |
| 8          | 0.0959 ± .0009 | .2599 ± .0009  |
| 9          | 0.0951 ± .0009 | .2811 ± .0009  |
Figure 6: Average value of $\mathcal{P}_T$ as a function of the number of analyses included. The five lines show the behaviour of $\langle \mathcal{P}_T \rangle$ for different amplitudes of systematic errors and in the case of no background subtraction.
This shows that even large systematic errors on the efficiency are not significant while the same uncertainties on the background play a role. In the case of huge systematic errors (40%) the sensitivity degrades considerably including analyses with high level of background. If one has to deal with such a situation it is obviously better to reject analyses with too low signal to background ratio (in our example between 0.1 and 0.25).

Finally in Table 6 we show the values that would be obtained if we neglected the existence of background and we compared the outcome of the experiment with signal only MC experiments. If we did that the addition of high background analyses would definitely deteriorate the sensitivity as can be clearly seen from Figure 6.

### 7 Discoveries

To estimate the analysis sensitivity for discoveries we proceed exactly in the same way as previously shown when optimizing the analysis sensitivity for exclusions.

The only difference is that we set the discovery $CL$ at the requested probability for the measurement to be consistent with the background only hypothesis.

In Table 7 we show the probability to discover our signal at different levels of significance (1%, 0.1% and 0.01%) as a function of the number of analyses included.

From this Table we can see that the gain due to the inclusion of low purity analyses is much less than for the case of exclusion as shown in Table 2. There we had a remarkable gain including analyses with signal/background ratio as low as 0.1, while in Table 7 we have a remarkable gain only including analyses with signal/background ratio not lower than 1.

### 8 Measurements and other issues

Using the same estimator described before is possible to directly measure the rate of a given process. It can easily be seen that the optimization method here proposed also improves the errors on the measurement.

Another issue which follows naturally from this optimization method is the combination of results from different experiments. From what we have described it should be clear that

| Last analysis included | Discovery at $\leq 0.01$ | Discovery at $\leq 0.001$ | Discovery at $\leq 0.0001$ |
|------------------------|--------------------------|---------------------------|---------------------------|
| 1                      | 0.4747 ± 0.2580          | 0.2168 ± 0.1381           | 0.0786 ± 0.0552           |
| 2                      | 0.6088 ± 0.0779          | 0.3492 ± 0.0414           | 0.2183 ± 0.0499           |
| 3                      | 0.6318 ± 0.0002          | 0.3997 ± 0.0071           | 0.2366 ± 0.0195           |
| 4                      | 0.6292 ± 0.0021          | 0.3988 ± 0.0027           | 0.2312 ± 0.0089           |
| 5                      | 0.6339 ± 0.0011          | 0.3989 ± 0.0076           | 0.2261 ± 0.0143           |
| 6                      | 0.6326 ± 0.0030          | 0.3991 ± 0.0092           | 0.2063 ± 0.0245           |
| 7                      | 0.6338 ± 0.0031          | 0.3973 ± 0.0090           | 0.2453 ± 0.0246           |
| 8                      | 0.6296 ± 0.0030          | 0.3877 ± 0.0144           | 0.2237 ± 0.0120           |
| 9                      | 0.6345 ± 0.0030          | 0.4006 ± 0.0101           | 0.2254 ± 0.0209           |

Table 7: Discovery probability at different $CL$. The first row includes only the first analysis, while following rows include every time a new analysis for a total of 9 analyses in the last row.
different experiments can be treated on the same footing just as different analyses with their own efficiencies, backgrounds and systematic errors.

9 Conclusions

We propose a new method, which can be applied to searches and to any cross section measurement.

Using a large variety of estimators we are able to devise an intrinsically optimized analysis which is the same for discovery (and relative cross section measurement) and for exclusion.

Using this method the sensitivity of the analysis is improved compared to most of previously used methods.

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