ORDERING ALGORITHMS AND CONFIDENCE INTERVALS IN THE PRESENCE OF NUISANCE PARAMETERS

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We discuss some issues arising in the evaluation of confidence intervals in the presence of nuisance parameters (systematic uncertainties) by means of direct Neyman construction in multi-dimensional space. While this kind of procedure provides rigorous coverage, it may be affected by large overcoverage, and/or produce results with counterintuitive behavior with respect to the uncertainty on the nuisance parameters, or other undesirable properties. We describe a choice of ordering algorithm that provides results with good general properties, the correct behavior for small uncertainties, and limited overcoverage.

1. Introduction

A conceptually straightforward method to incorporate systematics into Confidence Limits is to apply the usual Neyman construction directly on the complete pdf of the problem, including the set of additional parameters $\nu$ describing the systematic effects, and then project the solution on the space of parameters of interest $\mu$. Systematic uncertainties may take the form of an allowed range for the $\nu$'s, or may be defined by the observables of the problem. Although the method can be applied to a more general situation, we will assume in the following discussion that measurements are available of some (“subsidiary”) observable(s) $y$, whose only purpose is to provide information on the systematic parameters, through the dependence of their pdf on $\nu$. In this case, one will consider the overall pdf:

$$p((x, y)|(\mu, \nu))$$

that gives the joint probability of observing the value of the “physics observables” $x$ plus all “systematic measurements” $y$, given all unknown parameters, physics and systematics. One starts by deriving Confidence Limits in the larger $(\mu, \nu)$ space from the observed values of $(x, y)$ with the same procedure that could have been used in absence of systematics to derive limits on $\mu$: one simply needs to sample a number of points inside the parameter space and require coverage for each of them. Then, in order to get results containing only the physical parameters, one needs to project the confidence region in $(\mu, \nu)$ onto the $\mu$ space, so as to get rid of unwanted information on the nuisance parameters.

Although the above procedure is general, conceptually simple, and rigorous, other methods have been preferred in the vast majority of problems in physics. This can be ascribed to a few important difficulties with this method. To begin with, the problem of numerical calculation of Confidence Regions (CRs) in multi-dimensional spaces is often quite complex and CPU-consuming. Then there is a non-trivial question of what ordering algorithm to use in the Neyman construction. There is an issue of “efficiency”, or power, of the solution, because projecting the band on the $\mu$ space effectively means to inflate a limited region in $(\mu, \nu)$ to an unlimited band in the $\nu$ direction, thereby increasing the coverage for all additional points $(\mu, \nu)$ included. This means that the final limits quoted on $\mu$ will almost always overcover, and sometimes badly, especially when $\nu$ has many dimensions; this is indeed the case with standard choices of ordering\(^1\). A related additional problem is that the behavior of the limits when the systematic uncertainty approaches zero is in many cases unsatisfying. It often happens that the limit for small systematics is quite different from the result one would quote in absence of that systematic; this problem, however, is not unique to the projection method.

If the above problems could be alleviated, this methodology could find greater use in HEP.

2. A Benchmark problem

Our discussion, although general, will be centered on a specific problem that has been the initial motivation for this work: a Poisson distributed signal in presence of a known background, with a systematic uncertainty on the signal normalization (efficiency).
We have:

\[ x \sim \text{Pois}(\epsilon \mu + b) \quad , \quad e \sim G(\epsilon, \sigma) \]  

(2)

where \( \epsilon \) is the result of a subsidiary measurement with resolution \( \sigma \) of the unknown efficiency \( \epsilon \), which is intended to be a generic “normalization factor”, not necessarily smaller than one. In the following we will mostly assume a normal distribution for \( G \) for simplicity; the possibility of negative values of the efficiency estimate does not pose any problems to the algorithms discussed in this document. This can actually occur, for instance, when the efficiency measurement implies some sort of background subtraction procedure.

3. Looking for an optimal band

What one would like to accomplish is to find a clever enough rule for constructing the initial Confidence Band, to minimize the amount of unnecessary coverage added when the band is projected onto the “interesting parameters” space. It is not obvious what the minimum is for a particular problem, because the frequentist requirement of minimum coverage for every possible true value of the parameters may imply some minimum amount of overcoverage, which is unavoidable regardless of the algorithm used in the construction, much in the way overcoverage occurs in discrete problems. Therefore, there is no reason for being a-priori discouraged about the capability of the projection method to provide powerful solutions (that is, narrow intervals). A striking demonstration of this is provided by the use of the projection method, with an appropriately designed algorithm for band construction, in producing a more efficient solution to a classical, well-explored problem like the ratio of Poisson means.

It is intuitively obvious that in order to obtain an efficient solution, the initial confidence band must extend as far as possible along the direction of the nuisance parameter. This is not trivial to achieve, since the band needs to be built in the \((x, \epsilon)\) space, while the objective is to produce a desired shape in the \((\mu, \epsilon)\) space. A good general requirement to impose is that, given any two sections of the band at two fixed values of the nuisance parameter \( \epsilon \), one must be completely included in the other. It is intuitive that a band cannot be optimal if it does not satisfy this requirement, because if one had to take one of the two sections and expand it to completely include the other, the projected confidence region in \( \mu \) would be unaffected, and conversely one could exploit the coverage gained in this way to trim a part of the exceeding part of the chosen section, thus creating the conditions for a tightening of the projected confidence region.

4. Ordering Algorithm

One way to define how to construct the confidence band in the complete space is to derive it from an ordering function \( f(x, e; \mu, \epsilon) \), so that the confidence band is defined by the inequality \( f(x, e; \mu, \epsilon) > c(\mu, \epsilon) \), where the threshold \( c \) is determined for each value of the parameters from the usual Neyman’s requirement of coverage:

\[ \int_{f(x,e;\mu,\epsilon) > c(\mu,\epsilon)} p(x, e | \mu, \epsilon) dx de \geq CL \]  

(3)

where \( CL \) is the desired Confidence Level. It is worth noting that this is not the only conceivable way to define a band satisfying the coverage condition, but it is attractive for reasons of simplicity. A simple way to implement in an ordering algorithm the requirement of inclusion formulated in the previous section is to impose that \( f(x, e; \mu, \epsilon) \) is independent of \( e \): \( f(x, e; \mu, \epsilon_1) = f(x, e; \mu, \epsilon_2) \). In this way, sections taken at different \( \epsilon \) for the same value of \( \mu \) will only differ in the value of \( c(\mu, \epsilon) \), and will therefore be included in one another. This requirement is also very convenient from the point of view of computing, as it implies that the ordering function \( f \) need only be calculated once for every \( \mu \).

As an additional requirement, we want the projected confidence regions to converge to the results in absence of systematic uncertainty when the size of the uncertainty goes to zero. We do not restrict to a specific ordering (one may want to be able to choose, for instance, between central and upper limits), so we start from a given generic ordering function \( f_0(x; \mu) \) in the restricted space. This defines the behavior of the ordering function along the direction of observable \( x \), but careless extension of any such rule to the

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This simple and common example has been selected by the CDF statistics committee as a benchmark in performing comparisons between a number of different methods. A minor difference from the current example is that a positive, Poisson–like distribution is assumed for the subsidiary measurement instead of a Gaussian, in order to avoid problems with Bayesian treatment.

whole \((x, e)\) space will not work. As an example, extending the trivial ordering used to achieve upper limits \((f_0(x; \mu) = x)\) results in substantial overcoverage (see fig.1a). We need additional criteria to ensure proper behavior in the subsidiary observable \(e\). We don’t want to give special preference to any values, because this will amount to attempting to extract information on the nuisance parameter, while we want to maximize information on the physical parameter \(\mu\). We do this by choosing the following ordering function:

\[
f(x, e; \mu) = \int_{f_0(x')}^{f_0(x)} p(x'|e; \mu, \hat{e}(e))dx' \tag{4}
\]

where \(\hat{e}(e)\) is the maximum–Likelihood estimate of \(e\) for the given \(e\). That implies that the same integrated conditional probability will be contained in the band for each value of \(e\).

We make an exception to the rule of being indifferent to the value of \(e, e\) for very unlikely values: we select an interval of values \([e_{\text{min}}, e_{\text{max}}]\) such that the probability for a measurement to fall outside is \(<1 - CL\), and assign lowest rank to all points lying outside this interval. From the above conditions, they will never be reached by the ordering procedure, so they can simply be ignored, which saves computation. This clipping technique has already been advocated as a help in keeping the projections small; in our context however it seemed to have no significant effects beyond saving computation.

5. Results

We have applied the ordering rule of equation (4) to our problem of choice (sec. 2), with an ordering \(f_0\) corresponding to upper limits. Fig. 1b shows that this time very little overcoverage is obtained, except from some discretization–related “ripples”. It is interesting to note that these limits are tighter than the limits obtained with other popular methods (compare, for instance, the coverage obtained for the same problem with Bayesian\(^2\) or Cousins–Highland methods\(^5, 6\)), although guaranteed by construction to cover for every possible value of both \(\mu\) and \(e\). This confirms the capability of the projection method to produce powerful results, when used in conjunction with an appropriate ordering algorithm, as per Eq. (4).

The procedure we have described can be used with any other desired ordering. If we apply it to Unified Intervals\(^7\), we find an interesting fact: because of the Likelihood Ratio theorem, ensuring the independence of the distribution from true parameter values, the ordering algorithm defined by Eq. (4) is approximately equivalent to ordering based on the ratio of profile Likelihoods. That quantity has been suggested as a good intuitive ordering to use in handling systematics since \(^8\), and has been used in neutrino experiments\(^1, 9\) (with a conditional frequentist motivation), and in a problem very similar to ours, the Poisson with uncertainty on background\(^4\). It reappears here as an approximation of the more general rule defined by Eq. (4). Fig 2 shows that coverage plot for our benchmark problem, which is close to the nominal constant 0.9, indicating that there is very little to be further gained.

6. Continuity

One of our initial goals was to obtain a continuous behavior when \(\sigma_{\text{syst}} \to 0\). In previous examples, although the limit is approximated much better than with other frequentist methods (see for instance\(^10\)), there is still a slight difference. For instance, the upper limit with the Unified method at 90% for \(n = 4, b = 3\) is \(5.6\), while our results approach \(\approx 5.47\) when \(\sigma \to 0\). More annoyingly, the limit found with systematics is lower. This is a well known problem, tied to the transition between discrete and continuous regime\(^11\), and is pretty much independent of the specific algorithm. However, our method for evaluating limits allows a very simple fix, requiring no alterations to the ordering: all that is needed is to keep the size of the grid used in the numerical calculations from becoming too small in the direction of the nuisance observable. This has a natural justification under the same principles that guided the general design of our algorithm: we are trying to disregard detailed information on the the subsidiary observable, in favor of information on the physics parameter \(\mu\). In our problem, by choosing a minimum step \(\Delta e = 0.1\) we obtain perfect continuity at zero (fig. 3). A side effect of this limitation is to save some computing time.

7. Systematic uncertainties given as ranges

The approach we have described has wider application than the examples mentioned above. For in-
stance, it can handle in a natural way the important situations in which no subsidiary measurement in available to provide information on the nuisance parameter. This often occurs in real life: the systematic uncertainty may be due to a physical constraint, or related to a choice within a range (discrete or continuous) of theoretical predictions or assumptions, or can otherwise be specified in a way that is not detailed enough to uniquely identify a probability distribution. In these cases, usually the only available information on $\epsilon$ is represented by a range of admissible values.

This situation is automatically handled by our approach: one simply has one less observable to worry about, but the rest of the construction works exactly in the same way. In fact, calculations are much faster with the lack of a subsidiary measurement, so that when dealing with small systematics it is actually more convenient to transform any possible nuisance measurement into an appropriate range for the nuisance parameter, and simply use that information as input, in order to save computing time. Again, our tests yielded very limited overcoverage, compatible with what was required simply by the discrete nature of the problem.

It is worth noting that a range of values is not at all equivalent to a uniform distribution, which implies more precise knowledge. For instance, by comparing the limits obtained in the two cases, it is seen that the limits for the range case are looser than in the uniform distribution case, as intuitively expected due to the smaller information content in a statement about a range (see Table 1). This is in contrast with what happens in a Bayesian approach, where a prior function is always required, and a uniform distribution is often chosen to represent lack of information.

In general, treating systematic uncertainties as ranges is a good candidate approach to problems with many nuisance parameters, as it allows big savings in CPU time, in addition to avoiding the trouble of having to worry about the accuracy of the distributions assumed to represent the systematic uncertainties.

8. Conclusions

We have presented a general method to incorporate systematic uncertainties in a limit calculation in a rigorous frequentist way, which is powerful (does not produce large overcoverage), has the right limit for small uncertainties, can be used even with uncertainties given as ranges, and can easily be calculated in practice. This is based on projection of a traditional Neyman construction with an ordering algorithm specified by Eq. (4). We have applied it to the specific problem of Poisson measurement with an uncertainty on the efficiency.

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Table 1. Confidence Limits for Poisson+background with systematic uncertainty on the efficiency, obtained by extending Unified Limits through Eq.(4). Results are given for $b = 3$, $e = 1.0$, and various models of uncertainty on $\epsilon$ (see text).

| $n_{obs}$ | Without systematics | Gaussian $\sigma = 0.1$ | Uniform $\pm 0.15$ | Range $\pm 0.15$ |
|-----------|---------------------|-------------------------|---------------------|------------------|
| 0         | 0.00 , 1.08         | 0.0 , 1.1               | 0.0 , 0.9           | 0.0 , 1.0        |
| 1         | 0.00 , 1.88         | 0.0 , 1.9               | 0.0 , 1.7           | 0.0 , 1.9        |
| 2         | 0.00 , 3.04         | 0.0 , 3.0               | 0.0 , 2.7           | 0.0 , 3.0        |
| 3         | 0.00 , 4.42         | 0.0 , 4.4               | 0.0 , 4.0           | 0.0 , 4.5        |
| 4         | 0.00 , 5.60         | 0.0 , 5.9               | 0.0 , 5.4           | 0.0 , 6.0        |
| 5         | 0.00 , 6.99         | 0.0 , 7.4               | 0.0 , 6.9           | 0.0 , 7.4        |
| 6         | 0.15 , 8.47         | 0.0 , 8.9               | 0.2 , 8.2           | 0.1 , 8.9        |
| 7         | 0.89 , 9.53         | 0.9 , 10.3              | 1.0 , 9.6           | 0.8 , 10.4       |
| 8         | 1.51 , 10.99        | 1.4 , 11.7              | 1.5 , 10.9          | 1.3 , 11.8       |
| 9         | 1.88 , 12.30        | 2.0 , 13.1              | 2.1 , 12.3          | 1.9 , 13.1       |

Fig. 2. Coverage plot for Unified limits, Gaussian uncertainty, $b = 3, \sigma = 0.1$.

Fig. 3. Behavior of upper limit when $\sigma \to 0$, same problem as in Fig. 2.

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