

# Physics 403

Credible Intervals, Confidence Intervals, and Limits

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# Parameter Intervals

- ▶ We often want to make a statement about some parameter  $\mu$  whose true value  $\mu_t$  (in the frequentist sense) is unknown.
- ▶ We measure an **observable**  $x$  whose PDF depends on  $\mu$ . I.e., we have  $p(x|\mu) = \mathcal{L}(x|\mu)$
- ▶ From Bayes' Theorem, we want to calculate

$$p(\mu_t|x) = \frac{\mathcal{L}(x|\mu_t) p(\mu_t)}{p(x)}$$

- ▶ A **Bayesian interval**  $[\mu_1, \mu_2]$  corresponding to a confidence level  $\alpha$  is constructed by requiring

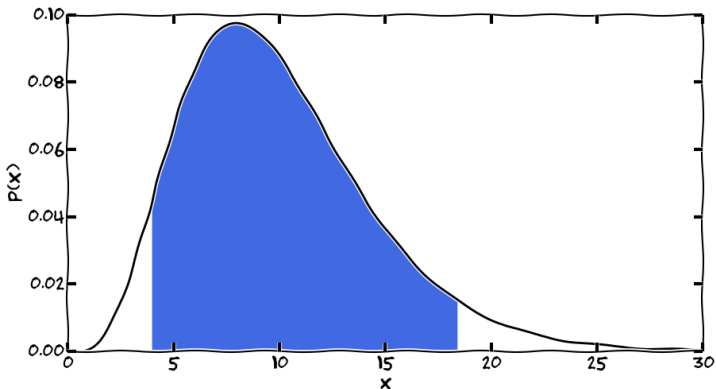
$$\int_{\mu_1}^{\mu_2} p(\mu_t|x) d\mu_t = \alpha$$

This is called the **credible interval** of  $\mu_t$

# Bayesian Credible Intervals

## Central Interval

Given the posterior PDF, it is easy to quote a range for a parameter:

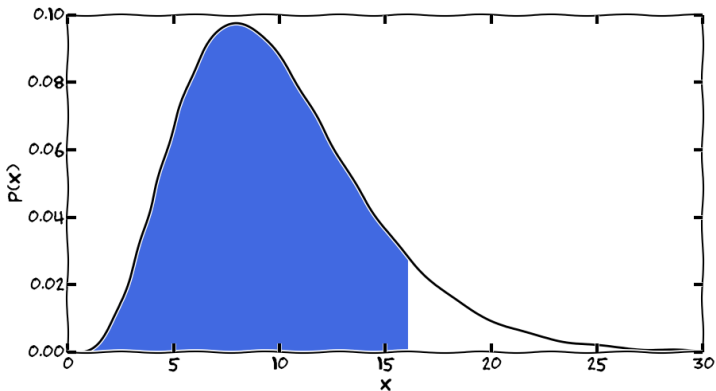


Central 90% of the PDF gives a **credible region**  $x \in [4.0, 18.4]$ .

# Bayesian Credible Intervals

## Upper Limit

If you wanted to quote an **upper limit** instead you would just integrate to find the 90<sup>th</sup> percentile:



Here  $x \in [0, 16.0]$ , or, “the upper limit of  $x$  at 90% C.L. is 16.0”

# Advantages and Disadvantages of the Bayesian Approach

- ▶ With the Bayesian approach you can account for **prior knowledge** when calculating the credible region, which can be very useful for quoting limits near a physical boundary
- ▶ Example from Cowan [1]: you measure  $m^2 = E^2 - p^2$ . Because of measurement uncertainties the **maximum likelihood estimator**  $\hat{m}^2 < 0$
- ▶ A Bayesian would be able to use a prior that vanishes for  $m < 0$ , so you don't have to publish an unphysical value. This option is not available to a frequentist
- ▶ However, a 90% Bayesian credible interval may not mean that 90% you will measure a value in a certain range, because the PDF does not have to refer to long-run frequencies
- ▶ The frequentist range (**confidence interval**) is sometimes what you want, but interpreting it is tricky

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# Classical Confidence Intervals

- ▶ Since frequentists do not work with posterior PDFs, **classical intervals are not statements about  $\mu_t$  given an observable  $x$**
- ▶ For a frequentist, the range  $[\mu_1, \mu_2]$ , called the **confidence interval**, is a member of a set such that

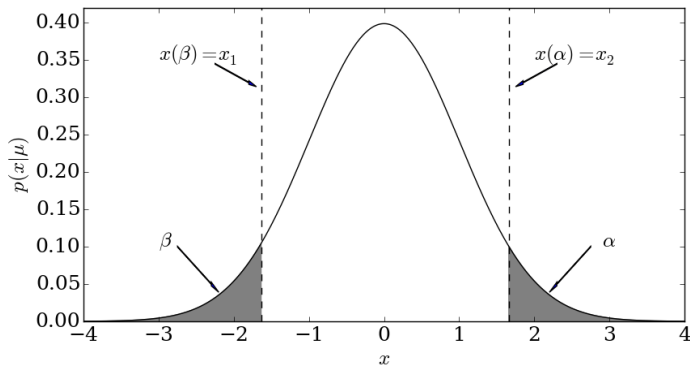
$$p(\mu \in [\mu_1, \mu_2]) = \alpha$$

- ▶ The values  $\mu_1$  and  $\mu_2$  are functions of  $x$ , and refer to the **varying intervals** from an ensemble of experiments with **fixed  $\mu$**
- ▶ Frequentist:  $[\mu_1, \mu_2]$  contains the **fixed, unknown  $\mu_t$**  in a fraction  $\alpha$  of hypothetical experiments
- ▶ Bayesian: the degree of belief that  $\mu_t$  is in  $[\mu_1, \mu_2]$  is  $\alpha$
- ▶ These views *can* correspond, but they don't have to



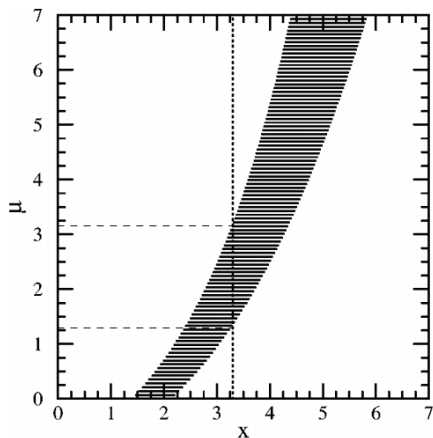
## Constructing a Neyman-Pearson Interval

To construct a confidence interval, we begin with  $p(x|\mu)$ , the PDF of the observable given a **fixed value of the parameter  $\mu$** :



The observable  $x$  has probability  $1 - \alpha - \beta$  to fall in the unshaded region. We define a **central confidence interval** by setting  $\alpha = \beta$

# Constructing a Confidence Belt



- ▶ Since  $\mu$  varies, we now repeat this procedure for different values of  $\mu$
- ▶ Construct a **confidence belt** by calculating  $x_1$  and  $x_2$  such that

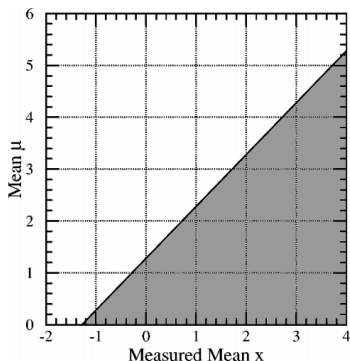
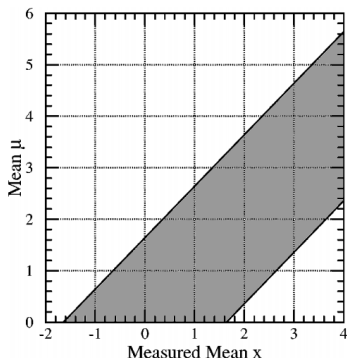
$$\begin{aligned} p(x < x_1 | \mu) &= p(x > x_2 | \mu) \\ &= (1 - \alpha) / 2 \end{aligned}$$

for each value of  $\mu$

- ▶ If we observe  $x_0$ , the confidence interval  $[\mu_1, \mu_2]$  is the **union of all values of  $\mu$  defined by the vertical slice through the belt**

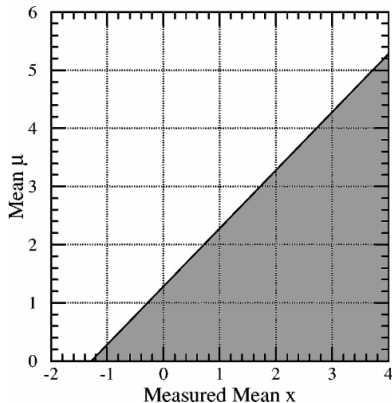
## Central and Upper Intervals

To construct an upper interval, calculate  $p(x < x_1 | \mu) = 1 - \alpha$  for all  $\mu$ .



Left: confidence belt for **90% C.L. central intervals** for the mean of a Gaussian with a boundary at 0. Right: confidence belt for **90% C.L. upper limits** for the mean  $\mu$  (from [2])

## Using an Upper Limit



This plot was constructed using the PDF

$$p(x|\mu) = \frac{1}{\sqrt{2\pi}} \exp \left[ -\frac{(x - \mu)^2}{2} \right].$$

Only positive values of  $\mu$  are physically allowed, so the plot cuts off at  $\mu < 0$ .

This is perfectly valid, but what happens when the measurement is  $x = -1.8$ ?

Draw a vertical line at  $x = -1.8$ ; the confidence interval is an **empty set**. How can we interpret this?

# Interpreting the Confidence Interval

- ▶ **Problem:** we set up the problem to ignore  $\mu$  in the **non-physical region**  $\mu < 0$ , but observed  $x = -1.8$  and found that  $[\mu_1, \mu_2] = \emptyset$
- ▶ **Temptation:** we might want to conclude that all values of  $\mu$  are **ruled out** by the measurement. Is this correct?

# Interpreting the Confidence Interval

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- ▶ **Temptation:** we might want to conclude that all values of  $\mu$  are **ruled out** by the measurement. Is this correct?
- ▶ Nope! Remember what the 90% confidence interval tells you: given an ensemble of identical experiments, you should expect to construct an interval that contains the **true value of  $\mu$**  90% of the time
- ▶ If  $[\mu_1, \mu_2] = \emptyset$  then conclude that you have conducted one of the 10% of experiments that **fail to contain the true value**
- ▶ It's a common mistake to conclude that the confidence interval tells you about the true value  $\mu_t$ . **It doesn't.** A frequentist test won't tell you about  $\mu_t$ , just the long-run outcome of many identical experiments

# Frequentist Coverage

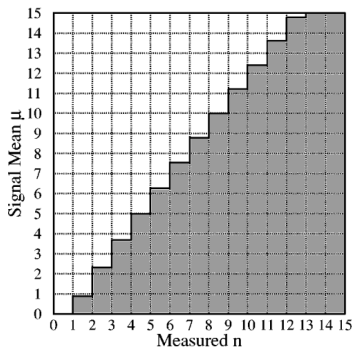
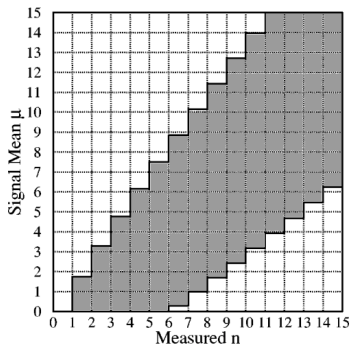
- ▶ If  $p(\mu \in [\mu_1, \mu_2]) = \alpha$  is satisfied, one says that the intervals **cover  $\mu$  at the stated confidence** (or equivalently, that the intervals have the correct “coverage”)
- ▶ **Undercoverage**: there exists a  $\mu$  such that  $p(\mu \in [\mu_1, \mu_2]) < \alpha$
- ▶ **Overcoverage**: there exists a  $\mu$  such that  $p(\mu \in [\mu_1, \mu_2]) > \alpha$
- ▶ Undercoverage is a serious problem because it can lead to a Type I error, i.e., **failure to accept a true null hypothesis (false discovery)**
- ▶ If a set of intervals overcovers for some values of  $\mu$  but never undercovers it is called **“conservative”**
- ▶ Conservative intervals are not considered as big of a problem, but they result in Type II errors, i.e., **failure to reject a false null hypothesis (loss of power)**

# Poisson Process with Background

## Built-in Overcoverage

Suppose you are counting discrete events  $x \rightarrow n$  where  $n$  consists of **signal events** with unknown mean  $\mu$  and **background events** with known mean  $b$ :

$$p(n|\mu) = (\mu + b)^n \exp[-(\mu + b)]/n!$$





# Poisson Process with Background

## Built-in Overcoverage

- ▶ Because in the Poisson process  $n$  is an integer, we will sometimes find that

$$p(\mu \in [\mu_1, \mu_2]) \neq \alpha$$

simply because the **discrete intervals cannot cover  $\mu$**

- ▶ Convention: for the Poisson process, instead choose to satisfy

$$p(\mu \in [\mu_1, \mu_2]) \geq \alpha$$

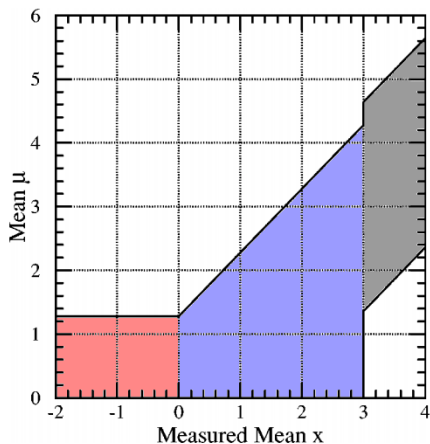
in all edge cases. I.e., **systematically overcover** when necessary

- ▶ This is pretty sub-par. We want a 90% interval to fail to contain the true value 10% of the time. Overcoverage means this happens less than that
- ▶ Unfortunately, the overcoverage in the Poisson case is **not done by choice**. It's a consequence of the discreteness of the counts

## Other Limits on Producing Confidence Intervals

- ▶ There is a serious limitation with classical confidence intervals: for coverage to be meaningful, **you must decide ahead of time what kind of interval to calculate**
- ▶ If it is *determined before conducting an experiment* that an upper limit is appropriate, then the triangular confidence belt shown earlier is perfectly fine
- ▶ If it is *determined before conducting an experiment* that a central limit is appropriate, then the central confidence belt shown earlier is perfectly fine
- ▶ But, if the experimenter decides to publish an upper or central interval *based on the results of the experiment* – a completely reasonable thing to do, by the way – then **things go bad very quickly**

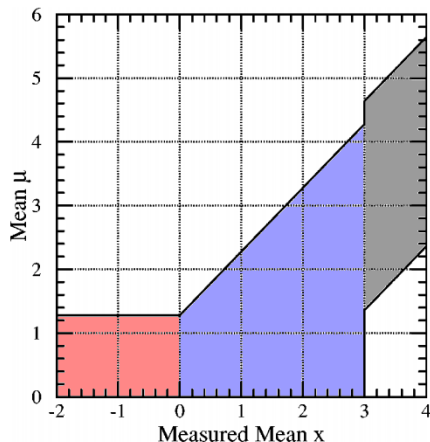
# Flip Flopping



Suppose a physicist measures a quantity  $x$  and decides to publish results about  $\mu$  as follows:

- ▶ If  $x < 0$ , publish an upper limit on  $\mu$  to be “conservative” (red)
- ▶ If the measurement of  $x$  is  $< 3\sigma$ , calculate an upper limit on  $\mu$  (blue)
- ▶ If the measurement of  $x$  is  $\geq 3\sigma$ , calculate a central confidence interval (gray)
- ▶ We say the physicist “flip-flops” between publishing central intervals and upper limits

# The Problem with Flip Flopping



- ▶ Flip-flopping shows up as kinks in the confidence belt. It's a problem because  $\mu$  is undercovered if  $x < 3\sigma$
- ▶ For  $\mu = 2$ , the interval  $[x_1 = 2 - 1.28, x_2 = 2 + 1.64]$  contains only 85% of the probability defined by

$$p(x|\mu) = \frac{1}{\sqrt{2\pi}} \exp \left[ -\frac{(x - \mu)^2}{2} \right]$$

- ▶ Hence, most of the intervals on this plot don't cover  $\mu$  and are not conservative

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# Alternative Methods of Constructing a Confidence Interval

There is quite a bit of freedom in how you can construct a confidence interval, so there are several approaches for how to draw the 90% interval over  $x$  for a fixed  $\mu$ :

- ▶ **Upper or lower limits:** add all  $x$  greater than or less than a given value
- ▶ **Central intervals:** draw a central region with equal probability of  $x$  falling above or below the region
- ▶ **Ranking:** starting from  $x$  which maximizes  $p(x|\mu)$ , keep adding values of  $x$ , ranked by  $p(x|\mu)$ , until the interval contains 90% of the probability

This last ordering scheme is closely related to the so-called **Feldman-Cousins method**, which can be used to get around the flip-flopping problem [2]

# The Feldman-Cousins Method

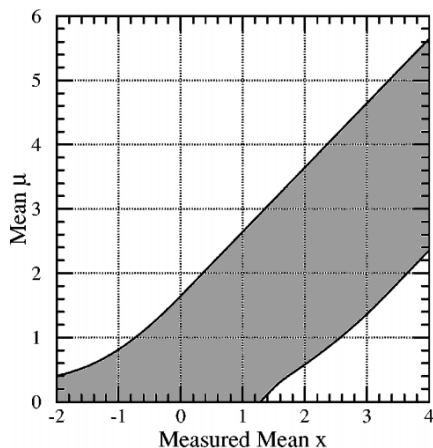
- ▶ For each  $x$ , let  $\hat{\mu}$  be the **physically allowed** value of the mean  $\mu$  which maximizes  $p(x|\mu)$ . I.e.,  $\hat{\mu}$  is the MLE
- ▶ Then calculate the likelihood ratio

$$R = \frac{p(x|\mu)}{p(x|\hat{\mu})}$$

- ▶ For  $\mu$  fixed, add values of  $x$  to the interval from higher to lower  $R$  until the desired probability content is realized, e.g., 90%
- ▶ Gaussian example:  $\hat{\mu} = x$  if  $x \geq 0$  and  $0$  if  $x < 0$ . So

$$R = \frac{p(x|\mu)}{p(x|\hat{\mu})} = \begin{cases} \exp\left[-\frac{(x-\mu)^2}{2}\right] / 1 & x \geq 0 \\ \exp\left[-\frac{(x-\mu)^2}{2}\right] / \exp\left[-\frac{x^2}{2}\right] & x < 0 \end{cases}$$

# A Feldman-Cousins Interval



- ▶ Left: Feldman-Cousins confidence interval for a Gaussian  $\mu$  with a boundary at 0
- ▶ The ratio ensures that the confidence interval is never an empty set
- ▶ There are **no more kinks** in the confidence belt; it transitions smoothly between upper limits and central intervals given a measurement  $x$
- ▶ Procedure: take data and calculate the FC interval. If  $x$  is small, then the method **automatically** returns  $\mu_1 = 0$



# Using Feldman-Cousins Intervals in Practice

Common application: quote a limit on the size of a signal given a known background:

$$p(\mu|b, n_0) = (\mu + b)^{n_0} \exp[-(\mu + b)]/n_0!$$

$n_0 \setminus b$	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

The lookup table for 90% C.L. is reprinted from the Feldman-Cousins paper [2]. For  $b = 4$ , we have to observe at least  $n_0 = 8$  events before  $\mu_1 \neq 0$ . We'd then say that we exclude  $\mu = 0$  at the 90% C.L.

## Remaining Conceptual Problems

Problems remain with the interpretation of data when the number of events are fewer than the expected background

### Example

Experiment 1:  $b = 0, n_0 = 0 \implies \mu \in [0.00, 2.44]$  at 90% C.L.

Experiment 2:  $b = 15, n_0 = 0 \implies \mu \in [0.00, 0.92]$  at 90% C.L.

What's going on here? Experiment 1 worked hard to remove their background. Experiment 2 did not and expected a much higher background.

Neither experiment observed any events, but Experiment 2, by common sense the “worse” of the two experiments, has a **smaller Feldman-Cousins confidence interval** than Experiment 1. Seems pretty unfair, no?

# Don't Confuse Intervals with Posterior Probabilities

- ▶ The origin of the paradox is that it's easy to think of the smaller confidence interval as a **tighter constraint on  $\mu_t$**
- ▶ But that is thinking about the interval as if it is equivalent to

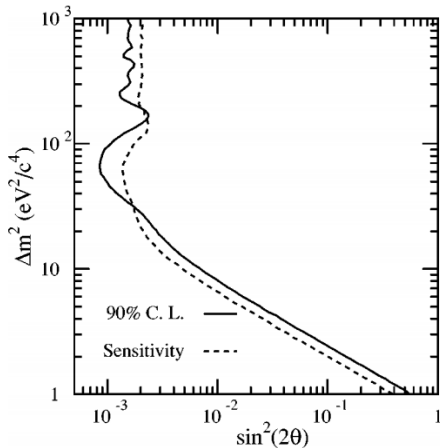
$$p(\mu_t|x_0) = \text{posterior probability of } \mu_t$$

- ▶ Remember, we are calculating  $p(x_0|\mu)$ . I.e.,  **$\mu$  is fixed**. If we need to make an inference about  $\mu_t$ , we should be using a Bayesian framework (according to Feldman and Cousins themselves [2])
- ▶ So why even bother constructing a frequentist interval? Perhaps the question answers itself...
- ▶ If you're interested in the **long-run behavior** of many identical experiments, frequentist intervals are useful. But it's really easy to make basic conceptual mistakes when using them

# Reporting Sensitivity

If  $n_0 < b$ , report the “sensitivity,” the **average upper limit obtained with an ensemble of background-only experiments**, as well as calculated limits [2]

$b$	68.27% C.L.	90% C.L.	95% C.L.	99% C.L.
0.0	1.29	2.44	3.09	4.74
0.5	1.52	2.86	3.59	5.28
1.0	1.82	3.28	4.05	5.79
1.5	2.07	3.62	4.43	6.27
2.0	2.29	3.94	4.76	6.69
2.5	2.45	4.20	5.08	7.11
3.0	2.62	4.42	5.36	7.49
3.5	2.78	4.63	5.62	7.87
4.0	2.91	4.83	5.86	8.18
5.0	3.18	5.18	6.32	8.76
6.0	3.43	5.53	6.75	9.35
7.0	3.63	5.90	7.14	9.82
8.0	3.86	6.18	7.49	10.27
9.0	4.03	6.49	7.81	10.69
10.0	4.20	6.76	8.13	11.09
11.0	4.42	7.02	8.45	11.46
12.0	4.56	7.28	8.72	11.83
13.0	4.71	7.51	9.01	12.22
14.0	4.87	7.75	9.27	12.56
15.0	5.03	7.99	9.54	12.90



# Reporting Sensitivity

Back to the example:

## Example

Experiment 1:  $b = 0, n_0 = 0 \implies \mu \in [0.00, 2.44]$  at 90% C.L. The sensitivity is **2.44** at 90% C.L.

Experiment 2:  $b = 15, n_0 = 0 \implies \mu \in [0.00, 0.92]$  at 90% C.L. The sensitivity is **4.83** at 90% C.L.

The upper limit from Experiment 2 (0.92) is **much smaller than its sensitivity** (4.83), implying that the experiment benefitted from a huge and rather unlikely downward fluctuation in  $n_0$ .

Fluctuations happen, even into non-physical regions (remember the  $m^2$  example). Frequentists have to publish these fluctuations no matter what since the results from many experiments is of interest. Failure to do so will **bias meta-analyses** of the literature

## Summary

Constructing a frequentist confidence interval means that you identify some confidence level  $\alpha$  and then **build a set**  $[\mu_1, \mu_2]$  that has probability  $\alpha$  of containing  $\mu_t$ . Unfortunately:

- ▶ Sometimes the confidence interval is an empty set
- ▶ Intervals have kinks if you flip-flop between upper limits and central measurements
- ▶ You can't simply cut data in unphysical regions

If your data imply an unphysical result, too bad; you ran one of the  $1 - \alpha$  fraction of experiments with an interval that doesn't contain  $\mu_t$ .

The Feldman-Cousins method exploits the fact that you can construct a Neyman interval in several ways. **Ranking  $x$  by its likelihood ratio** allows you to fix some of the pathologies in interval construction

# References I

- [1] Glen Cowan. *Statistical Data Analysis*. New York: Oxford University Press, 1998.
- [2] Gary J. Feldman and Robert D. Cousins. “A Unified approach to the classical statistical analysis of small signals”. In: *Phys.Rev. D57* (1998), pp. 3873–3889. arXiv: [physics/9711021](https://arxiv.org/abs/physics/9711021) [[physics.data-an](https://arxiv.org/abs/physics/9711021)].