Testing for a Signal

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Abstract
We describe a statistical hypothesis test for the presence of a signal based on the likelihood ratio statistic. We derive the test for one case of interest and also show that for that case the test works very well, even far out in the tails of the distribution. We also study extensions of the test to cases where there are multiple channels.

1 Introduction

In recent years much work has been done on the problem of setting limits, beginning with the seminal paper by Feldman and Cousins [1]. A fairly comprehensive solution for limits on the signal rate in the presence of background and efficiency, both measured with some uncertainty, was given in Rolke, López and Conrad [2]. In this paper we will study a related problem, namely that of claiming a new discovery, say of a new particle or decay mode. Statistically this falls under the heading of hypothesis testing. We will describe a test derived in a fairly standard way called the likelihood ratio test. The main contribution of this paper is the study of the performance of this test. This is essential for two reasons. First, discoveries in high energy physics require a very small false-positive, that is the probability of falsely claiming a discovery has to be very small. This probability, in statistics called the type I error probability α, is sometimes required to be as low as $2.87 \cdot 10^{-7}$, equivalent to a 5σ event. The likelihood ratio test is an approximate test, and whether the approximation works this far out in the tails is a question that needs to be investigated. Secondly, in high energy physics we can often make use of multiple channels, which means we have problems with as many as 30 parameters, 20 of which are nuisance parameters. The sizes of the samples needed to insure that the likelihood ratio test works need to be determined.

2 Likelihood Ratio Test

We will consider the following general problem: we have data $\mathbf{X}$ from a distribution with density $f(\mathbf{x};\theta)$ where θ is a vector of parameters with $\theta \in \Theta$ and Θ is the entire parameter space. We wish to test the null hypothesis $H_0 : \theta \in \Theta_0$ (no signal) vs the alternative hypothesis. $H_a : \theta \in \Theta_0^c$ (some signal), where Θ_0 is some subset of Θ. The likelihood function is defined by

$$L(\theta|\mathbf{x}) = f(\mathbf{x};\theta)$$

and the likelihood ratio test statistic is defined by

$$\lambda(\mathbf{x}) = \frac{\sup_{\Theta_0} L(\theta|\mathbf{x})}{\sup_{\Theta} L(\theta|\mathbf{x})}$$

Intuitively we can understand the statistic in the case of a discrete random variable. In this case the numerator is the maximum probability of the observed sample if the maximum is taken over all parameters allowed under the null hypothesis. In the denominator we take the maximum over all possible values of the parameter. The ratio of these is small if there are parameter points in the alternative hypothesis for which the observed sample is much more likely than for any parameter point in the null hypothesis. In that case we should reject the null hypothesis. Therefore we define the likelihood ratio test to be: reject the null hypothesis if $\lambda(\mathbf{x}) \leq c$, for some suitably chosen c, which in turn depends on the type I error probability α.

How do we find c? For this we will use the following theorem: under some mild regularity conditions if $\theta \in \Theta_0$ then $-2\log\lambda(\mathbf{x})$ has a chi-square distribution as the sample size $n \to \infty$. The degrees of freedom of the chi-square distribution is the difference between the number of free parameters specified by $\theta \in \Theta_0$ and the number of free parameters specified by $\theta \in \Theta$.

A proof of this theorem is given in Stuart, Ord and Arnold [3] and a nice discussion with examples can be found in Casella and Berger [4].

3 A Specific Example: A Counting Experiment with Background and Efficiency

We begin with a very common type of situation in high energy physics experiments. After suitably chosen cuts we find n events in the signal region, some of which may be signal events. We can model n as a random variable N with a Poisson distribution with rate $es+b$ where b is the background rate, s the signal rate and e the efficiency on the signal. We also have an independent measurement y of the background rate, either from data sidebands or from Monte Carlo and we can model y as a Poisson with rate τb, where τ is the relative size of the sidebands to the signal region or the relative size of the Monte Carlo sample to the data sample, so that y/τ is the point estimate of the background rate in the signal region. Finally we have an independent measurement of the efficiency z, usually from Monte Carlo, and we will model z as a Gaussian with mean e and standard deviation σ_e. So we have the following probability model:

$$N \sim Pois(es+b) \qquad Y \sim Pois(\tau b) \qquad Z \sim N(e, \sigma_e)$$

In this model s is the parameter of interest, e and b are nuisance parameters and τ and σ_e are assumed known. Now the joint density of N, Y and Z is given by

$$f(n,y,z;e,s,b) = \frac{(es+b)^n}{n!}e^{-(es+b)}\frac{(\tau b)^y}{y!}e^{-\tau b}\frac{1}{\sqrt{2\pi\sigma_e^2}}e^{-\frac{1}{2}\frac{(z-e)^2}{\sigma_e^2}}$$

Finding the denominator of the likelihood ratio test statistic λ means finding the maximum likelihood estimators of e, s, b. They are given by $\widehat{s} = n - y/\tau$, $\widehat{b} = y/\tau$ and $\widehat{e} = z$.

We wish to test $H_0 : s = 0$ vs $H_a : s > 0$, so under the null hypothesis we have

$$\begin{aligned}\log f(n,y,z;0,b,e) &= n\log(b) - \log(n!) - b + \\ & y\log(\tau b) - \log(y!) - (\tau b) - \tfrac{1}{2}\log(2\pi\sigma_e^2) - \tfrac{1}{2}\frac{(z-e)^2}{\sigma_e^2}\end{aligned}$$

and we find that this is maximized for $\widetilde{b} = \frac{n+y}{1+\tau}$ and $\widetilde{e} = z$. Now

$$\lambda(n,y,z) = \frac{\sup\ L(0,b,e|n,y,z)}{\sup\ L(s,b,e|n,y,z)} = \frac{f(n,y,z|0,\widetilde{b},\widetilde{e})}{f(n,y,z|\widehat{s},\widehat{b},\widehat{e})} =$$

$$\frac{\left(\frac{n+y}{1+\tau}\right)/n!\exp\left(-\frac{n+y}{1+\tau}\right)\left(\tau\frac{n+y}{1+\tau}\right)^{y}/y!\exp\left(-\tau\frac{n+y}{1+\tau}\right)\frac{1}{\sqrt{2\pi\sigma_e^2}}e^{-\frac{1}{2}\frac{(z-z)^2}{\sigma_e^2}}}{n^n/n!\exp(-n)\,y^y/y!\exp(-y)\frac{1}{\sqrt{2\pi\sigma_e^2}}e^{-\frac{1}{2}\frac{(z-z)^2}{\sigma_e^2}}} =$$

$$\frac{\left(\frac{n+y}{1+\tau}\right)^{n+y}\tau^y}{n^n y^y}$$

One special case of this needs to be studied separately, namely the case $y = 0$. In this case we can not take the logarithm and the maxima above have to be found in a different way. It turns out that the maximum likelihood estimators are $\widehat{s} = n$, $\widehat{b} = 0$, $\widehat{e} = z$, and under the null hypothesis we find $\widetilde{b} = \frac{n}{1+\tau}$ and $\widetilde{e} = z$. With this we find $\lambda(n,0,z) = (1+\tau)^{-n}$.

First we note that the test statistic does no involve z, the estimate of the efficiency. This is actually clear: the efficiency is for the detection of signal events, but under the null hypothesis there are none. Of course the efficiency will affect the power curve: if e is small the observed n will be small and it will be much harder to reject the null hypothesis.

Now from the general theory we know that $-2\log\lambda(N, Y, Z)$ has a chi-square distribution with 1 degree of freedom because in the general model there are 3 free parameters and under the null hypothesis there are 2. So if we denote the test statistic by $L(n, y)$ we get

$$L(n,y) = -2\log\lambda(n,y,z) = \begin{cases} 2\left[n\log(n) + y\log(y) - (n+y)\log\left(\frac{n+y}{1+\tau}\right) - y\log(\tau)\right] & \text{if } y > 0 \\ 2n\log(1+\tau) & \text{if } y = 0 \end{cases}$$

and we have $L(N, Y) \sim \chi^2_1$, approximately.

Obviously we will only claim a disovery if there is an excess of events in the signal region, and so the test becomes: reject H_0 if $n > y/\tau$ and $L(n, y) > c$. Now it can be shown that c is the $(1 - 2\alpha)$ quantile of a chi-squared distribution with one degree of freedom.

The situation described here has previously been studied in Rolke, López and Conrad [2] in the context of setting limits. They proposed a solution based on the profile likelihood. This solution is closely related to the test described here. In fact it is the confidence interval one finds when inverting the test described above.

4 Multiple Channels

In high energy physics we can sometimes make use of multiple channels. There are a number of possible extensions from one channel. We will consider the following model: there are k channels and we have $N_i \sim Pois(e_i s_i + b_i)$, $Y_i \sim Pois(\tau_i b_i)$, $i = 1, .., k$, all independent. We will again find that the efficiencies do not affect the type I error probability. We will discuss two ways to extend the methods above to multiple channels, both with certain advantages and disadvantages.

4.1 Method 1: (Full LRT)

We can calculate the likelihood ratio statistic for the full model. It turns out that the test statistic L_k is given by

$$L_k(\mathbf{n}, \mathbf{y}) = \sum_{i=1}^{k} L(n_i, y_i) I(n_i > y_i/\tau_i)$$

where I is the indicator function, that is $I(n > y/\tau) = 1$ if $n > y/\tau$, and 0 otherwise. In other words the test statistic is simply the sum of the test statistics for each channel separately. The test is then as follows: we reject H_0 if $L_k(\mathbf{n}, \mathbf{y}) > c$. It can be shown that the distribution of the test statistic under the null hypothesis is a linear combination of chi-square distributions. Tables of critical values as well as a routine for calculating them are available from the authors.

4.2 Method 2: (Max LRT)

Here we will use the following test: reject H_0 if $M = \max_i\{L(n_i, y_i)I(n_i > y_i/\tau_i\} > c$, that is, we claim a discovery if there is a significant excess of events in any one channel. For this method the critical value c is found using Bonferroni's method, see for example Casella and Berger [4]. We therefore reject H_0 if $M > c$, where c is the $(1 - 2(1 - \sqrt[k]{1-\alpha}))$ quantile of a chi-square distribution with one degree of freedom.

As we shall see soon, which of these two methods performs better depends on the experiment.

5 Performance

How do the above tests perform? In order to be a proper test they first of all have to achieve the nominal type I error probability α. If they do we can then further study their performance by considering their power function $\beta(s)$ given by

$$\beta(s) = P(\text{reject } H_0| \text{ true signal rate is } s)$$

Of course we have $\alpha = \beta(0)$. $\beta(s)$ gives us the discovery potential, that is the probability of correctly claiming a discovery if the true signal rate is $s > 0$.

In simple cases the true type I error probability α and the power $\beta(s)$ can be calculated explicitly, in more difficult cases we generally need to use Monte Carlo. Moreover, if Monte Carlo is used a technique called importance sampling makes it possible to find the true type I error probability even out at 5σ.

First we will study the true type I error probability as a function of the background rate. In figure 1 we calculate α (expressed in sigma's) for background rates ranging from $b = 5$ to $b = 50$. Here we have used $\tau = 1$ and α corresponding to 3σ, 4σ and 5σ.

It is clear that even for moderate background rates (say $b > 20$) the true type I error is basically the same as the nominal one. For smaller background rates, the method is conservative, that is, the true significance of a signal is actually even higher than the one claimed, and it is therefore safe to use the method even for small b.

In figure 2 we have the power curves for $b = 50$, $\tau = 1$, $e = 1$, s from 0 to 100 and α corresponding to 3σ, 4σ and 5σ. This clearly shows the "penalty" of requiring a discovery threshold of 5σ: at that level the true signal rate has to be 83 for a 90% chance of making a discovery. If 3σ is used a rate of 52 is sufficient, and for 4σ it is 67.

Let us now consider the case of multiple channels. In figure 3 we have the results of the following simulation: There are 5 channels, all with the same background, going from 10 to 100, and the same $\tau = 1$. Again we see that the test achieves the nominal α even for small background rates.

For the last study we will compare the two methods for multiple channels. In figure 4 we have the power curves for the following situations: we have 5 channels with $b = 50$, $e = 1$, and $\tau = 1$ for all channels. In case 1 the signal rate s goes from 0 to 75 and is the same in all channels. In case 2 we have s_1 going from 0 to 100 and $s_2 = .. = s_5 = 0$. All simulations are done using $\alpha = 5\sigma$. Clearly in case 1 Full LRT does better whereas in case 2 it is Max LRT.

This is not surprising because the maximum makes this method more sensitive to the "strongest" channel whereas the sum makes Full LRT more sensitive to a "balance" of the channels. In practice, of course, a decision on which method to use has to be made before any data is seen. A discussion of the optimum strategy for making such a decision is beyond the scope of this paper.

6 Further Extensions

Our extension to multiple channels assumes possibly different signal rates in each channel. The most common situation involves different decay channels of a particle whose existence is being tested. In that case, the different signal rates are due to different branching ratios such that $si = ris$ with a common s. A detailed discussion of this case along with the inclusion of information on certain variables in each event (a technique generally known as marked Poisson) will be found in an upcoming paper.

7 Summary

We have discussed a hypothesis test for the presence of a signal. For the case of a Poisson distributed signal with a background that has either a Poisson or a Gaussian distribution we have carried out the calculations and done an extensive performance study. We have shown that the test achieves the nominal type I error probability α, even at a 5σ level. We extended the test to the case of multiple channels with two possible tests and showed that both achieve the nominal α. Either one or the other has better performance depending on the specific experiment.

References

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[3] A. Stuart, J.K.Ord and S. Arnold, "*Advanced Theory of Statistics, Volume 2A: Classical Inference and the Linear Model*", 6^{th} Ed., London Oxford University Press (1999)

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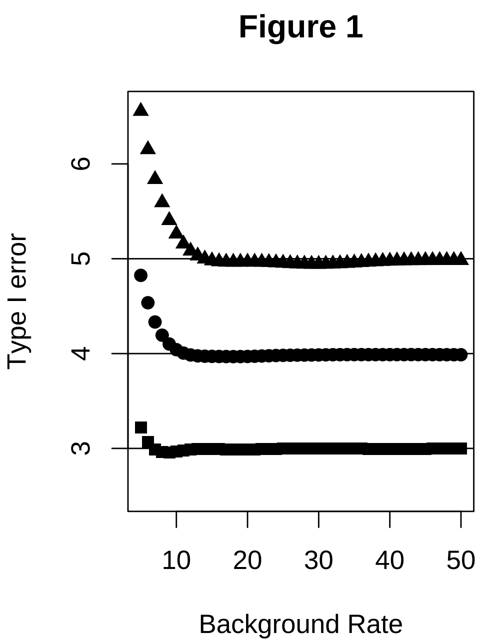

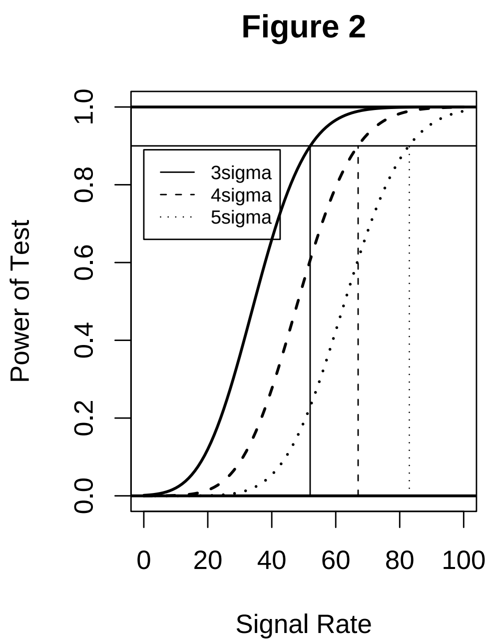

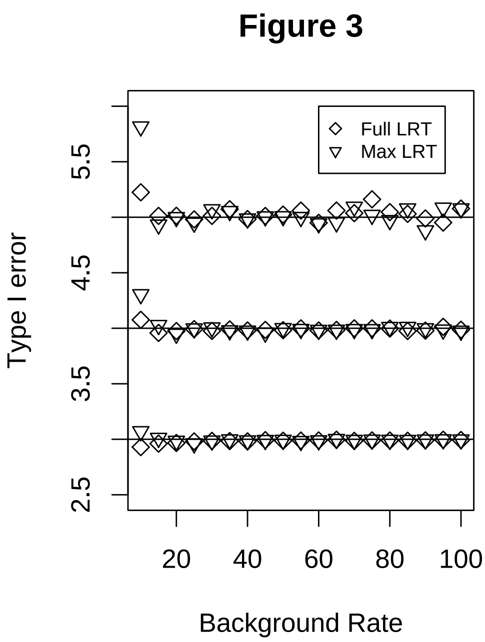

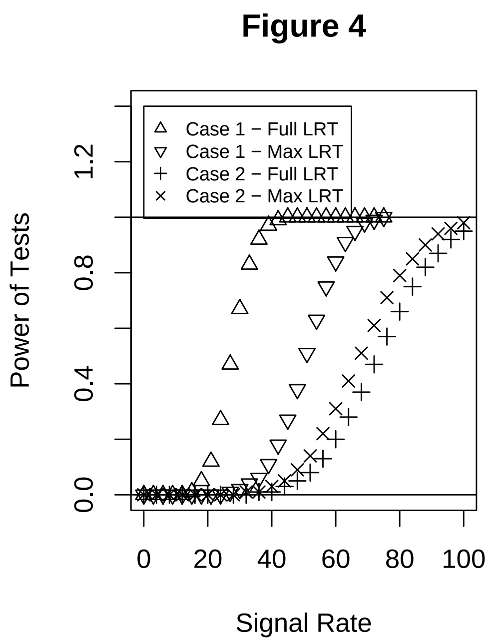

Fig. 1: Type I error probability α for different values of the background rate b
Fig. 2: Power of Test for $b = 50, \tau = 1$
Fig. 3: Type I error probability α for different values of the background rate b for the 5 channel case.
Fig. 4: Power of two methods with 5 channels. Case 1 has equal signal in all channels, case 2 has signal in channel one and no signals in the others.