A Test for the Presence of a Signal, with Multiple Channels and Marked Poisson

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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 a special case of interest. We study extensions of the test to cases where there are multiple channels and to marked Poisson distributions. We show the results of a number of performance studies which indicate that the test works very well, even far out in the tails of the distribution and with multiple channels and marked Poisson.

\textit{Key words:} Likelihood ratio test, type I error probability, power of a test, Monte Carlo
1. Introduction

One of the main goals of the upcoming experiments at the Large Hadron Collider at CERN will be to make discoveries, for example of the Higgs boson. To do so it will be necessary to make use of all available information, that means we will need to use data from multiple channels as well as auxiliary measurements. In this paper we will describe a test capable of doing so, based on the likelihood ratio test statistic. The main contribution of this paper is the study of the performance of this test.

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 $\alpha$, is sometimes required to be as low as $2.87 \cdot 10^{-7}$, equivalent to a $5\sigma$ event. The likelihood ratio test is an approximate test, and what sample sizes are necessary for the approximation to work, especially this far out in the tail, is a question that needed to be investigated.

2. Likelihood Ratio Test

The general problem of discovery is as follows: we have data $X$ from a distribution with density $f(x; \theta)$ where $\theta$ is a vector of parameters with $\theta \in \Theta$ and $\Theta$ 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 $\Theta_0$ is some subset of $\Theta$. The likelihood function is given by

$$Like(\theta|x) = f(x; \theta)$$
and the likelihood ratio test statistic is defined by

$$\lambda(x) = \frac{\sup_{\Theta_0} \text{Like}(\theta|x)}{\sup_{\Theta} \text{Like}(\theta|x)}$$

Because $\text{Like}(\theta|x) \geq 0$ and because the supremum in the numerator is taken over a subset of the supremum in the denominator we have $0 \leq \lambda(x) \leq 1$. The likelihood ratio test rejects the null hypothesis if $\lambda(x) \leq c$, for some suitably chosen $c$, which in turn depends on the type I error probability $\alpha$.

How do we find $c$? There is of course a famous theorem that states that under some mild regularity conditions, if $\theta \in \Theta_0$ then $L(x) = -2 \log \lambda(x)$ 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 [1] and a nice discussion with examples can be found in Casella and Berger [2]. Unfortunately the theorem does not apply to our case, nevertheless as we shall see the conclusion does.

3. An Example: A Counting Experiment with Background, Efficiency and Acceptance

We begin with a very common type of situation in high energy physics experiments. This is a search for a particle by observing a particular decay channel. 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 \( res + b \) where \( b \) is the background rate, \( s \) the signal rate for the production of the particle, \( e \) the efficiency for observing the particular decay channel and \( r \) the branching fraction to that channel. 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 Gaussian random variable \( Y \) with rate \( b \) and standard deviation \( \sigma_b \). Finally we have an independent measurement of the efficiency \( z \), usually from Monte Carlo, and we will model \( z \) as a Gaussian random variable \( Z \) with mean \( e \) and standard deviation \( \sigma_e \). \( \sigma_b, \sigma_e \) as well as the branching fraction \( r \) are assumed to be known. So we have the following probability model:

\[
N \sim \text{Pois}(res + b) \quad Y \sim N(b, \sigma_b) \quad Z \sim N(e, \sigma_e)
\]

In this model \( s \) is the parameter of interest and \( e \) and \( b \) are nuisance parameters.

Now the joint density of \( N, Y \) and \( Z \) is given by

\[
P(N = n, Y = y, Z = z) dydz = f(n, y, z; e, s, b) = \frac{(res+b)^n}{n!} e^{-(res+b)} \cdot \frac{1}{\sqrt{2\pi\sigma_b^2}} \cdot e^{-\frac{(y-b)^2}{2\sigma_b^2}} \cdot \frac{1}{\sqrt{2\pi\sigma_e^2}} \cdot e^{-\frac{(z-e)^2}{2\sigma_e^2}}
\]

Finding the likelihood ratio test statistic \( \lambda \) means maximizing the density above (now viewed as the likelihood) twice, once over all parameters and then again assuming \( s = 0 \). We find

\[
L(n, y, z) = (-2) \log \left\{ \frac{\sup_{\{b,e\}} \text{Like}(0, b, e; n, y, z)} {\sup_{\{s,b,e\}} \text{Like}(s, b, e; n, y, z)} \right\} = 2n \log \left( \frac{n}{\bar{b}} \right) + 2\bar{b} - 2n + \frac{(y-\bar{b})^2}{\sigma_\bar{b}^2}
\]

where \( \bar{b} = \frac{1}{2} \left( y - \sigma_y^2 + \sqrt{(y - \sigma_y^2)^2 + 4n\sigma_b^2} \right) \)
First we note that the test statistic does not involve $z$, the estimate of the efficiency, nor does it involve $r$, the branching fraction. This is true for the one channel case but will no longer hold for multiple channels, although we will find that the test is sensitive only to the relative efficiencies and relative branching ratios between channels, quantities which are usually known more precisely than the absolute values.

Now from the general theory we know that $L(N, Y, Z)$ 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.

Large values of $L(n, y, z)$ indicate that the null hypothesis is wrong and should be rejected. Such large values happen if $n$ is much larger than $y$ but also if $n$ is much smaller. Here, though, we will only reject the null hypothesis if we have more events in the signal region than are expected from background, and therefore we reject the null hypothesis if $L(n, y, z) > q\chi^2_1(1 - 2\alpha)$ and also $n > y$. Here $q\chi^2_1(p)$ is the $p^{th}$ percentile of a chi-square distribution with one degree of freedom.

A similar problem, where the background is modeled as a Poisson rather than a Gaussian, is discussed in much more detail in Rolke, López. The closely related problem of setting limits was studied in Rolke, López and Conrad.
4. Extensions of the Model

4.1. Multiple Channels

In high energy physics we can sometimes make use of multiple channels. We will discuss the following model: there are \( k \) channels and we have \( N_i \sim \text{Pois}(r_i e_i s + b_i) \), \( Y_i \sim N(b_i, \sigma_{b_i}) \), \( Z_i \sim N(e_i, \sigma_{e_i}) \), for all \( i = 1, \ldots, k \), all independent.

The joint density is then found as follows: Let \( n = (n_1, \ldots, n_k) \), \( y = (y_1, \ldots, y_k) \), \( z = (z_1, \ldots, z_k) \), \( b = (b_1, \ldots, b_k) \), \( e = (e_1, \ldots, e_k) \), then

\[
f(n, y, z; s, b, e) = \prod_{i=1}^{k} \frac{(r_i e_i s + b_i)^{n_i}}{n_i!} e^{-\left(r_i e_i s + b_i\right)} \exp\left(-\frac{1}{2} \frac{(y_i - b_i)^2}{\sigma_{b_i}^2}\right) \exp\left(-\frac{1}{2} \frac{(z_i - e_i)^2}{\sigma_{e_i}^2}\right)
\]

The log-likelihood function is given by:

\[
\log \text{Like}(s, b, e; n, y, z) = \sum_{i=1}^{k} \left[ n_i \log (r_i e_i s + b_i) - \log(n_i!) - (r_i e_i s + b_i) - \frac{1}{2} \log(2\pi\sigma_{b_i}^2) + \frac{(y_i - b_i)^2}{\sigma_{b_i}^2} - \frac{1}{2} \log(2\pi\sigma_{e_i}^2) + \frac{(z_i - e_i)^2}{\sigma_{e_i}^2}\right]
\]

and taking derivatives we find the following system of equations for the maximum likelihood estimators:

\[
\sum_{i=1}^{k} \left( \frac{n_i r_i e_i}{r_i e_i s + b_i} - r_i e_i \right) = 0
\]

\[
\frac{n_i}{r_i e_i s + b_i} - 1 + \frac{y_i - b_i}{\sigma_{b_i}} = 0 \quad i = 1, \ldots, k
\]

\[
\frac{n_i r_i}{r_i e_i s + b_i} - r_i s + \frac{z_i - e_i}{\sigma_{e_i}} = 0 \quad i = 1, \ldots, k
\]

This system can not be solved analytically but it is fairly easy to do so numerically, for example with MINUIT. In addition, it can be shown analytically...
that the likelihood ratio test statistic depends not on the absolute values of the efficiencies and branching fractions but only on the ratios between the values for the different channels.

For the numerator of the likelihood ratio statistic we have \( s = 0 \) and the corresponding system has the solutions

\[
\tilde{b}_i = \frac{1}{2} \left( y_i - \sigma^2_{b_i} + \sqrt{(y_i - \sigma^2_{b_i})^2 + 4n_i \sigma^2_{b_i}} \right) \quad i = 1, \ldots, k
\]

\[
\tilde{e}_i = z_i \quad i = 1, \ldots, k
\]

As above we will claim a discovery only if there is an excess of events in the signal region. If we denote the test statistic by \( L(n, y, z) \) this means to reject the null hypothesis of no signal if \( L(n, y, z) > q \chi^2_{1}(1 - 2\alpha) \) and also \( \hat{s} > 0 \) where \( \hat{s} \) is the maximum likelihood estimator of the true signal \( s \).

4.2. Extension II: Marked Poisson

It is sometimes possible to include further information in this model. Consider the following case: in the \( i^{th} \) channel we observe \( n_i \) events in the signal region and \( y_i \) events in the background region. We have an independent measurement \( z_i \) of the efficiency. Furthermore we have measurements \( x_{ij}, j = 1, \ldots, n_i \) for each event in the signal region and we know the distributions of these measurements depending on whether an event is signal or background. This leads
to the following density function:

\[
\log \text{Like}(s, b; e; n, y, z) = \sum_{i=1}^{k} \left[ n_i \log (r_i e_i s + b_i) - \log(n_i!) - (r_i e_i s + b_i) - \frac{1}{2} \log(2\pi\sigma_{e_i}^2) - \frac{(y_i - b_i)^2}{\sigma_{b_i}^2} - \frac{(z_i - e_i)^2}{\sigma_{e_i}^2} \right] \\
+ \sum_{j=1}^{n_i} \log \left( \frac{r_i e_i s}{r_i e_i s + b_i} f^s_{ij}(x_{ij}) + \frac{b_i}{r_i e_i s + b_i} f^b_{ij}(x_{ij}) \right)
\]

where \(f^s_{ij}\) and \(f^b_{ij}\) are the densities of the signal and the background in the \(i^{th}\) channel, respectively. In this paper we will assume that \(f^s_{ij}\) and \(f^b_{ij}\) are fully known but it would be easy to let them depend on nuisance parameters as well. In some applications these densities might be estimated from the data, for example using neural networks. Furthermore, this model allows for a "mixture" case: if in some channels no measurements \(x_{ij}\) are available we only need to set \(f^s_{ij}\) and \(f^b_{ij}\) equal to 1.

The expression above simplifies somewhat if we set \(f_{ij} = \frac{f^b_{ij}(x_{ij})}{f^s_{ij}(x_{ij})}\) and omit any constant terms:

\[
\log \text{Like}(s, b; e; n, y, z) = \\
\sum_{i=1}^{k} \left[ - (r_i e_i s + b_i) - \frac{1}{2} \frac{(y_i - b_i)^2}{\sigma_{b_i}^2} - \frac{1}{2} \frac{(z_i - e_i)^2}{\sigma_{e_i}^2} + \sum_{j=1}^{n_i} \log (r_i e_i s + b_i f_{ij}) \right]
\]

Finding the maximum likelihood estimators now means solving the following nonlinear system of \(2k + 1\) equations:

\[
\sum_{i=1}^{k} r_i e_i \left( \sum_{j=1}^{n_i} \frac{1}{r_i e_i s + f_{ij} b_i} - 1 \right) = 0
\]

\[
\frac{y_i - b_i}{\sigma_{b_i}^2} - 1 + \sum_{j=1}^{n_i} \frac{f_{ij}}{r_i e_i s + f_{ij} b_i} = 0 \quad i = 1, ..., k
\]

\[
\frac{z_i - e_i}{\sigma_{e_i}^2} - r_i s + \sum_{j=1}^{n_i} \frac{r_i e_i}{r_i e_i s + f_{ij} b_i} = 0 \quad i = 1, ..., k
\]

Again this system can not be solved analytically. For the numerator of the likelihood ratio statistic we have \(s = 0\) and the corresponding system has the
same solutions as the corresponding system in section 4.1. The test is then again: reject the null hypothesis of no signal if \( L(n, y, z, x) > q_{\chi^2}(1 - 2\alpha) \) and \( \hat{s} > 0 \).

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

Performance studies for the case of one channel were previously done in Rolke-Lopez [3].

In high energy physics discoveries usually require a very small type I error probability, often as small as \( \alpha = 2.87 \times 10^{-7} \), equivalent to a 5\( \sigma \) event. A straightforward simulation study would therefore need to do about \( 10^9 \) runs. Instead of a simple MC study we will use a technique called importance sampling to estimate the true type I error probability. It works as follows. In a straightforward MC study we would generate \( N_i \sim \text{Pois}(b_i) \), \( Y_i \sim N(b_i, \sigma_{b_i}) \), \( Z_i \sim N(e_i, \sigma_{e_i}) \), \( X_{ij} \sim F_i^b \), where \( F_i^b \) is the distribution of the background events in channel \( i \), with \( i = 1, .., k, j = 1, .., N_i \). Then we would calculate \( L(N, Y, Z, X) \) and find the percentage of runs where \( L(N, Y, Z, X) > q_{\chi^2}(1 - 2\alpha) \) and \( \hat{s} > 0 \).
At $5\sigma$ though, this will only happen about 1 in every 3.5 million runs. So instead we will generate the MC data as if the true observed signal rate in every channel were $t$, that is we generate $N_s^i \sim \text{Pois}(t)$, $N_b^i \sim \text{Pois}(b_i)$, $Y_i \sim N(b_i, \sigma_b)$, $Z_i \sim N(e_i, \sigma_e)$, $X_{ij} \sim F^s_i$ for $j = 1, .., N_i^s$ and $X_{ij} \sim F^b_i$ for $j = N_i^s + 1, .., N_i^s + N_i^b$ ($= N_i$), respectively. For a suitably chosen $t$, $L(N, Y, Z, X)$ will be of the order of the critical value reasonably often. We generate $M$ MC samples and find the true type I error as

$$\hat{\alpha} = \frac{1}{M} \sum_{m=1}^{M} I[L(N, Y, Z, X) > q\chi^2_1(1 - 2\alpha), \hat{\sigma} > 0] w_m$$

where the weights $w_m$ are given by the likelihood ratio of the true density and the one used for the sampling:

$$w_m = \prod_{i=1}^{k} \frac{P(N = n_i | b_i)}{P(N = n_i | t + b_i)} = e^{kt} \prod_{i=1}^{k} \left( \frac{b_i}{t + b_i} \right)^{n_i}$$

For more on importance sampling see Srinivasan [5].

In figure 1 we have the result of the following study: we use 5 channels, the background rates $b$ vary from 2 to 100 and are the same in all channels, $\sigma_b = b/15$, $e = 0.9$, $\sigma_e = 0.1$, $r_i = 0.15$ in all channels. As we can see the test achieves the true type I error for all cases.

Next we will consider what happens when the number of channels grows. In figure 2 we have $k = 1$ to 50, in all channels $b = 25$ with $\sigma_b = 5/3$, $e = 0.9$ with $\sigma_e = 0.09$ and $r = 1/k$. Again we achieve the nominal type I error probability, even for 50 channels and at $5\sigma$.

In figure 3 we consider the power of the test. There are 10 channels, each with a background rate $b = 50$, $\sigma_b = 5$, efficiency $e = 0.9$, $\sigma_e = 0.09$ and
branching ratio $r = 0.05$. At the $5\sigma$ level the total signal rate has to be about 410 to have a 90% chance of claiming a discovery.

Now we turn to a study of the marked Poisson case. We will consider two examples. In the first we have some auxiliary measurement thought to be able to separate signal and background. The functions $f^s_i$ and $f^b_i$ have an (assumed to be known) parameter $\gamma$ and are given by

$$f^s(x) = \frac{1}{\gamma} e^{\frac{x}{\gamma}}, \quad 1 < x < 2$$
$$f^b(x) = \frac{1}{\gamma} e^{\frac{2-x}{\gamma}}, \quad 1 < x < 2$$

For small values of $\gamma$ there is a large distinction between signal and background, for larger values the separation becomes smaller. Two cases are shown in figure 4 in the top two panels with two different values of $\gamma$ corresponding to strong and almost no separation. $f^s_i$ is drawn in dashed lines and $f^b_i$ in solid lines.

In a different example we use the mass distributions themselves. We assume a flat background and a Gaussian signal with mean 0.5 and standard deviation $\delta$. Again two cases of different separation between signal and background are shown in figure 4, in the bottom panels. $f^s_i$ is drawn in dashed lines and $f^b_i$ in solid lines.

We begin as before with a study of the true type I error probability $\alpha$. In figure 5 we have 5 channels. Each channel has a background rate $b$ from 5 to 50, $\sigma_b = b/5$, an efficiency of $e = 0.9$, $\sigma_e = 0.1$ and $r = 0.15$. The + symbols are for example 1, $\gamma = 4$, $x$ for example 1, $\gamma = 0.33$, diamonds for example 2, $\delta = 0.25$ and upside down diamonds for example 2, $\delta = 0.05$. For all those cases the method achieves the true type I error probability $\alpha$. 
Finally, in Figure 6 we present a power study of those same marked Poisson examples. The signal rate goes from 0 to 200. For example 1 we use $\gamma = 2.0, 1.0$ and 0.5, for example 2 $\delta = 0.25, 0.15$ and 0.05, going from a large separation between signal and background by $f^b$ and $f^s$ to almost no separation. Figure 6 clearly shows how much improvement is possible by using the extra information contained in $f^b$ and $f^s$.

The studies here have used reasonable values for the parameters involved. For example, when using multiple channels, it is reasonable to use channels for which the product of efficiency times branching fraction is similar. In our studies these have been set equal. However, an exhaustive performance study is not possible because of the high dimensionality of the problem. Nevertheless, we believe that the uniformly excellent performance in studied cases is an indication that this test will perform very well in a wide range of cases. In general, though, we would recommend the practitioner to carry out their own simulation study for their specific problem to insure that the method also performs well there.

6. Summary

We have discussed a hypothesis test for the presence of a signal. We extended the test to the case of multiple channels as well as the use of auxiliary measurements using marked Poisson models. Studies of the performance of the test for typical cases yielded highly satisfactory results.
References

[1] A. Stuart, J.K. Ord and S. Arnold, “Advanced Theory of Statistics, Volume 2A: Classical Inference and the Linear Model”, 6th Ed., London Oxford University Press (1999)

[2] G. Casella and R.L. Berger, “Statistical Inference”, 2nd Ed., Duxbury Press, (2002)

[3] W.A. Rolke, A. López, “Testing for a Signal”, Proceedings of PHYS-TAT2007, CERN yellow report, physics/0006006

[4] W.A. Rolke, A. López and J. Conrad, “Limits and Confidence Intervals in the Presence of Nuisance Parameters”, Nuclear Instruments and Methods A, 551/2-3, 2005, pp. 493-503, physics/0403059

[5] R. Srinivasan, “Importance Sampling”, Springer, New York (2002)

7. Appendix
Figure 1: Study of type I error $\alpha$ for case of 5 channels. The background rates $b$ vary from 2 to 100 and are the same in all channels. $\sigma_b = b/15$, $\varepsilon = 0.9$, $\sigma_e = 0.1$, $r_i = 0.15$ in all channels.
Figure 2: Study of the effect of the number of channels on type I error. There are $k$ channels ($k = 1$ to 50). In all channels $b = 25$ with $\sigma_b = 5/3$, $e = 0.9$ with $\sigma_e = 0.09$ and $r = 1/k$. 
Figure 3: Study of the power of the test. There are 10 channels, each with a background rate $b = 50$, $\sigma_b = 5$, efficiency $e = 0.9$, $\sigma_e = 0.09$ and branching fraction $r = 0.05$. 

\[ \text{Power} \text{ vs. Signal Rate} \]
Figure 4: Examples for the two types of distributions used in the study of the marked Poisson case. In the upper two panels we have an auxiliary measurement for the events, in the lower two panels the actual mass distributions are used.
Figure 5: Study of type I error using multiple channels and marked Poisson. There are 5 channels. Each channel has a background rate $b$ from 5 to 50, $\sigma_b = b/5$, an efficiency of $e = 0.9$, $\sigma_e = 0.1$ and $r = 0.15$. The + symbols are for example 1, $\gamma = 4.0$, x for example 1, $\gamma = 0.33$, diamonds for example 2, $\delta = 0.25$ and upside down diamonds for example 2, $\delta = 0.05$. 
Figure 6: Power study for case of multiple channels and marked Poisson. We use 5 channels, each channel has a background rate $b = 50$, $\sigma_b = 5$, an efficiency of $e = 0.9$, $\sigma_e = 0.1$ and $r = 0.15$. The signal rate goes from 0 to 200. For example 1 we use $\gamma = 2$, 1, and 0.5, for example 2 $\delta = 0.25$, 0.15 and 0.05, going from a weak separation between signal and background by $f_b$ and $f^s$ to a strong separation.