How to Claim a Discovery

W.A. Rolke and A.M. López University of Puerto Rico - Mayaguez

We describe a statistical hypothesis test for the presence of a signal. The test allows the researcher to fix the signal location and/or width a priori, or perform a search to find the signal region that maximizes the signal. The background rate and/or distribution can be known or might be estimated from the data. Cuts can be used to bring out the signal.

1. INTRODUCTION

Setting limits for new particles or decay modes has been an active research area for many years. In high energy physics it received renewed interest with the unified method by Feldman and Cousins [1]. Giunti [2] and Roe and Woodroofe [3] gave variations of the unified method, trying to resolve an apparent anomaly when there are fewer events in the signal region than expected. They all discuss the problem of setting limits for the case of a known background rate. The case of an unknown background rate was discussed in a conference talk by Feldman [4] and a method for handling this case was developed by Rolke and López [5]. Little work has been done though on the question of claiming a discovery. This problem could be handled by finding a confidence interval and claiming a discovery if the lower limit is positive. Instead the question of a discovery should be done separately, by performing a hypothesis test with the null hypothesis H_o :"There is no signal present". Rejecting this hypothesis will then lead to a claim for a new discovery. In carrying out a hypothesis test one needs to decide on the type I error probability α , the probability of falsely rejecting the null hypothesis. This is of course equivalent to the major mistake to be guarded against, namely that of falsely claiming a discovery.

In practice a hypothesis test is often carried out by finding the p-value. This is the probability that an identical experiment will yield a result as extreme (with respect to the null hypothesis) or even more so given that the null hypothesis is true. Then if $p < \alpha$ we reject H_0 ; otherwise we fail to do so. For the test discussed here it is not possible to compute the p-value analytically, and therefore we will find the p-value via Monte Carlo.

Maybe the most important decision in carrying out a hypothesis test is the choice of α , or what we might call the discovery threshold. As we shall see, this decision is made much easier by the method described here because we will need only one threshold, regardless of how the analysis was done. What a proper discovery threshold should be in high energy physics is a question outside the scope of this paper, although we might suggest $\alpha = 0.001$ (roughly equivalent to 3σ). Sinervo [6] argues for a much stricter standard of 5σ , or $\alpha = 2.9 * 10^{-7}$. We believe that such extreme values were used in the past because it was felt that the calculated p values were biased downward by the analysis process, and a small α was needed in order to compensate for any unwittingly introduced biases. If we were to trust that our p-value is in fact correct, a 1 in 1000 error rate should to be acceptable.

A general introduction to hypothesis testing with applications to high energy physics is given in Sinervo [6]. A classic reference for the theory of hypothesis testing is Lehmann [7].

2. THE SIGNAL TEST

Our test uses T = x - b or $T = x - y/\tau$ as the test statistic, depending on whether the background rate b is assumed to be known or not. Here x is the number of observations in the signal region, y is the number of observations in the background region and τ is the probability that a background event falls into the background region divided by the probability that it falls into the signal region. Therefore y/τ is the estimated background in the signal region and $x - y/\tau$ is an estimate for the signal rate λ . T is the maximum likelihood estimator of λ , and it is the quantity used in Feldman and Cousins [1] without being set to 0 when $x - y/\tau$ is negative. This is not necessary here because a negative value of $x - y/\tau$ will clearly lead to a failure to reject H_0 .

Other choices for the test statistic are of course possible. For example, a measure for the size of a signal that is often used in high energy physics is S/\sqrt{b} . Under the null hypothesis this statistic is approximately Gaussian, at least if there is sufficient data. Unfortunately the approximation is not sufficiently good in the extreme tails where a new discovery is made, leading to p-values that are much smaller than is warranted. Even when using Monte Carlo to compute the true p-value, this test statistic can be shown to be inferior to the one proposed in our method because it has consistently lower power, that is its probability of detecting a real signal is smaller.

In order to find the p-value of the test we need to know the null distribution. In the simplest case of a known background rate and everything else fixed

this is given by the Poisson distribution, but in all other cases it is not possible to compute the null distribution analytically, and we will therefore find it via Monte Carlo. As an illustration consider the following case shown in figure 1: here we have 100 events on the interval [0, 1], with the signal region a priori set to be [0.44, 0.56]. There are 25 events in the signal region, and the background distribution is known to be flat. Therefore we find $x = 25, y = 75, \tau = 7.33$ and T = 14.77. Because we know that the background is flat on [0, 1], and because under the null hypothesis all 100 events are background we can simulate this experiment by drawing 100 observations from a uniform distribution on [0,1] and computing T for this Monte Carlo data set. Repeating this 150000 times we find the histogram of Monte Carlo T values shown in figure 2, case 1. In this simulation 8 of the 150000 simulation runs had a value of T greater than 14.77, or p = 0.000053. Using $\alpha = 0.0001$ we would therefore reject the null hypothesis and claim a discovery. Note that in addition to rejecting the null hypothesis we can also turn the p-value into a significance by using the Gaussian distribution and claim that this signal is a 3.87σ effect.

How would things change if the signal region had not been fixed a priori but instead was found by searching through all signal regions centered at 0.5 and we would have accepted any signal with a width between 0.01 and 0.2? That is if we had kept the signal location fixed but find the signal width that maximizes T, the estimate of the number of signal events? Again we can find the null distribution via Monte Carlo, repeating the exact analysis for each simulation run individually. The histogram of T values for this case is shown in figure 2, case 2. Here we find a value of T larger than 14.77 in 570 of the 150000 runs for a p-value of 0.0038 or 2.67σ . At a discovery threshold of $\alpha = 0.001$ we would therefore not find this signal significant anymore.

Even more, what if we also let the signal location vary, say anywhere in [0.2, 0.8]? That is for any pair of values (L, H) we define [L, H] as the signal region and [0, L), (H, 1] as the background region, compute $T_{L,H}$ for this pair and then maximize over all possible values of L and H. Note that because $T_{L,H}$ is monotonically increasing in τ as long as all the observations stay either in the signal or in the background region, we can find the maximum fairly quickly by letting L and H be the actual observations. The histogram of $T_{L,H}$ values for this case is shown in figure 2, case 3. We find a value of T larger than 14.77 in 9750 of the 150000 runs for a p-value of 0.065 or 1.51σ , clearly not significant.

It was necessary in the second and third cases above to limit the search region somewhat, to the interval [0.2, 0.8] and to signals at least 0.01 and at most 0.2 wide, because otherwise the largest value of T is almost always found for a very wide signal region, even when a clear narrow signal is present. This restriction will not induce a bias as long as the decision on where to search are made a priori.

In the general situation where the background is not flat on [0, 1] we can make use of the probability integral transform. Of course this requires knowledge of the background distribution F, but if it is not known we can estimate it from the data, either using a parametric function fitted to the data or even using a nonparametric density estimator. Again all calculations are done under the null hypothesis so we do not need to worry about the signal or its distribution.

As long as we copy exactly for the Monte Carlo events what was done for the real data we will find the correct p-value. This includes using cuts used to improve the signal to noise ratio, but it then requires the ability to correctly Monte Carlo all the variables used for cutting, including their correlations.

3. PERFORMANCE OF THE METHOD

As an illustration for the performance of the signal test consider the following experiment: we generate 100 events from a linear background on [3, 5] and (if present) a Gaussian signal at 3.9 with a width of 0.05. Then we find the signal through a variety of situations, from the one extreme where everything is fixed a priori to the other where the largest signal of any width is found. The background density is found by fitting and the background rate is estimated. The power curves are shown in figure 3. No matter what combination of items were fixed a priori or were used to maximize the test statistic, and with it the signal to noise ratio, all cases achieved the desired type I error probability, $\alpha = 0.05$. Not surprisingly the more items are fixed a priori, the better the power of the test.

4. CONCLUSION

We have described a statistical hypothesis test for the presence of a signal. Our test is conceptually simple and very flexible, allowing the researcher a wide variety of choices during the analysis stage. It will yield the correct type I error probability as long as the Monte Carlo used to find the null distribution exactly mirrors the steps taken for the data. Monte Carlo studies have shown that this method has satisfactory power.

Acknowledgments

This work was partially supported by the Division of High Energy Physics of the US Department of Energy.



Figure 1: 100 Events on [0,1], with the signal region a priori set to be [0.44, 0.56]. There are 25 events in the signal region, and the background distribution is assumed to flat.



Figure 2: Histograms of T values of Monte Carlo simulation.



Peak	Width	Param.	Rate
1: fixed	fixed	fixed	estimated
2: fixed	fitted	fixed	estimated
3: fitted	fitted	fixed	estimated
4: fixed	fixed	fixed	exact
5: fixed	fitted	fixed	exact
6: fitted	fitted	fixed	exact
7: fixed	fixed	fitted	estimated
8: fixed	fitted	fitted	estimated
9: fitted	fitted	fitted	estimated
10:fitted	fitted	fitted	exact
Linear background on [3,5]			
Gaussian Peak at 3.9, s=0.1			
Sample Size :100			

Figure 3: Power curves for 10 different cases such as signal location fixed a priori or not, same for signal width, background estimated or ect. alpha=0.05 is used.

References

- R.D. Cousins, G.J. Feldman, "A Unified Approach to the Classical Statistical Analysis of Small Signals", Phys. Rev, D57, (1998)
- [2] 3873.C. Giunti, "A new ordering principle for the classical statistical analysis of Poisson processes with background", Phys. Rev D59, 053001 (1999).
- [3] B.P. Roe, M.B. Woodroofe, "Improved Probability Method for Estimating Signal in the Presence of Background", Phys. Rev D60 053009 (1999)
- [4] G. Feldman, "Multiple measurements and parameters in the unified approach", talk at Fermilab Workshop on Confidence Limits 27-28 March,

2000, http://conferences.fnal.gov/cl2k/, p. 10-14.

- [5] W.A. Rolke, A.M. López, "Confidence Intervals and Upper Bounds for Small Signals in the Presence of Background Noise", Nucl. Inst. and Methods A458 (2001) 745-758
- [6] P.K. Sinervo, "Signal Significance in Particle Physics", Proceedings of the Conference: Advanced Statistical Techniques in Particle Physics, Institute for Particle Physics Phenomenology, University of Durham, UK, 2002, 64-76.
- [7] E.L. Lehmann "Testing Statistical Hypotheses", 2nd Ed. (1986) Wiley, New York.