

## Finding an upper limit in the presence of an unknown background

S. Yellin\*

*Department of Physics, University of California, Santa Barbara, Santa Barbara, California 93106*

(Received 5 April 2002; published 20 August 2002)

Experimenters report an upper limit if the signal they are trying to detect is nonexistent or below their experiment's sensitivity. Such experiments may be contaminated with a background too poorly understood to subtract. If the background is distributed differently in some parameter from the expected signal, it is possible to take advantage of this difference to get a stronger limit than would be possible if the difference in distribution were ignored. We discuss the "maximum gap" method, which finds the best gap between events for setting an upper limit, and generalize to the "optimum interval" method, which uses intervals with especially few events. These methods, which apply to the case of relatively small backgrounds, do not use binning, are relatively insensitive to cuts on the range of the parameter, are parameter independent (i.e., do not change when a one-one change of variables is made), and provide true, though possibly conservative, classical one-sided confidence intervals.

DOI: 10.1103/PhysRevD.66.032005

PACS number(s): 06.20.Dk, 14.80.-j, 14.80.Ly, 95.35.+d

### I. INTRODUCTION

Suppose we have an experiment whose events are distributed along a one-dimensional interval. The events are produced by a process for which the expected shape of the event distribution is known, but with an unknown normalization. In addition to the signal, there may also be a background whose expectation value per unit interval is known, but one cannot completely exclude the possibility of an additional background whose expectation value per unit interval is non-negative, but is otherwise unknown. If the experimenters cannot exclude the possibility that the unknown background is large enough to account for all the events, they can only report an upper limit on the signal. Even experimenters who think they understand a background well enough to subtract it may wish to allow for the possibility that they are mistaken by also presenting results without subtraction. Methods based on likelihood, such as the approach of Feldman and Cousins [1], or Bayesian analysis, cannot be applied because the likelihood associated with an unknown background is unknown. An example of this situation is the analysis of an experiment which tries to detect recoil energies  $E_{\text{recoil}}$  deposited by weakly interacting massive particles (WIMPs) bouncing off atoms in a detector. For a given WIMP mass, and assumed WIMP velocity distribution, the shape of the distribution in  $E_{\text{recoil}}$  can be computed, but the WIMP cross section is unknown, and it is hard to be certain that all backgrounds are understood. The simplest way of dealing with such a situation is to pick an interval in, say,  $E_{\text{recoil}}$ , and take as the upper limit the largest cross section that would have a significant probability, say 10%, of giving as few events as were observed, assuming all observed events were from WIMPs. One problem with this naive method is that it can be very sensitive to the interval chosen. It is typical for the bottom of a detector's range of sensitivity to be limited by noise or other backgrounds. Thus if the interval extends to an especially low  $E_{\text{recoil}}$ , there will be many events, leading to a

weaker (higher) upper limit than is required by the data. On the other hand, experimenters could inadvertently bias the result by choosing the interval's end points to give especially few events, with an upper limit that is lower than is justified by the data. In order to avoid such a bias, it might be thought best to avoid using the observed events to select the interval used. But the procedures discussed here take the opposite approach. The range is carefully chosen to include especially few events compared with the number expected from a signal. The way the range is chosen makes the procedure especially insensitive to unknown background, which tends to be most harmful where there are especially many events compared with the number expected from a signal. It would be a mistake to compute the upper limit as if the interval were selected without using the data; so the computation is designed to be correct for the way the data are used.

While the methods described here cannot be used to identify a positive detection, they are appropriate for obtaining upper limits from experiments whose backgrounds are very low, but nonzero. These methods have been used by the CDMS experiment [2].

### II. MAXIMUM GAP METHOD

Figure 1 illustrates the maximum gap method. Small rectangles along the horizontal axis represent events, with position on the horizontal axis representing some measured parameter, say, "energy,"  $E$ . The curve shows the event spectrum  $dN/dE$  expected from a proposed cross section  $\sigma$ . If there is a completely known background, it is included in  $dN/dE$ . But whether or not there is a completely known background, we assume there is also an unknown background contaminating the data. To set an upper limit, we vary the proposed size of  $\sigma$  until it is just high enough to be rejected as being too high. We seek a criterion for deciding if a proposed signal is too high. Since there are especially many events at low  $E$ , while  $dN/dE$  is not especially high there, those events must be mostly from the unknown background. If we looked only at the low energy part of the data, we would have to set an especially weak (high) upper limit.

\*Email address: yellin@slac.stanford.edu

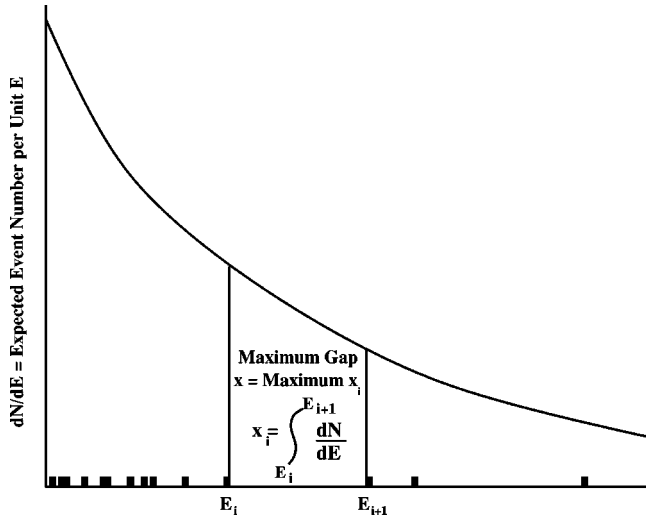


FIG. 1. Illustration of the maximum gap method. The horizontal axis is some parameter “ $E$ ” measured for each event. The smooth curve is the signal expected for the proposed cross section, including any known background. The events from signal, known background, and unknown background are the small rectangles along the horizontal axis. The integral of the signal between two events is “ $x_i$ .”

To find the strongest (lowest) possible upper limit, we should look at energies where there are not many events, and therefore there is not much background.

Between any two events  $E_i$  and  $E_{i+1}$ , there is a gap. For a given value of  $\sigma$ , the “size” of the gap can be characterized by the value within the gap of the expected number of events,

$$x_i = \int_{E_i}^{E_{i+1}} \frac{dN}{dE} dE. \quad (1)$$

The “maximum gap” is the one with the greatest “size;” it is the largest of all the  $x_i$ . The bigger we assume  $\sigma$  to be, the bigger will be the size of the maximum gap in the observed event distribution. If we want, we can choose  $\sigma$  so large that there are millions of events expected in the maximum gap. But such a large  $\sigma$  would be experimentally excluded, for unless a mistake has been made, it is almost impossible to find zero events where millions are expected. To express this idea in a less extreme form, a particular choice of  $\sigma$  should be rejected as too large if, with that choice of  $\sigma$ , there is a gap between adjacent events with “too many” expected events. The criterion for “too many” is that, if the choice of  $\sigma$  were correct, a random experiment would almost always give fewer expected events in its maximum gap. Call  $x$  the size of the maximum gap in the random experiment. If the random  $x$  is lower than the observed maximum gap size with probability  $C_0$ , the assumed value of  $\sigma$  is rejected as too high with confidence level  $C_0$ . Since  $x$  is unchanged under a one-one transformation of the variable in which events are distributed, one may make a transformation at a point from whatever variable is used, say  $E$ , to a variable equal to the total number of events expected in the interval between the point and the lowest allowed value of  $E$ . No matter how

events were expected to be distributed in the original variable, in the new variable they are distributed uniformly with unit density. Thus any event distribution is equivalent to a uniform distribution of unit density. The probability distribution of  $x$  depends on the total length of this uniform unit density distribution, and in this new variable the total length of the distribution is equal to the total expected number of events,  $\mu$ , but it does not depend on the shape of the original event distribution.  $C_0$ , the probability of the maximum gap size being smaller than a particular value of  $x$ , is a function only of  $x$  and  $\mu$ :

$$C_0(x, \mu) = \sum_{k=0}^m \frac{(kx - \mu)^k e^{-kx}}{k!} \left( 1 + \frac{k}{\mu - kx} \right), \quad (2)$$

where  $m$  is the greatest integer  $\leq \mu/x$ . For a 90% confidence level upper limit, increase  $\sigma$  until  $\mu$  and the observed  $x$  are such that  $C_0$  reaches 0.90.

Equation (2) can be evaluated relatively quickly when  $C_0$  is near 0.9. When  $\mu$  is small, so is  $m$ , and when  $\mu$  is large, the series can be truncated at relatively small  $k$  without making a significant error. Equation (2) is derived in Appendix A.

While this method can be used with an arbitrary number of events in the data, it is most appropriate when there are only a few events in the part of the range that seems relatively free of background (small  $\mu$ ). The method is not dependent on a choice for binning because unbinned data are used. No Monte Carlo computation of the confidence level is needed because the same formula for  $C_0$  applies independent of the functional form for the shape of the expected event distribution. The result is a conservative upper limit that is not too badly weakened by a large unknown background in part of the region under consideration; the method effectively excludes regions where a large unknown background causes events to be too close together for the maximum gap to be there.

### III. OPTIMUM INTERVAL METHOD

If there is a relatively high density of events in the data, we may want to replace the “maximum gap” method by one in which we consider, for example, the “maximum” interval over which there is one event observed, or two events, or  $n$  events, instead of the zero events in a gap.

Define  $C_n(x, \mu)$  to be the probability, for a given cross section without background, that all intervals with  $\leq n$  events have their expected number of events  $\leq x$ . As for  $C_0$  of the maximum gap method, so long as  $x$  and  $\mu$  are fixed,  $C_n$  is independent of the shape of the cross section and the parameter in which events are distributed. But  $C_n(x, \mu)$  increases when  $x$  increases, and it increases when  $n$  decreases.  $C_n$  can be tabulated with the help of a Monte Carlo program, although the special case of  $n=0$  can be more accurately computed with Eq. (2). Once  $n$  is chosen,  $C_n$  can be used in the same way as  $C_0$  for obtaining an upper limit: For  $x$  equal to the maximum expected number of events taken over all intervals with  $\leq n$  events,  $C_n(x, \mu)$  is the confidence level with which the assumed cross section is excluded as being too high. But since we do not want to allow  $n$  to be chosen in

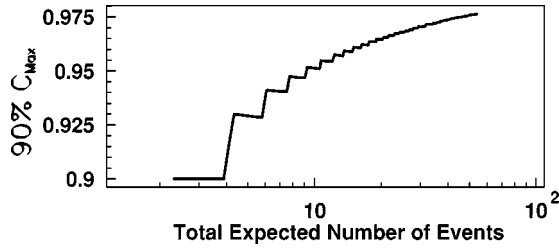


FIG. 2. Plot of  $\bar{C}_{\text{Max}}(0.9, \mu)$ , the value of  $C_{\text{Max}}$  for which the 90% confidence level is reached, as a function of the total number of events  $\mu$  expected in the experimental range.

a way that skews results to conform with our prejudices, the optimum gap method includes automatic selection of which  $n$  to use.

For each interval within the total range of an actual experiment, compute  $C_n(x, \mu)$  for the observed number of events,  $n$ , and expected number of events,  $x$ , in the interval. The bigger  $C_n$  is, the stronger will be the evidence that the assumed cross section is too high. Thus for each possible interval, one may quantify how strongly the proposed cross section is excluded by the data. The “optimum interval” is the interval that most strongly indicates that the proposed cross section is too high. The optimum interval tends to be one in which the unknown background is especially small. The overall test quantity used for finding an upper limit on the cross section is then  $C_{\text{Max}}$ , the maximum over all possible intervals of  $C_n(x, \mu)$ . A 90% confidence level upper limit on the cross section is one for which the observed  $C_{\text{Max}}$  is higher than would be expected from 90% of random experiments with that cross section and no unknown background.

The definition of  $C_{\text{Max}}$  seems to imply that its determination requires checking an infinite number of intervals. But given any interval with  $n$  events,  $x$ , and hence  $C_n(x, \mu)$ , can be increased without increasing  $n$  by expanding the interval until it almost hits either another event or an end point of the total experimental range. For determination of  $C_{\text{Max}}$  one need only consider intervals that are terminated by an event or by an end point of the total experimental range. If the experiment has  $N$  events, then there are  $(N+1)(N+2)/2$  such intervals, one of which has  $C_n(x, \mu) = C_{\text{Max}}$ .

The function  $\bar{C}_{\text{Max}}(C, \mu)$  is defined to be the value such that a fraction  $C$  of random experiments with that  $\mu$ , and no unknown background, will give  $C_{\text{Max}} < \bar{C}_{\text{Max}}(C, \mu)$ . Thus the 90% confidence level upper limit on the cross section is where  $C_{\text{Max}}$  of the experiment equals  $\bar{C}_{\text{Max}}(0.9, \mu)$ , which is plotted in Fig. 2.

A Monte Carlo program was used to tabulate  $C_n(x, \mu)$ . A FORTRAN routine interpolates the table to compute  $C_n(x, \mu)$  when  $n$ ,  $x$ , and  $\mu$  are within the tabulated range. The routine applies when  $0 < \mu < 54.5$  and when  $0 \leq n \leq 50$ .

The function  $\bar{C}_{\text{Max}}(C, \mu)$  has been computed by Monte Carlo and tabulated for  $\mu < 54.5$  and various  $C$ . Certain peculiarities of this function are discussed in Appendix B.

Routines to evaluate functions described in this paper, along with the tables they use, are available on the web [3].

#### IV. COMPARISONS OF THE METHODS

We compare the maximum gap ( $C_0$ ) and optimum interval ( $C_{\text{Max}}$ ) methods with each other, with the standard [4] way of finding an upper limit (“Poisson”), and with another method ( $p_{\text{Max}}$ ) described in Appendix C.

The standard “Poisson” confidence level  $C$  upper limit cross section is the one whose  $\mu$  would result in a fraction  $C$  of random experiments having more events in the entire experimental range than the  $n$  actually observed. This fraction  $C$  is

$$P(\mu, n+1) \equiv \sum_{k=n+1}^{\infty} \frac{\mu^k}{k!} e^{-\mu} = \int_0^{\mu} dt \frac{t^n}{n!} e^{-t}. \quad (3)$$

The last equality is proved by observing that both sides have the same derivative, and they have the same value at  $\mu = 0$ .  $P(x, a)$ , the incomplete gamma function, is in CERNLIB [5] as GAPNC( $a, x$ ), DGAPNC( $a, x$ ), and GAMDIS( $x, a$ ).

The description of the  $p_{\text{Max}}$  method is relegated to Appendix C because although  $p_{\text{Max}}$  is somewhat easier to implement than  $C_{\text{Max}}$ , it was found to be less powerful.

Two comparisons of the effectiveness of the methods were performed: tests (a) and (b). For test (a), 500 000 zero-background Monte Carlo experiments were generated for each of 40 assumed cross sections.  $C_0$ ,  $p_{\text{Max}}$ ,  $C_{\text{Max}}$ , and the Poisson method were used to find the 90% confidence level upper limits on the cross section. For a given true cross section  $\sigma_{\text{True}}$ , there is a certain median value  $\sigma_{\text{Med}}$  that is exceeded exactly 50% of the time by the computed upper limit. Figure 3(a) shows  $\sigma_{\text{Med}}/\sigma_{\text{True}}$  as a function of  $\mu$ . The dotted curve used  $C_0$  to determine the upper limit, the dash-dotted curve used  $p_{\text{Max}}$ , the dashed one used  $C_{\text{Max}}$ , and the solid, jagged, curve used the Poisson method. The Poisson method gives a jagged curve because of the discrete nature of the variable used to calculate the upper limit, the total number of detected events. For any cross section shape, when there is no background,  $C_{\text{Max}}$  gives a stronger limit than  $p_{\text{Max}}$  in most random experiments, and both are stronger than  $C_0$ . Even without background, for some values of the true  $\mu$ ,  $C_{\text{Max}}$  gives a stronger (lower) upper limit than the Poisson method. This happens because the discrete nature of the Poisson method causes it to have greater than 90% coverage.

Although test (a) is presented as a comparison of methods in the absence of background, it can also be considered to be a comparison of methods when the background is distributed in the same way as the signal. If the unknown background happens to have the same distribution as the signal would have, essentially no sensitivity is lost by using the optimum interval method with  $C_{\text{Max}}$  instead of the Poisson method.

Test (b) was similar to test (a), but the Monte Carlo program simulated a background unknown to the experimenters, and distributed differently from the expected signal. The total experimental region was split into a high part and a low part, with background only in the low part. Half the expected signal was placed in the low part, where the simulated background was twice the expected signal. For this case, the two lowest curves are almost exactly on top of each other; Fig.

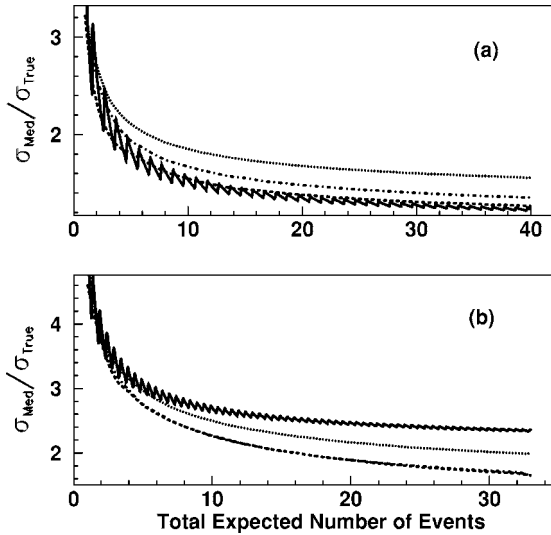


FIG. 3.  $\sigma_{\text{Med}}/\sigma_{\text{True}}$ , the typical factor by which the upper limit cross section exceeds the true cross section, when  $C_0$  is used (dotted lines), when  $p_{\text{Max}}$  is used (dash-dotted lines), when  $C_{\text{Max}}$  is used (dashed lines), and when the Poisson method is used (solid lines). These ratios are a function of  $\mu$ , the total number of events expected from the true cross section in the entire experimental range. For the upper figure (a) there is no background, and for the lower figure (b) there is just as much unknown background as there is signal, but the background is concentrated in a part of the experimental range that contains only half the total signal.

3(b) shows that  $C_{\text{Max}}$  and  $p_{\text{Max}}$  get equally strong upper limits.  $C_0$  produces a weaker limit, and the Poisson method is weakest of all.

From the definition of the 90% confidence level upper limit, test (a) results in an upper limit that is lower than the true value exactly 10% of the time; i.e., all methods except the Poisson make a mistake 10% of the time (the discrete nature of the Poisson distribution results in its making mistakes less than 10% of the time). But for test (b) the unknown background raises the upper limit; so all methods make a mistake less than 10% of the time. Figure 4 shows the fraction of mistakes with test (b) using  $C_0$  (dotted),  $p_{\text{Max}}$  (dash-dotted), and  $C_{\text{Max}}$  (dashed). Although  $C_{\text{Max}}$  and  $p_{\text{Max}}$  give equally strong upper limits for test (b),  $C_{\text{Max}}$  makes fewer mistakes.  $C_0$  makes the most mistakes of the tested methods. Not shown is the Poisson method; because its upper limit is so high, it makes almost no mistakes.

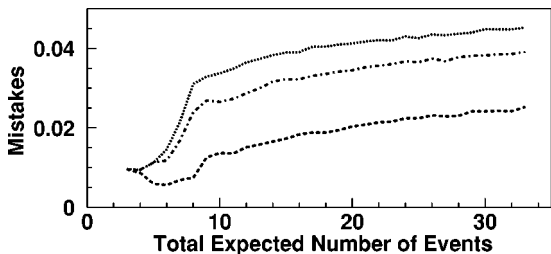


FIG. 4. Fraction of cases for test (b) (see text) in which the true cross section was higher than the upper limit on the cross section computed using  $C_0$  (dotted),  $p_{\text{Max}}$  (dash-dotted), and  $C_{\text{Max}}$  (dashed).

## V. CONCLUSIONS

Judging from the tests shown in Fig. 3 and Fig. 4, the best of the methods discussed here is the optimum interval method, with  $C_{\text{Max}}$ . This method is useful for experiments with small numbers of events when it is not possible to make an accurate model of the background, and it can also be used when experimenters want to show an especially reliable upper limit that does not depend on trusting their ability to model the background. Because the optimum interval method automatically avoids parts of the data range in which there are large backgrounds, it is relatively insensitive to placement of the cuts limiting the experimental range. Because the optimum interval method does not use binned data, it cannot be biased by how experimenters choose to bin their data. Unlike Bayesian upper limits with a uniform prior, the result of the optimum interval method is unchanged when a change in variable is made. The optimum interval method produces a true, though possibly conservative, classical (frequentist) confidence interval; at least 90% of the time the method is used its 90% confidence level upper limit will be correct, barring experimental systematic errors.

## ACKNOWLEDGMENTS

Thanks are due to Richard Schnee for useful discussions, for suggesting improvements of this paper, and for being the first to apply its methods to an experimental analysis. This work was supported by a grant from the U.S. Department of Energy No. DE-FG03-91ER40618.

## APPENDIX A: DERIVATION OF THE EQUATION FOR $C_0$

In order to derive Eq. (2), let us first find the probability that the maximum gap size is less than  $x$  when there are exactly  $n$  events, then get  $C_0$  by averaging  $n$  over a Poisson distribution.

We assume  $n$  events are distributed in some variable  $y$  according to a density distribution that integrates to a total of  $\mu$  expected events, and define  $P(x;n,\mu)$  to be the probability that the maximum gap size is less than  $x$ . As explained in Sec. II, one may make a change of variables to  $z(y)$  such that the density distribution is uniform over  $0 < z < \mu$ .  $P(x;n,\mu)$  is the probability that the maximum  $z$  coordinate distance between adjacent events is less than  $x$  given that there are exactly  $n$  events distributed randomly, independently, and uniformly between  $z=0$  and  $z=\mu$ . The function  $P$  depends only on  $x$ ,  $n$ , and  $\mu$ , but not on the shape of the original density distribution.

The problem of finding  $P(x;n,\mu)$  can be simplified by making a coordinate change  $w(z) = z/\mu$ . The new coordinate runs from 0 to 1 instead of 0 to  $\mu$ . With this coordinate change, any set of  $n$  events with  $x$  equal to the maximum gap between adjacent events becomes a set of  $n$  events, still uniformly distributed, but with maximum new coordinate distance between adjacent events equal to  $x/\mu$ . It follows that  $P(x/\mu;n,1) = P(x;n,\mu)$ , and we need only solve the problem of finding  $P$  for  $\mu=1$  to get the solution for any value of  $\mu$ . When  $\mu$  is understood to be 1, it will be dropped, and we will write  $P(x;n)$  to mean the same as  $P(x;n,1)$ . The prob-

lem has been reduced to one in which  $n$  points have been scattered randomly in independent uniform probability distributions on the interval  $(0,1)$ . We want to find the probability that the maximum empty interval has length less than  $x$ . We do this with the help of a recursion relation that allows one to compute  $P(x;n+1)$  from knowledge of  $P(x;n)$ .

$P(x;n+1)$  is the integral over  $t < x$  of the probability that the lowest event is between  $t$  and  $t+dt$  and that the rest of the  $n$  events in the remaining  $1-t$  range has no gap greater than  $x$ . The probability that the lowest event is between  $t$  and  $t+dt$  is (number of ways of choosing one particular event of the  $n+1$  events) times (probability that the particular event will be between  $t$  and  $t+dt$ ) times (probability that each of the other  $n$  events will be greater than  $t$ ). We get a factor in the integrand  $(n+1) \times dt \times (1-t)^n$ . The other factor in the integrand is the probability that there is no gap greater than  $x$  for the remaining  $n$  events:  $P(x;n,1-t) = P(x/(1-t);n)$ . The recursion relation for  $0 < x < 1$  is

$$P(x;n+1) = \int_0^x dt (n+1)(1-t)^n P\left(\frac{x}{1-t};n\right). \quad (A1)$$

It is convenient to distinguish between various pieces of the  $x$  range between 0 and  $\mu$ , for it will turn out that  $P(x;n,\mu)$  takes on different forms in different pieces of that range. If  $x$  is in the range  $\mu/(m+1) < x < \mu/m$ , we say  $P(x;n,\mu) = P_m(x;n,\mu)$ , and we say  $x$  is in the  $m$ th range. Let us again restrict ourselves to  $\mu=1$  and consider Eq. (A1). If  $x$  is in the  $m$ th range and, as in Eq. (A1),  $0 < t < x$ , then  $x/(1-t)$  is in either range  $m$  or range  $(m-1)$ . The boundary between these two ranges is at  $x/(1-t) = 1/m$ ; so  $t = 1 - mx$ . For  $m > 0$  Eq. (A1) becomes

$$\begin{aligned} \frac{P_m(x;n+1)}{n+1} &= \int_0^{1-mx} dt (1-t)^n P_m\left(\frac{x}{1-t};n\right) \\ &+ \int_{1-mx}^x dt (1-t)^n P_{m-1}\left(\frac{x}{1-t};n\right). \end{aligned} \quad (A2)$$

The appearance of  $m-1$  brings up the question of what happens if  $m=0$ . Let us interpret the  $m=0$  range to be the one with  $1/1 < x < 1/0 = \infty$ . Since the empty space between events is certainly less than the length of the whole interval,  $P_0(x;n) = 1$ .

For  $m \geq 0$  it can be shown that

$$P_m(x;n) = \sum_{k=0}^m (-1)^k \binom{n+1}{k} (1-kx)^n. \quad (A3)$$

In this equation, we interpret  $\binom{n}{k}$  as

$$\binom{n}{k} = \frac{n!}{k!(n-k)!} \equiv \frac{\Gamma(n+1)}{\Gamma(k+1)\Gamma(n-k+1)}.$$

The gamma function is meaningful when analytically continued, in which case  $\binom{n}{k}$  is zero if  $k$  is an integer that is less than zero or greater than  $n$ . In  $P(x;0)$ , the maximum (and

only) gap is always 1; so  $P_0(x;0) = 1$  for  $x > 1$ , while for  $m > 0$ , when  $0 < x < 1$ ,  $P_m(x;0) = 0$ . Since Eq. (A3) is easily verified to be correct for all  $m \geq 0$  when  $n=0$ , one may use induction with Eq. (A2) to prove Eq. (A3) for all other  $n > 0$ . The simple but somewhat tedious manipulations of sums will not be given here, except for a useful identity in the induction step:

$$\binom{n}{k} + \binom{n}{k-1} = \binom{n+1}{k}.$$

It follows from Eq. (A3) that

$$P_m(x;n,\mu) = \sum_{k=0}^m (-1)^k \binom{n+1}{k} (1-kx/\mu)^n. \quad (A4)$$

Let us now compute  $C_0$ , the probability for the maximum empty space between events in  $(0,\mu)$  being less than  $x$  given only that events are thrown according to a uniform unit density. Average Eq. (A4) over a Poisson distribution with mean  $\mu$  to get

$$C_0 = \sum_{k=0}^m \sum_{n=0}^{\infty} e^{-\mu} \frac{\mu^n}{n!} (-1)^k \binom{n+1}{k} (1-kx/\mu)^n, \quad (A5)$$

which can be summed over  $n$  (again the manipulations will not be shown here) to give Eq. (2).

## APPENDIX B: PECULIARITIES OF $\bar{C}_{\text{Max}}$

The function  $\bar{C}_{\text{Max}}(0.9,\mu)$  has certain peculiarities. For example, it cannot be defined for  $\mu < 2.3026$ . Random experiments with  $\mu < 2.3026$  either give the largest possible value of  $C_{\text{Max}}$ , which occurs for zero events, with probability  $e^{-\mu} > 10\%$ , or give smaller values with probability  $1 - e^{-\mu} < 90\%$ . There is therefore no number  $\bar{C}_{\text{Max}}(0.9,\mu)$  for which there is exactly 90% probability of  $C_{\text{Max}} < \bar{C}_{\text{Max}}(0.9,\mu)$ . No cross section resulting in  $\mu < 2.3026$  can be excluded to as high a confidence level as 90%.

Another peculiarity of  $\bar{C}_{\text{Max}}(0.9,\mu)$  is that it is not especially smooth; it tends to increase rapidly near certain values of  $\mu$ . To understand this behavior, note that for a given value of  $\mu$ , the maximum possible value of  $x$  is  $x = \mu$ . Thus the maximum possible value over all  $x$  of  $C_n(x,\mu)$  is  $C_n(\mu,\mu)$ . If  $C_n(\mu,\mu)$  is less than  $\bar{C}_{\text{Max}}(0.9,\mu)$  then intervals with  $n$  events cannot have  $C_{\text{Max}} = C_n$  for that value of  $\mu$ . Furthermore, since  $C_n(x,\mu)$  decreases with increasing  $n$ , intervals with  $m > n$  events also have  $C_m < C_{\text{Max}}$ . For low enough  $\mu$ , only intervals with  $n=0$  need be considered. In this case, the 90% confidence upper limit for  $C_{\text{Max}}$  occurs when  $x$  in  $C_0(x,\mu)$  is equal to  $x_0(0.9,\mu)$ , where  $x_0(C,\mu)$  is the inverse of  $C_0(x,\mu)$ ; it is defined as the value of  $x_0$  for which  $C_0(x_0,\mu) = C$ . Thus for low enough  $\mu$  (but above 2.3026)

$$\bar{C}_{\text{Max}}(0.9,\mu) = C_0(x_0(0.9,\mu),\mu). \quad (B1)$$

TABLE I. Threshold  $\mu$  for which intervals with  $\geq n$  events need not be considered when computing  $C_{\text{Max}}$ .

$n$	$\mu(n)$	$\mu(n+1)$	$\mu(n+2)$	$\mu(n+3)$	$\mu(n+4)$
0	2.303	3.890	5.800	7.491	9.059
5	10.548	12.009	13.433	14.824	16.196
10	17.540	18.891	20.208	21.520	22.821
15	24.119	25.400	26.669	27.926	29.197
20	30.457	31.690	32.972	34.203	35.422
25	36.632	37.849	39.108	40.333	41.546
30	42.768	43.978	45.164	46.351	47.544
35	48.734	49.944	51.139	52.314	53.488

$C_0(x_0(0.9, \mu), \mu) = 0.9$  from the definitions of  $C_0$  and  $x_0$ . This formula for  $\bar{C}_{\text{Max}}$  breaks down as soon as  $\mu$  is large enough to have  $C_1(\mu, \mu) > \bar{C}_{\text{Max}}(0.9, \mu)$ , for at this value of  $\mu$  it is possible for an interval with  $n=1$  to be  $C_{\text{Max}}$ . In general, the threshold  $\mu$  for intervals with  $n$  points being able to produce  $C_{\text{Max}}$  for confidence level  $C$  is where

$$C_n(\mu, \mu) = \bar{C}_{\text{Max}}(C, \mu). \quad (\text{B2})$$

Every time a threshold in  $\mu$  is passed that allows another value of  $n$  to participate in producing  $C_{\text{Max}}$ , the value of  $\bar{C}_{\text{Max}}(C, \mu)$  spurts upward.

If one considers all intervals with  $\leq n$  events, then the largest expected number of events is less than  $\mu$  if and only if there are more than  $n$  events in the entire experimental range. Thus  $C_n(\mu, \mu)$  is the probability of  $> n$  events in the entire experimental range:  $C_n(\mu, \mu) = P(\mu, n+1)$  of Eq. (3). This equation, with Eq. (B2), can be used to compute the thresholds in  $\mu$  where  $n$  events first need to be included when trying to find  $C_{\text{Max}}$  in a calculation of the 90% confidence level. These thresholds are tabulated in Table I. As an example of usage of this table, if you are evaluating  $C_{\text{Max}}$  for a 90% confidence level calculation with  $\mu = 20$ , you can ignore intervals with more than 11 events.

The many rapid increases in  $\bar{C}_{\text{Max}}(0.9, \mu)$  of Fig. 2 occur when thresholds given in Table I are crossed.

### APPENDIX C: PROBABILITY OF MORE EVENTS THAN OBSERVED IN AN INTERVAL

Instead of using  $C_n(x, \mu)$  as a measure of how strongly a given interval with  $n$  events excludes a given cross section, one may use  $p_n(x)$ , the calculated Poisson probability of there being more events in a random interval of that size than were actually observed. This probability is  $P(x, n+1)$ , as defined in Eq. (3). If  $p_n$  is too large, then the cross section used in the calculation must have been too large. For a given cross section, find the interval that excludes the cross section most strongly; i.e., find the interval that gives the largest calculated probability of there being more events in the interval than were actually observed. In other words, as was done with  $C_{\text{Max}}$  of the optimum interval method, define  $p_{\text{Max}}$  to be the maximum over the  $p_n$  for all possible intervals. If random experiments for the same given cross section would



FIG. 5. Plot of  $\bar{p}_{\text{Max}}(0.9, \mu)$ , the value of  $p_{\text{Max}}$  for which the 90% confidence level is reached, as a function of the total number of events  $\mu$  expected in the experimental range.

give a smaller  $p_{\text{Max}}$  90% of the time, then the cross section is rejected as too high with 90% confidence level. The function  $\bar{p}_{\text{Max}}(C, \mu)$  is defined as the  $p_{\text{Max}}$  for which the confidence level  $C$  is reached at the given  $\mu$ .

Although this method may not be as effective as the optimum gap method, it is much easier to calculate  $p_n(x) = P(x, n+1)$  than it is to calculate  $C_n(x, \mu)$ .

Much of the reasoning applied to the optimum interval method applies here. As was the case for the optimum interval method,  $\bar{p}_{\text{Max}}(C, \mu)$  depends only on  $C$  and  $\mu$ , but not otherwise on the shape of the cross section. As for the optimum interval method,  $\bar{p}_{\text{Max}}(0.9, \mu)$  is not defined for  $\mu < 2.3026$ . For sufficiently low  $\mu$  above 2.3026 Eq. (B1) becomes

$$\bar{p}_{\text{Max}}(0.9, \mu) = p_0(x_0(0.9, \mu)) = e^{-x_0(0.9, \mu)}. \quad (\text{C1})$$

For the threshold  $\mu$  at which intervals with  $n$  points become able to contribute to  $p_{\text{Max}}$  for confidence level  $C$ , Eq. (B2) becomes

$$P(\mu, n+1) \equiv p_n(\mu) = \bar{p}_{\text{Max}}(C, \mu). \quad (\text{C2})$$

A Monte Carlo program was used to compute a table of  $\bar{p}_{\text{Max}}(0.9, \mu)$  for  $\mu \leq 70$ , and the function is plotted in Fig. 5.

Table II shows approximate values of the threshold  $\mu$  calculated using Eq. (C2) with  $C=0.9$  for each  $n$  from 0 to

TABLE II. Threshold  $\mu$  below which intervals with  $\geq n$  events need not be considered when computing  $p_{\text{Max}}$  for the 90% confidence level.

$n$	$\mu(n)$	$\mu(n+1)$	$\mu(n+2)$	$\mu(n+3)$	$\mu(n+4)$
0	2.303	5.156	7.584	9.661	11.599
5	13.427	15.193	16.900	18.559	20.176
10	21.771	23.355	24.880	26.419	27.922
15	29.428	30.891	32.359	33.808	35.251
20	36.701	38.100	39.519	40.913	42.317
25	43.700	45.091	46.465	47.827	49.193
30	50.561	51.902	53.255	54.589	55.926
35	57.264	58.603	59.920	61.237	62.549
40	63.868	65.179	66.478	67.791	69.080

44. The third digit of  $\mu$  does not really deserve to be trusted since  $\bar{p}_{\text{Max}}$  was computed from a Monte Carlo generated table.

Appendix B explained why the value of  $\bar{C}_{\text{Max}}(0.9, \mu)$  spurts upward when  $\mu$  crosses a threshold where intervals with more points can contribute to  $C_{\text{Max}}$ . A much less obvi-

ous similar effect occurs with  $\bar{p}_{\text{Max}}(0.9, \mu)$ . Notice the irregularity in the curve of Fig. 5 just after  $\mu = 5.156$ , where  $n = 1$  first begins to contribute. Between  $\mu = 2.3026$  and  $\mu = 5.156$ , Eq. (C1) applies, but after  $\mu = 5.156$ ,  $\bar{p}_{\text{Max}}$  shoots above this form. The smaller irregularity above  $\mu = 7.584$ , where  $n = 2$  begins to contribute, is barely visible.

- 
- [1] G.J. Feldman and R.D. Cousins, Phys. Rev. D **57**, 3873 (1998).  
 [2] D. Abrams *et al.*, astro-ph/0203500.  
 [3] <http://www.slac.stanford.edu/~yellin/ULsoftware.html>  
 [4] Particle Data Group, R.M. Barnett *et al.*, Phys. Rev. D **54**, 1 (1996). See especially p. 164. In subsequent reviews the Particle Data Group dropped its discussion of upper limits of Pois-

son processes, probably because the procedure of Feldman and Cousins [1] is now generally accepted as preferable when, as is usually assumed in discussions of confidence regions, backgrounds are well understood.

- [5] <http://wwwinfo.cern.ch/asdoc/shortwrupsdir/index.html>