STRONGER CLASSICAL CONFIDENCE LIMITS

Giovanni Punzi[*]
Scuola Normale Superiore and INFN - Pisa

Abstract
A new way of defining limits in classical statistics is presented. This is a natural extension of the original Neyman's method, and has the desirable property that only information relevant to the problem is used in making statistical inferences. The result is a strong restriction on the allowed confidence bands, excluding in full generality pathologies as empty confidence regions or unstable solutions. The method is completely general and directly applicable to all problems of limits. Some examples are discussed. In the well-known problem of Poisson processes with background it gives limits that do not depend on background in the case of no observed events.

1. INTRODUCTION

I belong to that class of physicists which prefer a classical approach to statistical inferences from physics experiments. I will not discuss in this contribution my motivations for this preference, since they are very eloquently described by other contributors to this workshop (see [5]).

However, I do believe that several difficulties with the current methods for setting confidence limits pointed out by critics of Bayesian inclination are reasons for real concern. This is because I am convinced that any method for quoting limits, in order to have interest for a physicist, must have some minimally good intuitive properties (for instance, better experiments should be able to set tighter limits). We just can't help the simple fact that classical limits are not statements on p(parameter|data) (see [5] for a very clear explanation of this point). But I think we should try to make sure they are indeed statements about *something* related to the parameter. I do believe that the coverage requirement is a very important property: I am very reluctant to accept any method for summarizing the information under the form of an accepted region per the parameters that does not guarantee a minimum rate of correct results. It is simply too good a property to give it up.

Unfortunately, we all know that coverage is not *sufficient*. It does not prevent paradoxical results to be obtained, otherwise there would have been no motivation for developing so many different methods for choosing limits. If one had to take the attitude that the coverage property is sufficient reason to justify any limit, however counterintuitive, then there would be no reason for not simply accepting an empty set as a possible result of a measurement. As a matter of fact, most physicists do not accept that, because that kind of results *tells them nothing* about the parameter.

Luckily, the range of methods allowed in classical statistics is potentially much wider than the currently explored solutions, so there is ample space for looking for better behaved confidence bands. I have described in [2] the rationale for a novel classical method for setting confidence limits that addresses all concerns I had with classical limits. I will briefly summarize here the proposed method and argue that its properties are better than that of all other known methods, referring the reader to [2] for a more complete discussion. I also apply the method to the now famous problem of Poisson plus background.

2. DEFINITION OF 'STRONG CONFIDENCE LEVEL'

The essence of the proposal is to quote limits by replacing (or supplementing) the usual CL as defined by Neyman[1] with a similarly formulated, but much more restrictive concept, which I called "strong CL".

[*]E-mail address: punzi@pi.infn.it

The strong CL is by construction always *smaller* than plain CL, therefore a band at a given sCL is also a legal band at the corresponding CL, so the standard Neyman's coverage is guaranteed, possibly with some *overcoverage*. One can view it either as just another way of choosing a particular band in the ample set of possibility left by Neyman's requirement of correct coverage, or as a radically different idea, that still preserves the standard coverage requirement. As a difference with other proposed methods, the band is not necessarily uniquely identified.

The definition runs as follows: a confidence band is said to have strong Confidence Level equal to sCL if it complies with the following requirement[2]:

for every possible value of the parameters μ and every subset of possible values for the observable x (χ):

$$\frac{p(x \in \chi, \mu \notin B(x)|\mu)}{\sup_\mu \ p(x \in \chi|\mu)} \leq 1 - sCL. \tag{1}$$

whenever the denominator is non–zero. Here $B(x)$ represents the accepted region for μ, given the observed x.

For comparison, the standard definition of CL, when written in the same form is:

for every possible value of the parameters μ:

$$p(\mu \notin B(x)|\mu) \leq 1 - CL. \tag{2}$$

The definition of strong CL is graphically illustrated in Fig. 1.

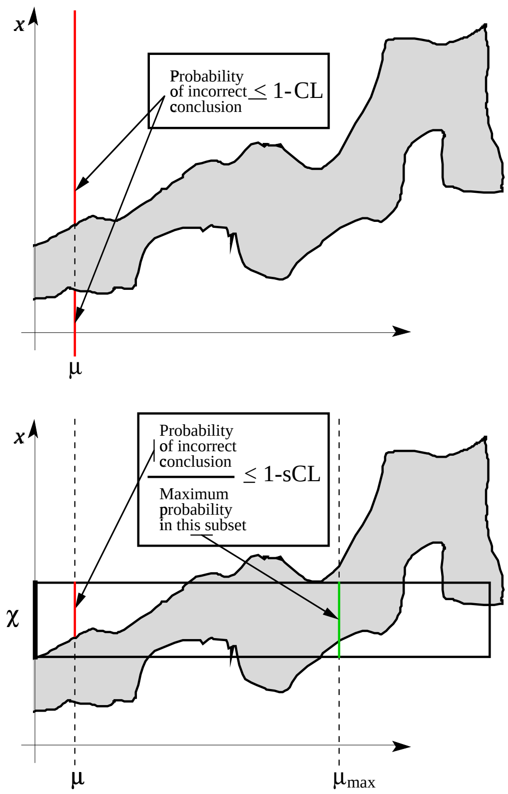

Fig. 1: Graphical illustration of the standard definition of CL (upper) and the new concept of "strong CL" (lower). The property illustrated for strong-CL must hold for *every* possible set χ of observable values.

It is interesting to note that this condition can be seen simply as the application of a generalized Neyman condition to every possible subsets of the observable space. As the standard CL, strong CL also has an intuitive interpretation in terms of expected frequency of reporting wrong conclusions: if one focuses on any particular subset of observable values, *the frequency of wrong results is limited to a small fraction (1-sCL) of the maximum expected rate of results in that category*.

The interesting novelty here is the guarantee that inferences from all possible experimental outcomes will have the same quality: the possibility of "unlucky results" is ruled out. This *uniformity of treatment* of all possible experimental outcomes is the basis of many good properties of confidence bands that satisfy this more restrictive requirement, which justify the additional computational effort.

3. PROPERTIES

Since it is not possible to explain in detail and formally prove the properties of strong CL in a single short talk, I will limit here just to list and quickly illustrate them with the help of a single very simple example, referring the interested reader to ref. [2] for details.

The example I will use is that of a trivial pdf that does not depend on the value of the unknown parameters. More precisely, let's consider the case of a parameter μ having only two possible discrete values, and an observable x also having only two possible discrete values, and let the pdf be given by the following table:

	$\mu 1$	$\mu 2$
$x1$	0.95	0.95
$x2$	0.05	0.05

(3)

Surprisingly, this trivial example allows many interesting considerations to be done.

3.1 Conceptual purity

Strong CL is a 100% pure classical method: it does not make any use of the concept of probability of an unknown parameter. Of course this is good to some, bad to others.

I think however that *purity* in itself should be appreciated by most people. Classical and Bayesian methods rest on very contrasting views of the very basic concepts, starting from the definition of probability itself, and it is difficult to avoid the suspect that any constructions made by a mix of the two (of which there are several examples) will eventually meet with contradictions and paradoxes.

3.2 Empty confidence regions are forbidden

Suppose one wants to find a 95% Confidence band for the above trivial pdf (3). Intuitively one expects not to be able to draw any conclusion, since the value of the parameter is irrelevant to the outcome of the experiment. In this simple case one can easily list all possible bands satisfying Neyman's definition of CL. They are four and shown in Fig 2. All but the first have some "overcoverage", that is they cover a larger region than strictly required by the definition of CL. Overcoverage is generally considered negatively, as a loss of power, therefore the first solution (a) is the most attractive from the point of view of its greater "discriminating power". Unfortunately, that is far from being intuitively satisfactory: if $x2$ is observed the absurd conclusion is that both values of the parameter are excluded.

Bands b) and c) are also intuitively repugnant. They imply one can draw a statistical conclusion at 95% on some parameter by measuring a totally unrelated quantity (I like to call those "Voodoo" bands). From the point of view of Neyman's requirement, they are just as good as any other band. This is a clear demonstration that mere coverage is not sufficient to ensure one will obtain meaningful limits.

a)

	$\mu 1$	$\mu 2$
x1	0.95	0.95
x2	0.05	0.05

b)

	$\mu 1$	$\mu 2$
x1	0.95	0.95
x2	0.05	0.05

c)

	$\mu 1$	$\mu 2$
x1	0.95	0.95
x2	0.05	0.05

d)

	$\mu 1$	$\mu 2$
x1	0.95	0.95
x2	0.05	0.05

Fig. 2: The set of all possible bands at 95% CL for a very simple "indifferent" pdf. The accepted region in each case is shown in grey.

If one looks at sCL, however, it is easy to verify that sCL is *zero* for band a), b) and c), while sCL=CL=100% for band (d), the intuitively correct conclusion. It can actually be proved rigorously[2] that the probability of an empty region is zero when using a strong band, whatever the pdf.

Are there other classical methods capable of avoiding this pitfall ? The most commonly used construction[10] looks explicitly for the narrowest band, so it yields (a) as the solution. If one looks at Likelihood Ratio ordering, one sees that all cells of the table get assigned the same rank in the ordering. If one had to follow exactly the prescription of ref. [3], one would start adding cells at random until attaining proper coverage: this yields randomly to any one of the four results. If one takes the attitude of ref. [4] then he is forced to add all cells together, and correctly finds (d).

While this is correct, it is a very near miss of paradoxical conclusions, compared with the clear cut, black-or-white answer provided by the strong CL. This difficulty in reaching the correct conclusion in a so simple case, should make one suspect that LR-ordering is not addressing the issue of empty region correctly. Indeed, it can be shown with more complex examples that LR ordering can actually yield empty confidence regions for wide ranges of observable values[2].

I feel that the RW modification of LR[9], based on removing ancillary variables, does correctly address the substance of this problem, but unfortunately it is not clear, to me at least, how it can be extended to more than a few specific cases. Incidentally, note that Bayes method is also exempt from this problem.

3.3 The question of correct sensitivity

We can learn even more by adding an infinitesimal perturbation to this simple pdf, as shown in Fig. 3. Band a) and c) are discarded by Neyman's condition since they now *undercover* and one is left just with options b) and d).

Now, both the narrowest band[10] and the LR criteria (whatever their flavor) choose solution b) without ambiguity ! (I am not sure about how to apply method [9] to this case).

b)

	$\mu 1$	$\mu 2$
x1	$0.95{+}\varepsilon$	$0.95{-}\varepsilon$
x2	$0.05{-}\varepsilon$	$0.05{+}\varepsilon$

d)

	$\mu 1$	$\mu 2$
x1	$0.95{+}\varepsilon$	$0.95{-}\varepsilon$
x2	$0.05{-}\varepsilon$	$0.05{+}\varepsilon$

Fig. 3: The set of all possible bands at 95% CL for a slightly perturbed indifferent pdf. The accepted region in each case is shown in grey.

This band is still very close to the "Voodoo" paradox of previous case. While now there is indeed a small sensitivity of x to the value of μ, it is worth reflecting on the fact that this result will be quoted at 95% CL, however small ϵ is.

Conversely, strong CL follows perfectly the intuitive perception of the situation: sCL is infinitesimally small for band b)[1] , while it is still $> 95\%$ for band d) (it is actually 100%).

I think this is a prototype case where the sensitivity of the experiment is not correctly reflected by the usual ways of quoting limits, just as it happens in the problem of Poisson with background. I think that criticisms as those raised by [6, 9] must be given proper attention if we wish classical methods to keep their current popularity. In my view, a limit that requires additional information about sensitivity to be quoted is lacking something: it is hard for a physicist to be happy with a limit figure that does not correctly account for the resolution of the experimental setup. The sCL does the job correctly and without the need for a separate parameter to represent the sensitivity of the experiment. This works also for the Poisson case (see below). A general statement requires a precise definition of the term 'sensitivity', but it is seen from the definition of sCL that a parameter value cannot be excluded unless its likelihood is small relative to the maximum.

3.4 Stability

It is worth noting the instability of all methods other than strong CL: if one changes the sign of ϵ in the above example, all probabilities change by infinitesimal quantities, but the decision on μ in case of observing $x2$ is suddenly reversed, however small ϵ is, and the conclusion is in both cases claimed at 95% CL !

Limits obtained from Strong CL are always stable for small perturbations of the pdf. This robustness is very important from a physicist point of view, and is due to the fact that sCL is based on *integrals* of probabilities. Conversely, the LR quantity depends on the *maxima* of the Likelihood function, which are sensitive to narrow local peaks and other possible small irregularities of the pdf.

3.5 Invariance under change of variable in the observable

This is another good property, since it removes an important element of arbitrariness. I think it is an important advantage of the classical methods that they are invariant under a change of variable in the parameter, and it is even better to have the same property in the observable space. The only classical methods I know of that have this property are the "unified method" [3] and the strong confidence described here.

3.6 Exclusion of 'irrelevant information' and the Likelihood Principle

Strong CL has the following property:

Take a subset of observable values. The set of *all possible* sCL limits for x inside this subset depends *only* on the Likelihood functions for values of x within that same subset (actually, even up to a multiplicative constant) (formal proof found in [2])

This is a more abstract, but I think highly significant property, probably the ultimate reason for all other good properties of Strong CL. It is remarkably close to the Likelihood Principle, and it is very good and far from obvious that this property can be attained simultaneously with the seemingly contrasting requirement of correct coverage. Note that the Bayesian method obviously has this good property, but *no classical method other than strong CL has it* (also proved in [2]).

It might seem at first sight that this property means that knowledge of the ensemble is not necessary to set sCL limits. Of course, this cannot be true, since sCL guarantees correct coverage. What is determined by the Likelihood function is a *set* of limits. A choice must be made, and the choices for

[1]It is exactly sCL=$\frac{2\epsilon}{0.05+\epsilon}$

different regions of x cannot be made independently, therefore knowledge of the ensemble is necessary. If one ignores the ensemble and simply makes a random choice based on the likelihood of the actual observation, the result is the effect called “flip-flopping” in ref. [3].

4. APPLICATION TO POISSON+BACKGROUND

An immediate consequence of the last mentioned property of strong CL is that the limits obtained when no events are observed cannot depend on expected background: this is because the likelihood function at $n = 0$ is independent of b, up to a constant factor.

I have explicitly calculated some strong bands for this distribution using the method outlined in [2] and compared with other choices. Fig. 4 shows a 90% sCL band for an expected background of 3.0 events, compared to FC[3] and RW[9] bands at 90% CL. It appears that the strong band is somewhat wider than both, even if it is not very different from RW for small n. The sCL band in case of no background is also shown, and it is seen to coincide at $n = 0$ with the sCL band for $b = 3.0$, as expected.

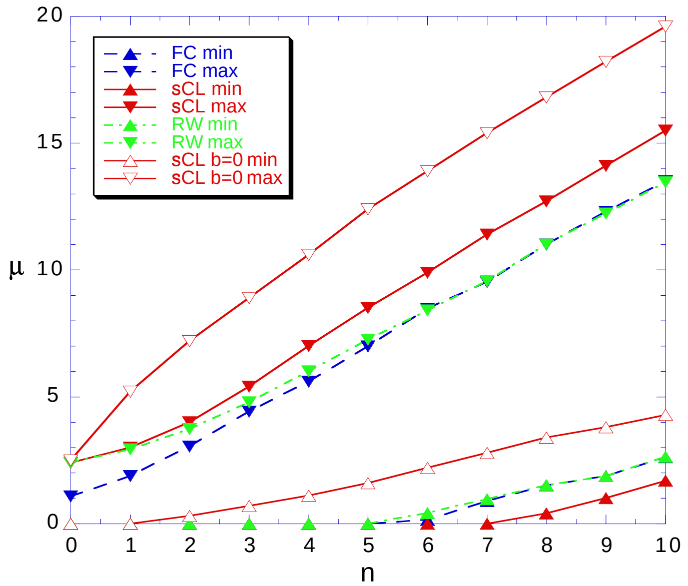

Fig. 4: Comparison of some bands at 90% CL for Poisson with mean expected background of 3.0 events. A strong band is shown together with FC and RW bands. The strong CL result for the zero-background case is also shown. It can be seen that the limits for $n = 0$ are the same for the two cases of $b = 0.0$ and $b = 3.0$.

Figure 5 shows that the strong band at 90% sCL is not too different from the FC band at 95% CL. Larger deviations at $n = 0$ must of course be expected at higher background levels, since the FC upper limit will approach zero.

5. CONCLUSIONS

The strong CL is a classical method for constructing confidence bands with very good properties. I suggest that whenever a confidence band is constructed using any method, one always evaluates its sCL as a way to check that the limits obtained will be physically sensible.

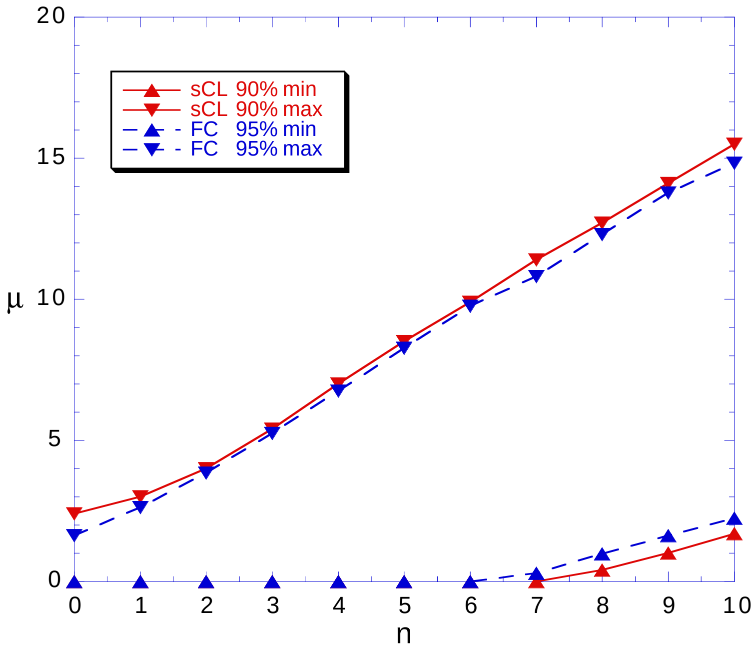

Fig. 5: Comparison of strong band at 90% sCL with FC band at 95% CL. The shapes are similar, with the exception of the point at $n = 0$.

Acknowledgements

I wish to thank G. Zech and H. Prosper for interesting comments and for making me appreciate the importance of the connection with the Likelihood Principle. I wish to thank the organizers of this workshop for creating this wonderful and unique opportunity for exchange of ideas.

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Discussion after talk of Giovanni Punzi. Chairman: Peter Igo-Kemenes.

H. Prosper

Just a couple of comments and a question. You made a comment that one of the reasons why you criticized the likelihood ratio method is that – I'm quoting a paper – 'the results can be counter-intuitive, and hard to interpret'. I'm just trying to imagine, two years from now, we're looking for the Higgs, and I try to use this method, and I try to explain to my colleagues what this means. It seems to me that we are already finding it very difficult to understand even the current methods, they're simply at a level of complexity that I think many people would find difficult. The reason you reject the Bayesian approach, I gather, is because it's subjective and you do not know what prior to use, and since you don't know what prior to use, you have to pick one out of a hat - that's subjective. However, reading your paper, it's quite clear that your reason for rejecting other confidence intervals is that you don't like their behaviour. Do you regard that as subjective? And if so why do you reject another method that's subjective? Are your motivations for doing what you do that basically you do not like the behaviour of the confidence limits calculated by, say, the likelihood ratio method or other methods (yes, yes - reply by Punzi); whatever you do not like, that's your motivation? You then invent a new method, and my question is, why is your method in that sense less subjective than any other method?

G. Punzi

Less subjective? Well, I don't know if it's less subjective, I think it has some good properties. Within classical methods, there are no other methods with such good properties, this at least is what appears to me. If one likes to do classical statistics, it looks like this gives you the best you can have. I'm not arguing Bayesian versus classical, I'm just saying 'if you want to be classical, this looks like a good way'.

H. Prosper

My problem with all these methods is this. Today we have very powerful computers, so I can imagine, I can say 'I don't like this particular set of limits.' It would be very easy to take the likelihood ratio limits, and then by brute force modify them until they behave the way I want, and I'm beginning to get very worried that we're moving in that direction. That is, we say: we don't particularly like this, but we modify them in some way so that I'm now happy, and I know how to do it. You could just take any sort of limits whatsoever and just perturb them, run my computer many many times until they behave the way I want. Why is that different from what you're doing?

G. Punzi

But this method I am proposing is general, Here you don't have to do any special treatment. You do the same thing every time.

H. Prosper

But your method requires, as I understand it, looking at every subset of the data, and therefore this is computationally intensive, so if I'm going to use a computer to do this, I might as well do it in a straightforward way, as I've suggested.

G. Punzi

Yes, it is possible. It is true that it takes more CPU, but, I don't know if this is your point, it is possible to write a program that automatically gives you the limit without having to worry case by case. This is possible. It's not something that you have to look at case by case, but it's a general requirement that you can run a program, maybe a CPU-heavy program, but it will automatically give you the limits, it doesn't require your judgement.

G. Zech

You give in your paper a corrolary which eventually says you have to fulfil a likelihood limit. Is this formula a necessary condition only, or is it also sufficient?

G. Punzi

No it is not sufficient. In fact I didn't show the plot, but I did draw the contour that I get by using only that formula, and the band that I get by forcing the general requirement, and I see that they are different.

F. James

In answer to Harrison's question. I think that what is interesting here is that you have a principle of local scale invariance which is apparently meaningful to theoreticians, perhaps less to us, and it's very difficult to calculate computationally because there are all these subsets, but at least there is a unifying principle behind it. On the other hand you claim it's classical in the sense that it doesn't use Bayesian reasoning, but usually we think of classical as having particular coverage. But your method is over-covering. Now you can do that if you want conditional coverage, for example, and conditional coverage we know over-covers unconditionally. If you don't like the fact that these limits get smaller as the expected background goes up, you can simply set them equal to a constant as expected background goes up, and that would give you a conditional coverage which is correct, but unconditional coverage which over-covers. And that one can do with other principles I think, that are easier to calculate.

G. Punzi

OK. It is true that this method sometimes over-covers. Not all the time, it depends on the *pdf*. But I think that the essential classical feature is not just in having exact strict coverage, but in having a way that doesn't make any assumption of what the parameter value is, or whether the parameter has, or not, a probability distribution. I think this is the thing that prevents classical statistics from even saying some things that Bayesians do, just because in classical statistics the concept of a distribution for the parameter is not allowed. Actually it is completely invariant with respect to the metric in the parameters, as I said. Of course you get some of the time some overcoverage, but my proposal looks even more classical because it's also invariant in observable space, since classical methods are invariant in all changes of the parameter. This is also invariant for all changes in the observed space, which looks like actually nice properties. So that's why I think it's better than just adjusting things in a way. Besides that, you are not really forced to use the band which has strong confidence of 95%. This depends on your choice. You can still decide, since they are both classical concepts, you have no problem in deciding. OK, you want to use a 95% confidence band, but among all possible bands, I choose the one which has the highest strong confidence and I impose that this be higher than some threshold. This is the important thing, because what happens is that among all possible bands with the correct coverage at a given confidence level, the ones which are bad for intuition all have very small values of strong confidence. So in a way you can take strong confidence as a measurement of whether your band is reasonable or not, and you may still decide to use the regular coverage criteria for deciding which one to use. This is still a possibility.

R. Cousins

I just wanted to address this point about the empty regions, because we have claimed that there are no empty regions, and you and somebody else claim there are empty regions. As you've shown in your table, the point arises when you have a tie when you're constructing the acceptance region. In our paper we do not give instructions as to what to do; the people who claim that there are empty null sets choose not to include all the ties. However, we can go to the book [shows transparency of beginning of Chapter 23 of Kendall's Advanced Theory of Statistics, in the new edition by Stuart and Ord], which actually defines this method. It defines the critical region for the test statistic by the condition with a less than or equal sign. So the textbook way is to include all the regions that have a tie. Then our understanding is that you will not have any empty regions.

G. Punzi

OK, I agree that this is a solution to that, this is an example where you have a tie between several values where you have the possibility of requiring this thing and solving this anyway, but what I wanted to show with that example was that the likelihood ratio ordering itself does not easily tell you what is good from what is bad. You get to the point where two things, one of which is reasonable and the other very bad, are put very very close at the same level and you need some special change to be able to distinguish between them. So, this point was made to try to convey these kinds of things, but there is also a stronger point. It is possible to make examples where you don't even have a tie. I don't know if you read this example in my paper. I didn't mention that because it's a bit more complicated, but I can make you a drawing. [Draws diagram of x against μ].

If you have read it, you already know, but suppose this is μ and this is the observable x. Suppose you have basically any *pdf* here; then you can do this trick, I admit it's not very natural but it doesn't matter. This is μ and this is x. Take this probability distribution and add a very narrow distribution with negligible area, like a ridge but made in this way. This is not very natural. Suppose this ridge has maybe some Gaussian distribution which is a very narrow peak of negligible area, and I superimpose on this plot here, where there is a *pdf* staying behind. Also, in addition to this complication, let me complicate it even more. Suppose that the height of the ridge is increasing in going towards infinity, while still keeping the same area. You can make it squeeze this region which is wiggling, you squeeze and you bring it to infinity with an ever increasing height. So if you look at any x here and if you look at the likelihood plot, there is some distribution with, superimposed on it, a series of narrow spikes which become increasingly high. The maximum of the likelihood is at infinity, if μ has an infinite range. So what happens is that all of these points get a rank according to the likelihood ratio ordering which is zero, including the point of the spike, because for every spike there is another which is much higher.

It is a rather mathematical example, and in this way all the points are of zero rank, so all points in this region with this spike here get zero rank, so they are considered last in the likelihood ratio ordering.

So what happens is that this region here is a small region which should not require you to take it into account, because of reasons of tolerance, so if you make 95% by integrating outside this band, these points are taken last in the likelihood ratio ordering, so all of this band is left out. So all of this band will give empty confidence bounds.

M. Woodroofe

Kendall and Stuart weren't always super-careful about stating their mathematical assumptions, but they meant to exclude pathological cases like that.

J. Bouchez

Actually you do not need to resort to these funny examples. When you said there was a tie, it is only for the value of the parameter which is bound. For higher values of the parameter there is no tie, and so you can define unambiguously the interval you choose. So it is only a question when you are at the boundary for the parameter that you can have a tie. When you go to this limit, you just do it by continuity. Or else you do what you said: There is a tie, so you take all the points. But it is no use, because instead of getting a narrow result, you will say that the value of the parameter is the value of the limit.

G. Punzi

It is true that if you use the strong confidence definition, whether you like it or not, this is also handled correctly.

G. Feldman

Even though this is pathological, I don't even understand why this fails, because even in this case the point with μ equal to infinity includes x in its region, so the region is not null.

G. Punzi

I assume that $\mu = \infty$ is not a value. In my mathematical example, the maximum of the likelihood does not exist for any real μ. It is a superior limit which exists. Infinity is not a real number. If you use the likelihood ratio ordering, whenever the maximum of the likelihood exists, then that value is always included. It still does not help you so much, even if you include the point at infinity. You are completely altering the previous confidence band because of a negligible probability perturbation of the *pdf*, which should actually be ignored completely. A reasonable man should not run after something that is negligibly small.

C. Giunti

Your last figures were most interesting. What happens to the lower limit, in the Poisson case? What is the difference of your method, as compared with other methods?

G. Punzi

Remember that strong confidence gives you a range of possible bands, not always a unique band. It is something similar to a new way of getting limits. It is not a single choice. In reality, for the case of a Poisson with background, the variation is very limited. However in most cases, both the lower and the upper limits are wider, for most values of the background, if you compare the same confidence level for strong confidence and for the usual one. This is a way of comparing them, because they are kind of different things. This is not a choice within the usual framework, it is really a different way of thinking.

B. Roe

It seems to me that we should express things in terms of real coverage. When you say 90%, it is a sort of artificial parameter. You should compare what your real coverage is with, for example, Feldman and Cousins, or with Roe and Woodroofe. Somehow we've got to compare apples and oranges, and we should try to get into the same ball-park.

G. Punzi

OK, but you should not use bands with very low strong confidence. If you have a band with very low strong confidence, that is bad.

B. Roe

Coverage is an important concept.

G. Punzi

I agree, I just think it is not everything.

Chairman

Let's stop on a point of agreement.