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Coverage: suppose  $\mu^{*}$  the true value

$$P(x_1(\mu^*) < x_0 < x_2(\mu^*)) = \alpha$$



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Upper limit (lower limit = 0) Suppose Poisson variable and n=0 is measured (no background)  $=> 0 \pm 0$  (freq) or  $1 \pm 1$  (Beyes)?

By construction the probability to measure  $x_0' < x_0$  if the true value  $\mu = \mu_1(x_0)$  is  $(1-\alpha)$  (only one limit) or the probability to measure  $x_0' > x_0$  if the true value  $\mu = \mu_1(x_0)$  is  $\alpha$ 



Methods in Experimental Particle Physics

### frequentist limits

The belt is limited on one side only, and for any result of a measurement  $n_0$  we identify  $s_{up}$  in such a way that if  $s_{true} = s_{up}$ , the probability to get a counting smaller than  $n_0$  is  $1 - \beta^{31}$ . By considering the Poisson statistics without background (b=0) we get:

$$\sum_{n=0}^{n_0} \frac{e^{-s_{up}} s_{up}^n}{n!} = 1 - \beta$$

If  $n_0 = 0$  we have

$$e^{-s_{up}} = 1 - \beta$$
$$s_{up} = \ln \frac{1}{1 - \beta}$$

from which we get the same numbers for  $s_{up}$  obtained in the bayesian case.

#### frequentist limits



FIGURE 19. Neyman construction for the case of an upper limit. In this case a segment between  $n_1(\theta)$  and  $\infty$  is drawn for each value of the parameter  $\theta$ . The segments define the confidence region. Once a value of n,  $n_0$  is obtained, the upper limit  $s_{up}$  is found. (For simplicity the discrete variable n is considered as a real number here).

#### frequentist limits

If b is not equal to 0 but is known,

(201) 
$$\sum_{n=0}^{n_0} \frac{e^{-(s_{up}+b)}(s_{up}+b)^n}{n!} = 1 - \beta$$

and from this equation upper limits can be evaluated for the different situations.

It has been pointed out that the use of eq.201 gives rise to some problems. In particular negative values of  $s_{up}$  can be obtained using directly the formula<sup>32</sup>. This doesn't happen in the bayesian context where the condition s > 0 is put directly by using the proper prior.

 $^{32}$ A rate is a positive-definite quantity. However, if a rate is 0 or very small with respect to the experimental sensitivity, the probability that  $n_0$  is larger than b is exactly equal to the probability that  $n_0$  is lower than b. This implies that a negative rate naturally comes out from an experimental analysis based on a difference between two counts. The acceptance of such results is a sort of "philosophical" question and is controversial.

## Flip-flop problem

$$\overline{m}^2 = -54 \pm 30 \text{ eV}^2$$

 $p(m_t^2/\overline{m}^2) = \frac{L(\overline{m}^2/m_t^2)\pi(m_t^2)}{\int dm_t^2 L(\overline{m}^2/m_t^2)}$ 



FIGURE 21. Example of the square neutrino mass. Construction of the upper limit in the frequentist approach (left plot) and in the bayesian approach (right plot). (left) The red gaussian is the experimental like-lihood, the blue gaussian corresponds to the 95% CL upper limit that leaves 5% of possible the experiment outcomes below the present experimental average. (right) The blue curve is the result of the Bayes theorem when a prior forcing to positive values is applied (eq.202).



FIG. 4. Plot of confidence belts implicitly used for 90% C.L. confidence intervals (vertical intervals between the belts) quoted by flip-flopping physicist X, described in the text. They are not valid confidence belts, since they can cover the true value at a frequency less than the stated confidence level. For  $1.36 < \mu < 4.28$ , the coverage (probability contained in the horizontal acceptance interval) is 85%.

$n_0 b$	0.0	0.5	1.0	1.5	2.0	2.5	3.0	3.5	4.0	5.0
0	0.00, 2.44	0.00, 1.94	0.00, 1.61	0.00, 1.33	0.00, 1.26	0.00, 1.18	0.00, 1.08	0.00, 1.06	0.00, 1.01	0.00, 0.98
1	0.11, 4.36	0.00, 3.86	0.00, 3.36	0.00, 2.91	0.00, 2.53	0.00, 2.19	0.00, 1.88	0.00, 1.59	0.00, 1.39	0.00, 1.22
2	0.53, 5.91	0.03, 5.41	0.00, 4.91	0.00, 4.41	0.00, 3.91	0.00, 3.45	0.00, 3.04	0.00, 2.67	0.00, 2.33	0.00, 1.73
3	1.10, 7.42	0.60, 6.92	0.10, 6.42	0.00, 5.92	0.00, 5.42	0.00, 4.92	0.00, 4.42	0.00, 3.95	0.00, 3.53	0.00, 2.78
4	1.47, 8.60	1.17, 8.10	0.74, 7.60	0.24, 7.10	0.00, 6.60	0.00, 6.10	0.00, 5.60	0.00, 5.10	0.00, 4.60	0.00, 3.60
5	1.84, 9.99	1.53, 9.49	1.25, 8.99	0.93, 8.49	0.43, 7.99	0.00, 7.49	0.00, 6.99	0.00, 6.49	0.00, 5.99	0.00, 4.99
6	2.21,11.47	1.90,10.97	1.61,10.47	1.33, 9.97	1.08, 9.47	0.65, 8.97	0.15, 8.47	0.00, 7.97	0.00, 7.47	0.00, 6.47
7	3.56,12.53	3.06,12.03	2.56,11.53	2.09,11.03	1.59,10.53	1.18,10.03	0.89, 9.53	0.39, 9.03	0.00, 8.53	0.00, 7.53
8	3.96,13.99	3.46,13.49	2.96,12.99	2.51,12.49	2.14,11.99	1.81,11.49	1.51,10.99	1.06,10.49	0.66, 9.99	0.00, 8.99
9	4.36,15.30	3.86,14.80	3.36,14.30	2.91,13.80	2.53,13.30	2.19,12.80	1.88,12.30	1.59,11.80	1.33,11.30	0.43,10.30
10	5.50,16.50	5.00,16.00	4.50,15.50	4.00,15.00	3.50,14.50	3.04,14.00	2.63,13.50	2.27,13.00	1.94,12.50	1.19,11.50
11	5.91,17.81	5.41,17.31	4.91,16.81	4.41,16.31	3.91,15.81	3.45,15.31	3.04,14.81	2.67,14.31	2.33,13.81	1.73,12.81
12	7.01,19.00	6.51,18.50	6.01,18.00	5.51,17.50	5.01,17.00	4.51,16.50	4.01,16.00	3.54,15.50	3.12,15.00	2.38,14.00
13	7.42,20.05	6.92,19.55	6.42,19.05	5.92,18.55	5.42,18.05	4.92,17.55	4.42,17.05	3.95,16.55	3.53,16.05	2.78,15.05
14	8.50,21.50	8.00,21.00	7.50,20.50	7.00,20.00	6.50,19.50	6.00,19.00	5.50,18.50	5.00,18.00	4.50,17.50	3.59,16.50
15	9.48,22.52	8.98,22.02	8.48,21.52	7.98,21.02	7.48,20.52	6.98,20.02	6.48,19.52	5.98,19.02	5.48,18.52	4.48,17.52
16	9.99,23.99	9.49,23.49	8.99,22.99	8.49,22.49	7.99,21.99	7.49,21.49	6.99,20.99	6.49,20.49	5.99,19.99	4.99,18.99
17	11.04,25.02	10.54,24.52	10.04,24.02	9.54,23.52	9.04,23.02	8.54,22.52	8.04,22.02	7.54,21.52	7.04,21.02	6.04,20.02
18	11.47,26.16	10.97,25.66	10.47,25.16	9.97,24.66	9.47,24.16	8.97,23.66	8.47,23.16	7.97,22.66	7.47,22.16	6.47,21.16
19	12.51,27.51	12.01,27.01	11.51,26.51	11.01,26.01	10.51,25.51	10.01,25.01	9.51,24.51	9.01,24.01	8.51,23.51	7.51,22.51
20	13.55,28.52	13.05,28.02	12.55,27.52	12.05,27.02	11.55,26.52	11.05,26.02	10.55,25.52	10.05,25.02	9.55,24.52	8.55,23.52

TABLE IV. 90% C.L. intervals for the Poisson signal mean  $\mu$ , for total events observed  $n_0$ , for known mean background b ranging from 0 to 5.



FIGURE 20. 90% limit  $s_{up}$  (Upper end of confidence interval for  $\mu$  in the figure) vs. *b* for different values of  $n_0$ . These are the upper limits resulting from a frequentist treatment in the framework of the so called "Unified approach". The dotted portions of the lines correspond to configuration where central intervals rather than upper limits should be given. The dashed portions of the lines correspond to very unlikely configuration (very small  $n_0$  when *b* is quite large, so that  $p(n_0)$  is below 1%). (taken from G.Feldmann, R.Cousins, Phys.Rev.D57 (1998) 3873)

7.4. A modified frequentist approach: the  $CL_s$  method. Now we consider a method, developed in the last years and applied in many analyses especially from LHC experiments, including the search for the Higgs boson. It is the modified frequentist approach to the problem of setting upper/lower limits in search experiments.

n<sub>i</sub> events and expected events  $y_i = \mu s_i + b_i$ 

Signal strength 
$$\mu = \frac{\sigma}{\sigma_{th}}$$
 Theory expectation  $\mu=1$ 

$$L(\underline{n}/\mu, \underline{\theta}) = \prod_{i=1}^{M} \frac{(\mu s_i + b_i)^{n_i} e^{-(\mu s_i + b_i)}}{n_i!}$$

Add histogram of control regions, mj, background enriched

 $E[m_j] = u_j(\underline{\theta})$  depending on the nuisance parameters (and not on  $\mu$ )

$$L(\underline{n}/\mu, \underline{\theta}) = \prod_{i=1}^{M} \frac{(\mu s_i + b_i)^{n_i} e^{-(\mu s_i + b_i)}}{n_i!} \prod_{j=1}^{K} \frac{u_j^{m_j} e^{-u_j}}{m_j!}$$

Define the test statistics

$$q_{\mu} = -2 \ln \frac{L(\mu, \hat{\underline{\hat{\theta}}})}{L(\hat{\mu}, \hat{\underline{\hat{\theta}}})}$$
 profile likelihood ratio.

symbols:  $\hat{\mu}$  and  $\hat{\underline{\theta}}$  are the best values of the parameters obtained by maximizing L;  $\hat{\underline{\theta}}$  are the values of the nuisance parameters obtained by maximizing L at  $\mu$  fixed. The test

7.4.2. Discovery. In order to falsify a null hypothesis  $H_0$  we need to test the backgroundonly hypothesis. This can be done by using the test statistics  $q_0$ , that is eq. 207 for  $\mu = 0$ 

(210) 
$$q_0 = -2\ln\frac{L(0,\hat{\underline{\hat{\theta}}})}{L(\hat{\mu},\hat{\underline{\theta}})}$$

If we call  $q_0^{obs}$  the value of  $q_0$  obtained using the data, we can easily define a *p*-value

(211) 
$$p_0 = \int_{q_0^{obs}}^{\infty} f(q_0/0) dq_0$$

that, for what we have seen in the previous paragraph, is essentially a  $\chi^2$  test. If  $p_0$  is below the defined limit we falsify the hypothesis and we have done the discovery.

7.4.3. Signal exclusion:  $CL_{s+b}$ . We consider now how the test statistics shown in eq. 207 can be used for the exclusion of a given theory. Eq. 207 is rewritten with  $\mu = 1^{36}$ 

(212) 
$$q_1 = -2\ln\frac{L(1,\underline{\hat{\theta}})}{L(\hat{\mu},\underline{\hat{\theta}})}$$

The lower is  $q_1$ , the more compatible the data are with the theory, and the less compatible the data are with the pure background expectations. The pdf of  $q_1$  can be evaluated starting from MC samples, either generated with  $\mu = 1$  or for samples of pure background events generated with  $\mu = 0$ . We call respectively  $f(q_1/1)$  and  $f(q_1/0)$  the two pdf's. A graphical example of these pdf's is shown in Figure 22. The separation between the two pdf's determines the capability to discriminate the searched model with respect to the background<sup>37</sup>.



FIGURE 22. Example of  $q_1$  distributions in the two hypotheses, namely  $\mu = 1$  and  $\mu = 0$ . The separation between the two distributions indicate the capability to discriminate the two hypotheses.

evaluate the **sensitivity** of the experiment. define  $\tilde{q}_1$  as the **median** of the  $f(q_1/0)$  function<sup>3</sup>

expected  $CL^{exp}_{s+b} = \int_{\tilde{q}_1}^\infty f(q_1/1) dq_1$ 



FIGURE 23. For the same example of alternative hypotheses shown in Fig. 22: construction of  $CL_{s+b}^{exp}$  (upper plot) and of  $CL_{s+b}^{obs}$  (lower plot). In both cases the CL is given by the blue area. In the upper plot the median  $q_1$  from background experiments is indicated as  $\tilde{q}_1$ ; in the lower plot the  $q_1$  obtained by data is indicated as  $q_1^{obs}$ .

However, we have determined the median CL only. In actual background-only experiments, we will have background fluctuations, in such a way that  $q_1$  values will be obtained distributed according to  $f(q_1/0)$ . So we can evaluate an interval of confidence levels, by repeating the procedure above for two positions of  $q_1$ ,  $\tilde{q}_1^{(1)}$  and  $\tilde{q}_1^{(2)}$  such that respectively:

(214) 
$$\int_{-\infty}^{\tilde{q}_1^{(1)}} f(q_1/0) dq_1 = \frac{1-\beta}{2}$$

(215) 
$$\int_{-\infty}^{q_1^{-\gamma}} f(q_1/0) dq_1 = \frac{1+\beta}{2}$$

with e.g.  $\beta = 68.3\%$  to have a gaussian one-std.deviation interval. Confidence levels are then evaluated applying eq. 213 to  $\tilde{q}_1^{(1)}$  and  $\tilde{q}_1^{(2)}$ .

## Observation

(216) 
$$CL_{s+b}^{obs} = \int_{q_1^{obs}}^{\infty} f(q_1/1) dq_1$$

and this is the **observed** confidence level. If it is below, say 5% we exclude the signal at 95% CL.



FIGURE 23. For the same example of alternative hypotheses shown in Fig. 22: construction of  $CL_{s+b}^{exp}$  (upper plot) and of  $CL_{s+b}^{obs}$  (lower plot). In both cases the CL is given by the blue area. In the upper plot the median  $q_1$  from background experiments is indicated as  $\tilde{q}_1$ ; in the lower plot the  $q_1$  obtained by data is indicated as  $q_1^{obs}$ .

7.4.4. Signal exclusion:  $CL_s$ . A problem in the procedure outlined in the previous section has been put in evidence, and a correction to it, the so called modified frequentist approach has been proposed. We discuss now this method, also called  $CL_s$  method that is now widely employed for exclusion of new physics signals.

Let's consider the situation shown in Figure 24 where the two pdf's  $f(q_1/0)$  and  $f(q_1/1)$  have a large overlap signaling a small sensitivity. If we evaluate in this situation  $CL_{s+b}^{exp}$  we find a large value, so that we do not expect to be sensitive to exclusion. However what happens if  $q_1^{obs}$  is the one shown in the same Figure ? The observed  $CL_{s+b}^{obs}$  is well below 5% and the signal has to be excluded at 95% CL. But, are we sure that we have to exclude it ? In the same Figure the quantity  $CL_b^{obs}$  is reported:

(217) 
$$CL_b^{obs} = \int_{q_1^{obs}}^{\infty} f(q_1/0) dq_1$$

that is also very small in this case. Apparently the signal is small and the background "under-fluctuates", so that  $q_1^{obs}$  is scarcely compatible with the signal+background hypothesis but also with the background-only hypothesis. So, we are excluding the signal, essentially because the background has fluctuated.

In order to avoid this somehow unmotivated exclusion, the  $CL_s$  procedure has been defined. The idea is to use, as confidence level, the  $CL_s$  quantity, either expected or



FIGURE 24. Same construction of Fig. 23 for a situation where the discrimination between the two hypotheses is particularly poor and the overlap between the two distributions is high. The  $CL_{s+b}^{exp}$  is high (upper plot) but for a particular experiment with a under fluctuation of the background the  $CL_{s+b}^{obs}$  can be small in such a way to reject the signal hypothesis (lower plot). In the lower plot the magenta area shows  $CL_b^{obs}$  from which  $CL_s$  is built. In this case using the  $CL_s$  prescription rather than the  $CL_{s+b}$  one the signal is not rejected.

$$CL_s = \frac{CL_{s+b}}{CL_b}$$

The  $CL_s$  method is also said **modified frequentist** approach. In fact, the confidence interval obtained in this way has not the coverage properties required by the "orthodox" frequentist paradigm. So if we build a confidence interval with a  $CL_s$  of  $\alpha$ , the coverage is in general larger than  $\alpha$ , so that the Type-I errors are less than  $1 - \alpha$ .

## **Basic Definitions: POWER**

•  $\alpha = \Pr{ob(reject H_0 | H_0)}$ 



Birnbaum (1977)

"A concept of statistical evidence is not plausible unless it finds 'strong evidence for  $H_1$  as against  $H_0$ '

with small probability ( $\alpha$ ) when  $H_0$  is true,

and with much larger probability  $(1-\beta)$  when  $H_1$  is true. "

Birnbaum (1962) suggested that  $\alpha / 1 - \beta$ (significance / power)should be used as a measure of the strength of a statistical test,rather than  $\alpha$  alone

$$\begin{array}{l} (H) \\ p = 5\% \rightarrow p' = 5\% / 0.155 = 32\% \\ H_0 \\ \end{array} \\ p' \equiv CL_s \\ p'_{\mu} = \frac{p_{\mu}}{1 - p_0} \end{array}$$

CLs



# p-value - testing the null hypothesis

When testing the b hypotheis (null=b), it is custom to set

 $\alpha = 2.9 \, 10^{-7}$   $\rightarrow$  if  $\rho_b < 2.9 \, 10^{-7}$  the b hypothesis is rejected  $\rightarrow$  Discovery

When testing the s+b hypothesis (null=s+b), set  $\alpha = 5\%$ if  $\rho_{s+b} < 5\%$  the signal hypothesis is rejected at the 95% Confidence Level (CL)  $\rightarrow$  Exclusion