Statistics Intro

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Introduction

These slides provide an overview of the kind of statistics we use in **`combine`** and are not an exhaustive list of statistics methods used in CMS or HEP

These form an introduction to

- **Likelihoods**
  - Parameters of interest and nuisance parameters
  - Profiling and marginalisation
- **Hypothesis testing**
  - Bayesian (credible) and Frequentist (confidence) intervals
  - Discovery test statistics
  - Asymptotic formulas

For more complete introductory guides to statistics (in HEP), you can refer, for example, to the following reading list…

- G. Cowan, “Probability/Statistics" (ch. 38 & 39) in "Review of particle physics", Chin. Phys. C 40, 100001 (2016)
- R.J. Barlow, Statistics: A Guide to the Use of Statistical Methods in the Physical Sciences (Manchester Physics Series, 1989)
- L. Lyons, N. Wardle, “Statistical issues in searches for new phenomena in High Energy Physics”, Journal of Physics G Nuclear and Particle Physics 45(3), (2018)
- R. Cousins, “Lectures on Statistics in Theory: Prelude to Statistics in Practice”, arXiv:1807.05996
- G. Cowan, Statistical Data Analysis, (Oxford University Press, Oxford, 1998)
- L. Lyons: Statistics for Nuclear and Particle Physicists, (Cambridge University Press, New York, 1986)
- George Casella and Roger L. Berger, "Statistical inference," 2nd ed., Duxbury, 2002

And the CMS Statistics Committee pages: https://twiki.cern.ch/twiki/bin/view/CMS/StatisticsCommittee

Likelihoods

The generic **likelihood** we use in combine is defined as

$$\mathcal{L}(\vec{\alpha}) \sim p(data|\vec{\alpha})$$

$\vec{\alpha}$ are the **parameters** of the likelihood

$p(data|\vec{\alpha})$ is the **probability to observe the data**, for a particular value of $\vec{\alpha}$

Likelihoods

The generic **likelihood** we use in combine is defined as

$$\mathcal{L}(\vec{\alpha}) \sim p(data|\vec{\alpha})$$

It's worth noting two things

- The likelihood function is defined by ***fixing the data*** - that is, it takes different values for different outcomes

- The likelihood is ***not a probability*** - there are various normalisation terms which we ignore throughout

Likelihoods

Often we want to separate parameters which are physics parameters of interest (POI = $\vec{\mu}$) vs uninteresting parameters (NP = $\vec{\theta}$)

$$\vec{\alpha} = \left(\vec{\mu}, \vec{\theta}\right)$$

Typically (though certainly not always!) the nuisance parameters are constrained by some external measurements (eg Jet energy scales) - we introduce ***constraint terms***

$$\pi(\vec{\theta}_0|\vec{\theta}) \sim p(\vec{\theta}|\vec{\theta}_0)$$

where again, we introduce some observed (or measured) values $\vec{\theta}_0$ to relate π to the probability to observe that outcome some value of the NPs

Likelihoods

So then we have

$$\mathcal{L}(\vec{\mu}, \vec{\theta}) \sim p(data|\vec{\mu}, \vec{\theta}) \cdot \pi(\vec{\theta}_0|\vec{\theta})$$

Let's look at a very simple setup with 1 parameter of interest μ, and one nuisance parameter θ

Imagine we had an analysis which, after making some cuts, just counts the number of events left over in pp collisions (a ***cut-and-count*** analysis).

Our "*data*" in this case is just the observed number of events n, and the probability term is just a ***Poisson probability***

$$p(n|\lambda) = \frac{\lambda^n e^{-\lambda}}{n!}$$

Likelihoods

Often, we want to determine some total cross-section for production of these events which populate our selection. Typically we have some reference theory (eg the SM) in mind which predicts a value σ for this cross-section. Our POI then would be the cross-section, relative to that prediction - i.e

$$\lambda = \mu \cdot \sigma(pp \rightarrow X) \cdot \varepsilon \cdot A \cdot L$$

$\mathcal{E}$ - The efficiency of our selection

A - The acceptance of the detector

L - The integrated luminosity of our dataset

Likelihoods

L - The integrated luminosity of our dataset

Any of these terms could have “uncertainties” associated to them. We can model this uncertainty by introducing nuisance parameters Eg.

Say, the luminosity is known to 10%*. We could think of this as saying the rate of events could increase by 10% (x1.1) or decrease by 10% (1/1.1)

$$L \rightarrow L(1+0.1)^{\theta}$$

When θ=0, we recover the nominal value
We identify $\theta = \pm 1$ as + or -1 sigma uncertainty so…

$$\pi(\theta) = e^{-\frac{1}{2}\theta^2}$$

*Clearly we usually know the luminosity better than this

Likelihoods

L - The integrated luminosity of our dataset

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This is known as a ***log-normal**** distributed nuisance parameter

$$\pi(\theta) = e^{-\frac{1}{2}\theta^2}$$

*Clearly we usually know the luminosity better than this

this is a very common, but ***not the only* distribution we use

Likelihoods

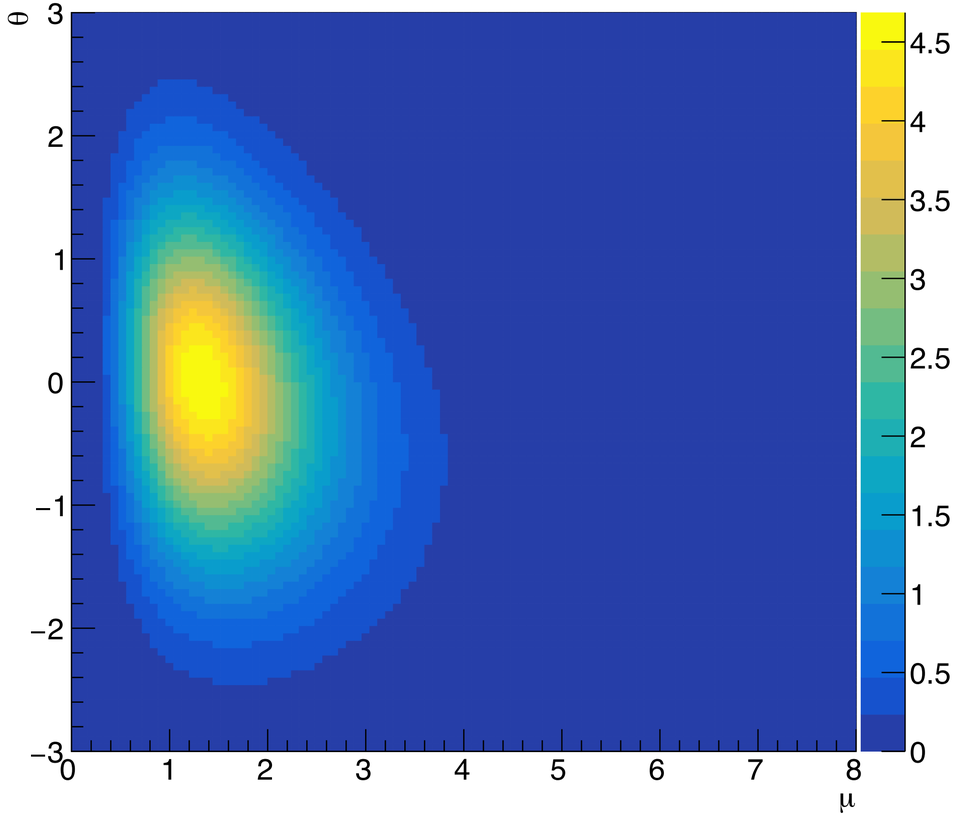
The likelihood is then $\mathcal{L}(\mu,\theta) = \lambda^n(\mu,\theta)e^{-\lambda(\mu,\theta)} \cdot e^{-\frac{1}{2}\theta^2}$

With $\lambda^n(\mu,\theta) = \mu\sigma(pp \to X)\varepsilon AL(1.1)^\theta$

Suppose in our experimental setup
A = 0.2, ε = 0.5, L = 30 fb^{-1} , σ = 1 fb

And we observe n = 4 events,
then our likelihood will look like …

You can see that the maximum of the likelihood is found at $\mu \sim 1.33$, θ = 0



*Clearly we usually know the luminosity better than this

Likelihoods

Notice that the maximum value of the likelihood doesn't mean anything

- Its > 1 so it cannot be a "probability"
- It's somewhat arbitrary - I could have included a normalisation term in $\pi(\theta)$ without changing the values of μ or θ at which the maximum of the likelihood is found

Instead, the relative values of likelihoods are useful (we will see why soon)

Also in general, we often have many more than one observation (eg multiple bins in a histogram, or unbinned data). These are simple to deal with by using the product rule for probability …

Multiple bins: $$p \to \prod_i p_i = \frac{\lambda_i^{n_i} e^{-\lambda_i}}{n_i!}$$

Unbinned: $$p \to \prod_i \int_{x_i}^{x_i+\delta x_i} f(x_i)dx \xrightarrow[\delta x_i \to 0]{} \prod_i f(x_i)\delta x_i = \prod_i f(x_i)$$

Where $f(x)$ is the probability density function for *x* and we have used the fact that the data is fixed to ignore the δx_i

Likelihoods

In general, we would also have many more than 1 nuisance parameter (usually, there is one per source of systematic uncertainty). In these cases, reporting the N-dim likelihood is not feasible and not interesting.

Instead, we tend to remove the nuisance parameters from the likelihood by one of two methods

Marginalisation or ***Profiling***

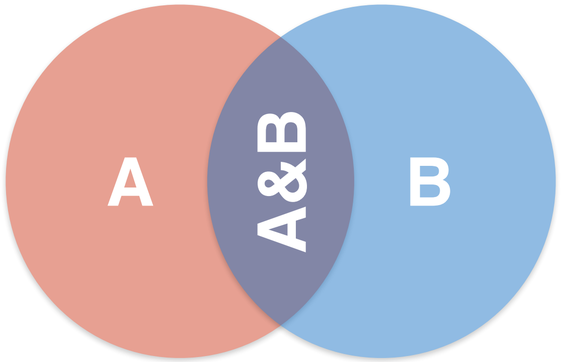
The two are often synonymous with **Bayesian** vs **Frequentist** methods

- We won't go into the long debate about which is better/worse/right/wrong etc, but rather just review the techniques we use in combine which are one or the other….

Marginalisation

Recall Bayes' theorem

$$p(A|B) = \frac{p(B|A)p(A)}{p(B)}$$



For our purposes, we can write this as

$$p(\mu|data) = \int \frac{p(data|\mu,\theta)p(\theta)p(\mu)}{p(data)} d\theta$$

since $p(\mu|data) = \int p(data|\mu,\theta)p(\theta)d\theta$, by the probability sum rule. $p(\mu|data)$ is know as the posterior probability of μ

Notice how the **likelihood** has appeared in the definition of the posterior!

Marginalisation

We have also introduced $p(\mu)$, the "***prior***" on μ.

$$p(\mu|data) = \int \frac{p(data|\mu,\theta)p(\theta)p(\mu)}{p(data)} d\theta$$

This is something we need to choose* - for now, lets assume a "flat prior" such that

$$p(\mu) = \begin{cases} 1/20 & \text{if } 0 \leq \mu \leq 20 \\ 0 & \text{if else} \end{cases}$$

Finally $p(data) = \int p(\mu|data)d\mu$ is just a normalisation term.

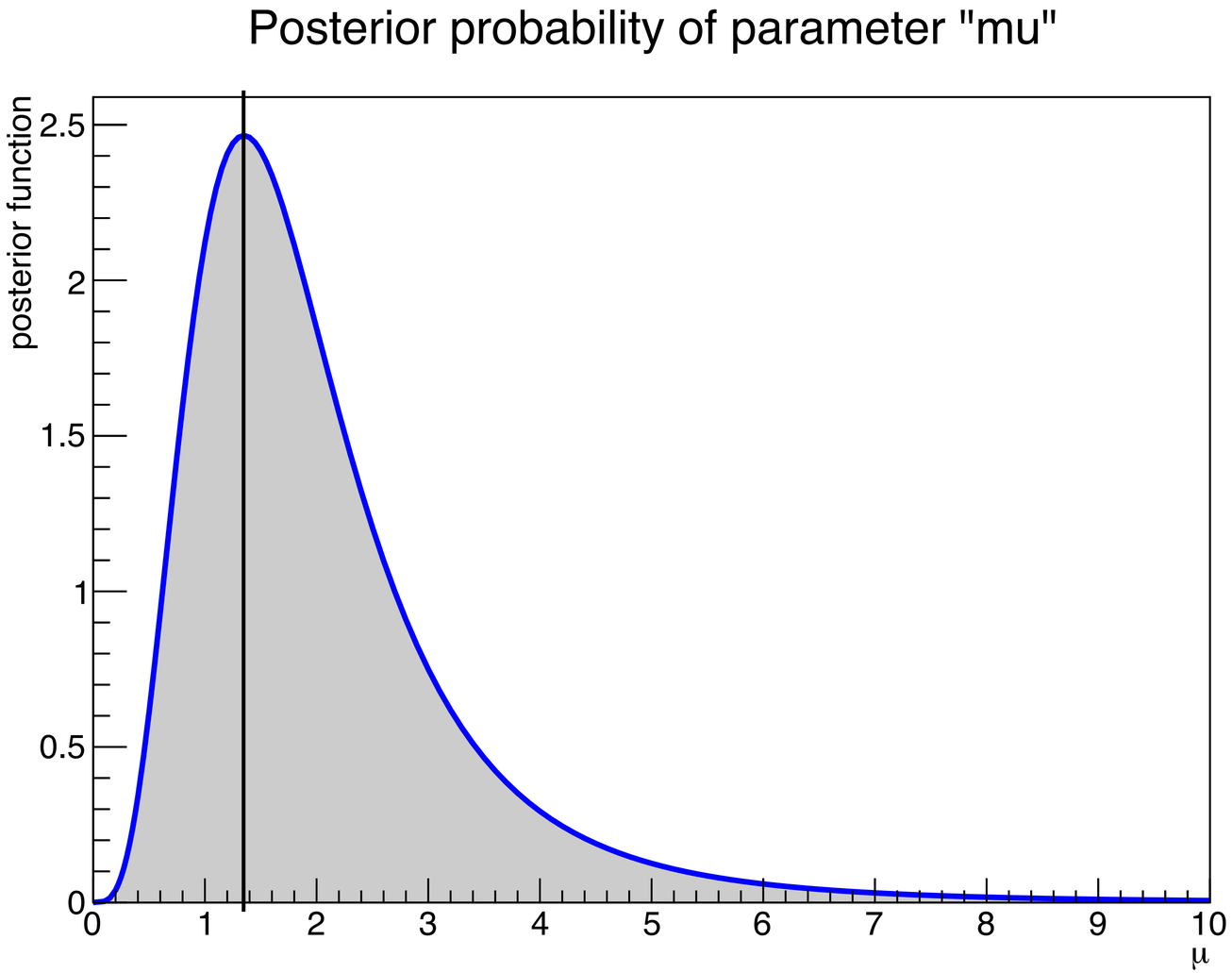
*The dependance of the results on this choice is something which must be checked in each analysis

Marginalisation

For our cut-and-count analysis, the posterior looks like …

The value of μ which is the most common is ~1.333!

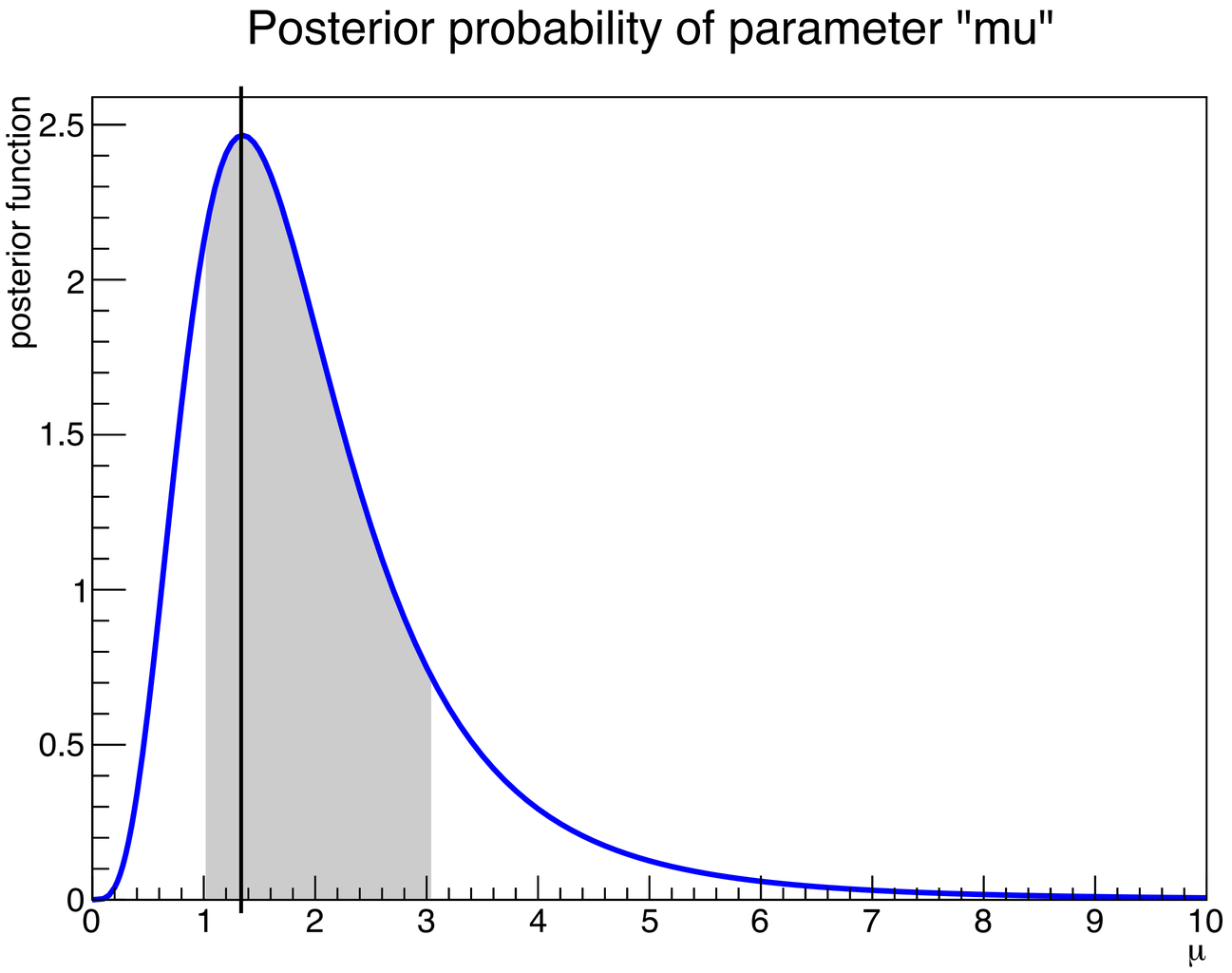
In this case, this is the same as the value which gave us the maximum likelihood value, when $\theta = 0$



Marginalisation

We could also ask which region contains 68% of the posterior distribution. This is known as a ***68% credible interval***

This is just one such example and another choice to be made is ***which*** such interval should be reported



Profiling

The other common method to remove nuisance parameters from the likelihood function is to find the value for θ which maximises the likelihood at each value of μ. This is known as ***profiling*** over the nuisance parameters

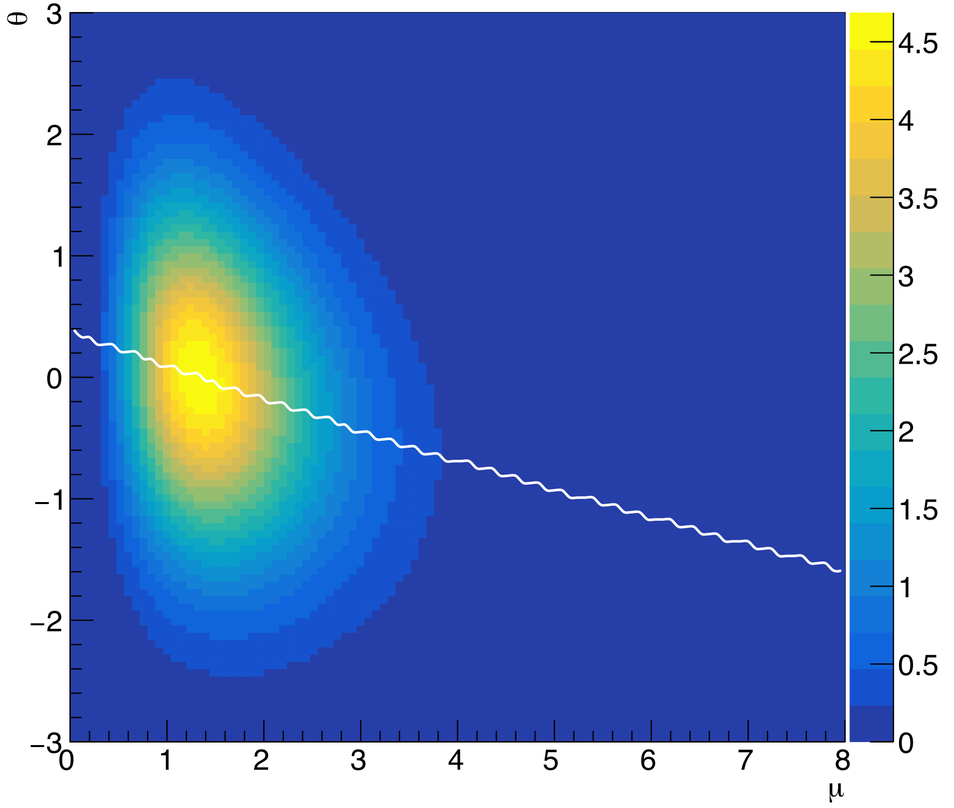
Taking our likelihood function, we can draw the line $\hat{\theta}(\mu)$, for which $\mathcal{L}(\mu, \theta)$ is maximum

The value of $\mathcal{L}(\mu, \theta)$, along this line is the "profiled likelihood"

$$\mathcal{L}(\mu, \theta) \rightarrow \mathcal{L}(\mu, \hat{\theta}(\mu)) := \max_{\theta} \mathcal{L}(\mu, \theta)$$

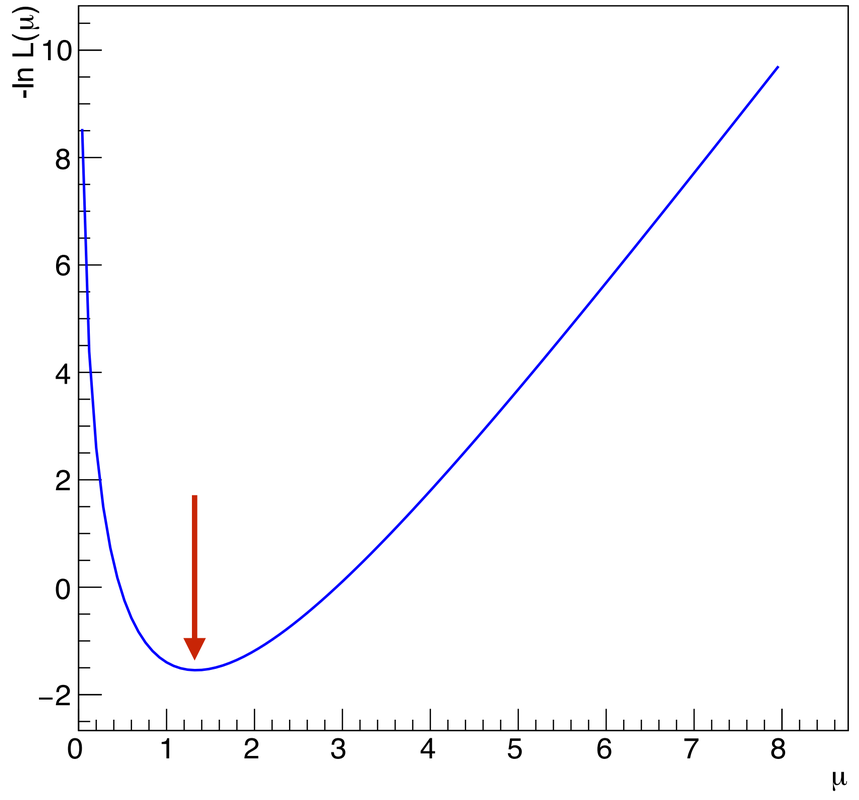
Or dropping, implicit dependencies,

$$\mathcal{L}(\mu, \theta) \rightarrow \mathcal{L}(\mu)$$



Profiling

Very often, to avoid dealing with small or large values of likelihoods (in this simple case it doesn't matter, but if we had many bins, the products can get quite small), we take negative logs of the likelihood —> maximum likelihood = ***minimum negative log likelihood***



$$\mathcal{L}(\mu) \rightarrow -\ln \mathcal{L}(\mu)$$

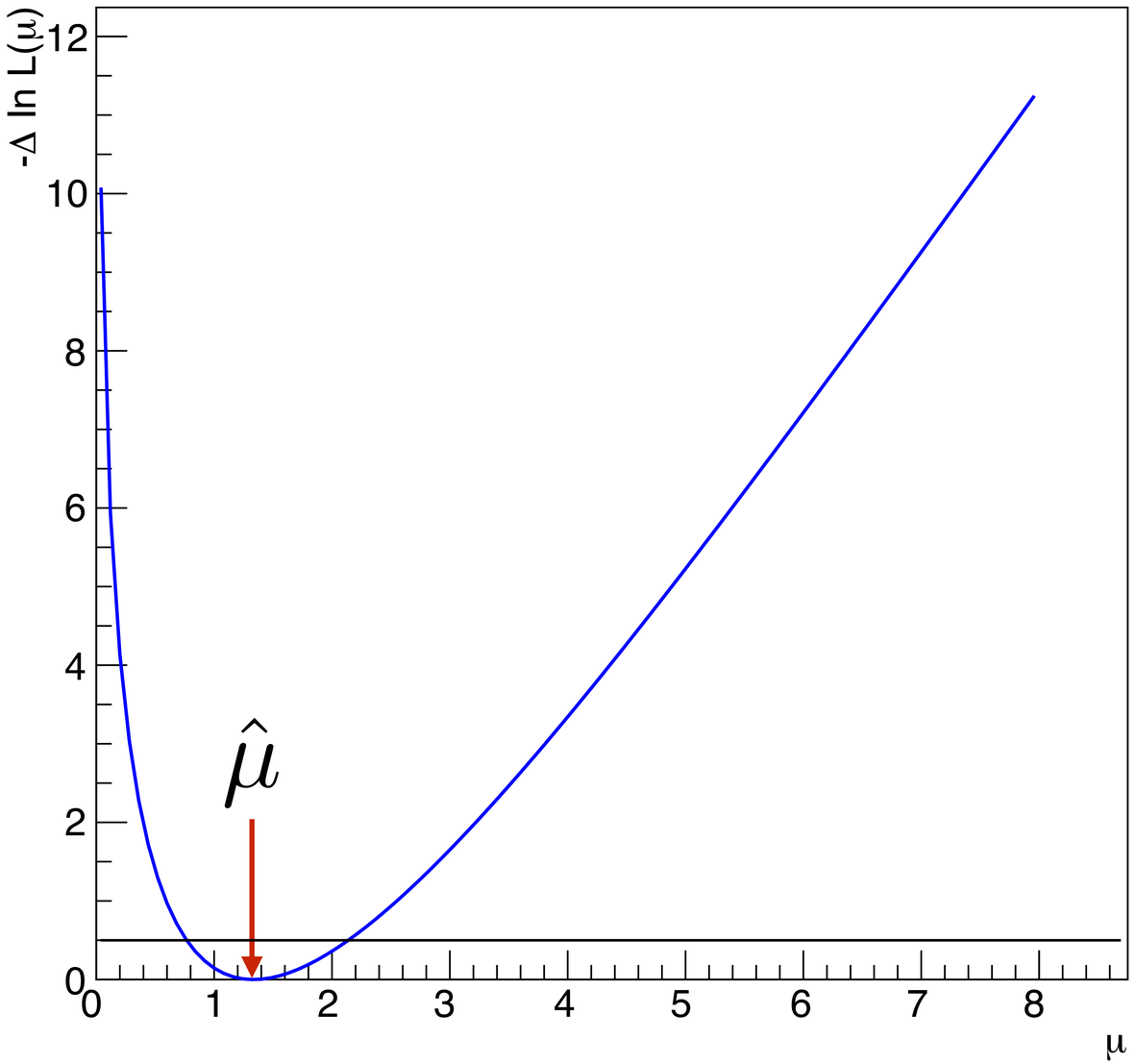
The minimum value of this curve is at $\hat{\mu}$ = 1.333!*

We often normalise this curve by subtracting the value at this minimum

$$-\ln \mathcal{L}(\mu) \rightarrow -\ln \mathcal{L}(\mu) - (-\mathcal{L}(\hat{\mu})) = -\Delta \ln \mathcal{L}(\mu)$$

* again the ^ notation indicates the value at which the likelihood (-ve log likelihood) is maximised (minimised)

Profiling



Wilkes' theorem* tells us that we can obtain a 68% confidence interval from the region for which

$$-\Delta \ln \mathcal{L}(\mu) < 0.5$$

Which we will call the "**minos**" method

What does that mean exactly?

*I won't go through why but think about taylor expanding the log-likelihood around the minimum

Frequentist intervals

So far, we have seen two methods for determining the value of the POI and ascribing a 68% confidence or credible interval

- For Bayesian thinkers, the 68% credible interval represents the probability that the parameter μ is in a certain region, given that we observed n=4 events.

- For frequentist thinkers, the interval we constructed was just one of many possibilities depending on the observation n. There is a little more work in defining what this interval means.

We can introduce the concept of ***coverage .***

"*When a 68% confidence interval has **good coverage** it means that 68% of intervals constructed in such a way will contain the **true** value of the POI.*"

This should hold regardless of the true value of the POI*. It is ***not*** a statement about the specific interval we constructed but rather a statement about the ***ensemble*** of intervals!

*And should also be true for any reasonable values of the nuisance parameters, but this is a subtlety which should be checked to hold

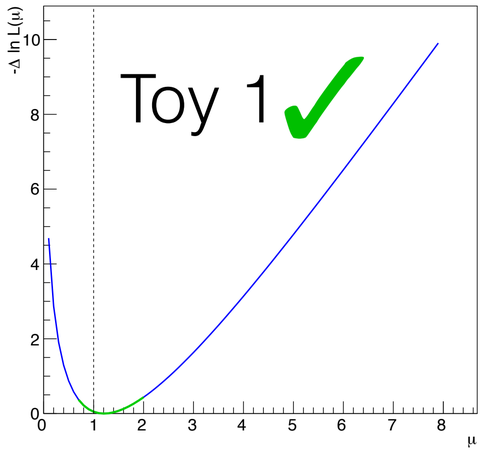
Frequentist intervals

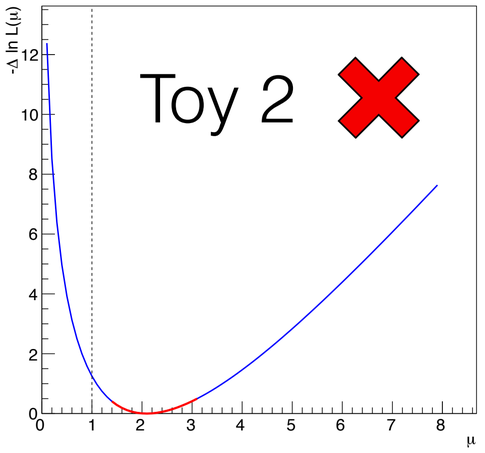
Let's suppose our true value of $\mu = 1$.

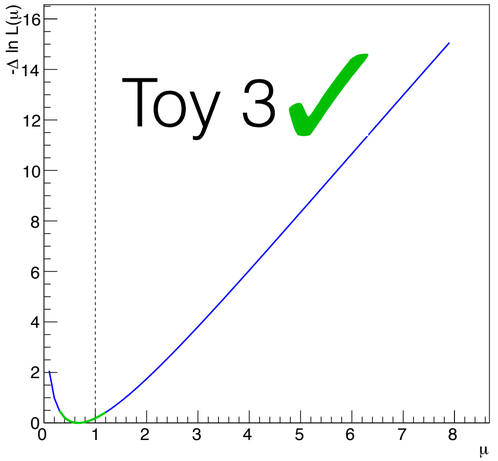
We can generate outcomes for n and for θ_0

- Remember that $\theta_0 = 0$ was the value we observed in our 1 measurement. We could imagine measuring other values, generated from $\pi(\theta_0|\theta)$
- We need to pick a value for θ to generate from however. The most obvious choice* would be $\hat{\theta}(\mu = 1) = 0.09$

For each generation (toy) we determine the 68% confidence interval and determine whether or not 1 is contained in the interval…



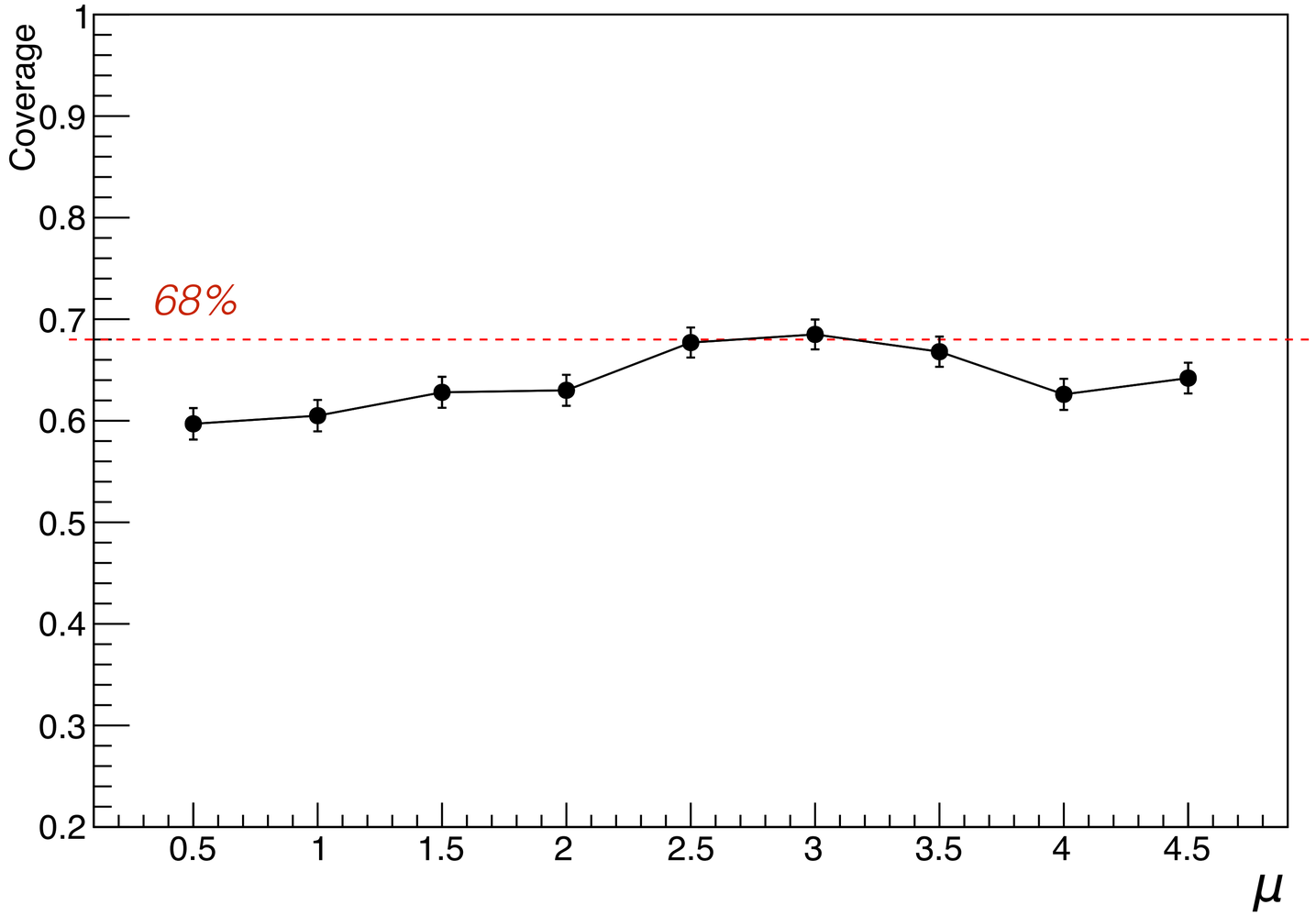




*Again, this is common practise, but we should check that the coverage property doesn't depend on this choice!

Frequentist intervals

What is the coverage as a function of μ ?



The intervals undercover for smaller values of μ .

This is not so surprising since Wilkes' theorem assumes the likelihood follows a Gaussian distribution.

This becomes more appropriate for large values of n but is less accurate when n is small

Frequentist intervals

We can do better using a Neyman construction…

1. Pick a true value of $\mu = \mu_T$, (set θ_0 to the value which maximises the original likelihood defined at $\mu = \mu_T$)
2. Generate toy values for n and θ_0 (for generating, again set θ to the value which maximises the original likelihood defined at $\mu = \mu_T$)
3. Evaluate $q = -\Delta \ln \mathcal{L}(\mu_T)$ (this is called a test-statistic) for each toy and enter into a histogram* -> $f(q)$

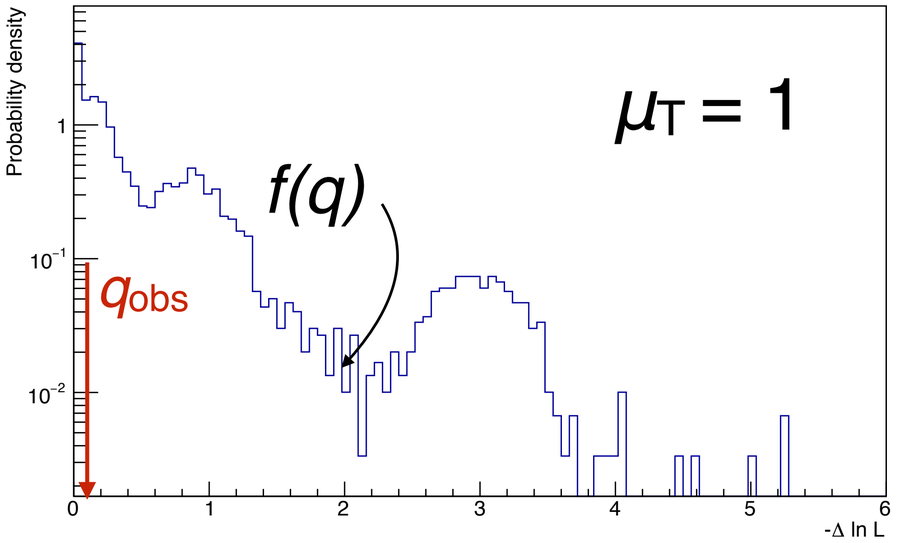
4. Calculate $p = \int_{q_{\rm obs}}^{+\infty} f(q) dq$ where $q_{\rm obs}$ is the value of q for the ***observed data***

5. If $p < 1 - 0.68$, then μ_T is in the 68% confidence interval, otherwise, its not
6. Start at 1. and repeat for another value of μ_T

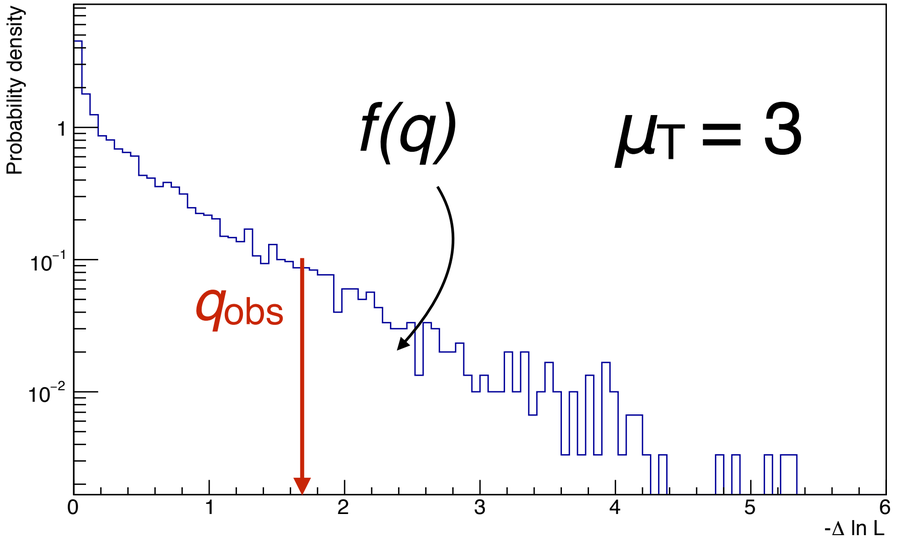
*note that in general, you need to choose an ordering principle for the outcomes, here we have used the Feldman-Cousins approach

Frequentist intervals

For a small value $\mu_T = 1$ (which means λ~3), we see the discrete nature of the Poisson probability appear in the distribution of q

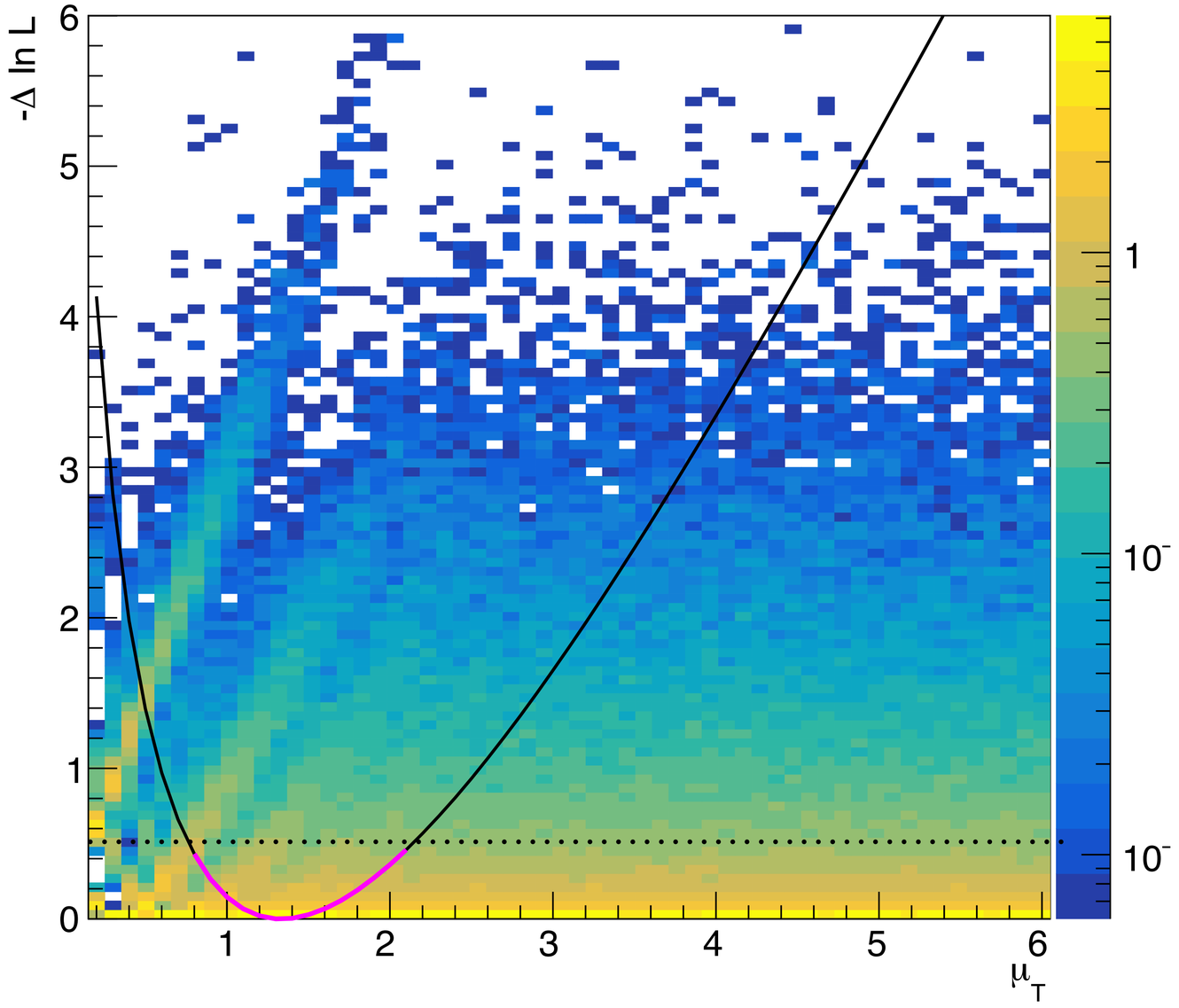


For large values $\mu_T = 3$ (which means λ~9) we see that the Poisson smooths out and the distribution of q looks like a χ^2 function with 1 degree of freedom. This is Wilkes' theorem kicking in !



Notice that the value of q_{obs} changes depending on μ. Of course, this is expected for our choice of procedure (test-statistic)

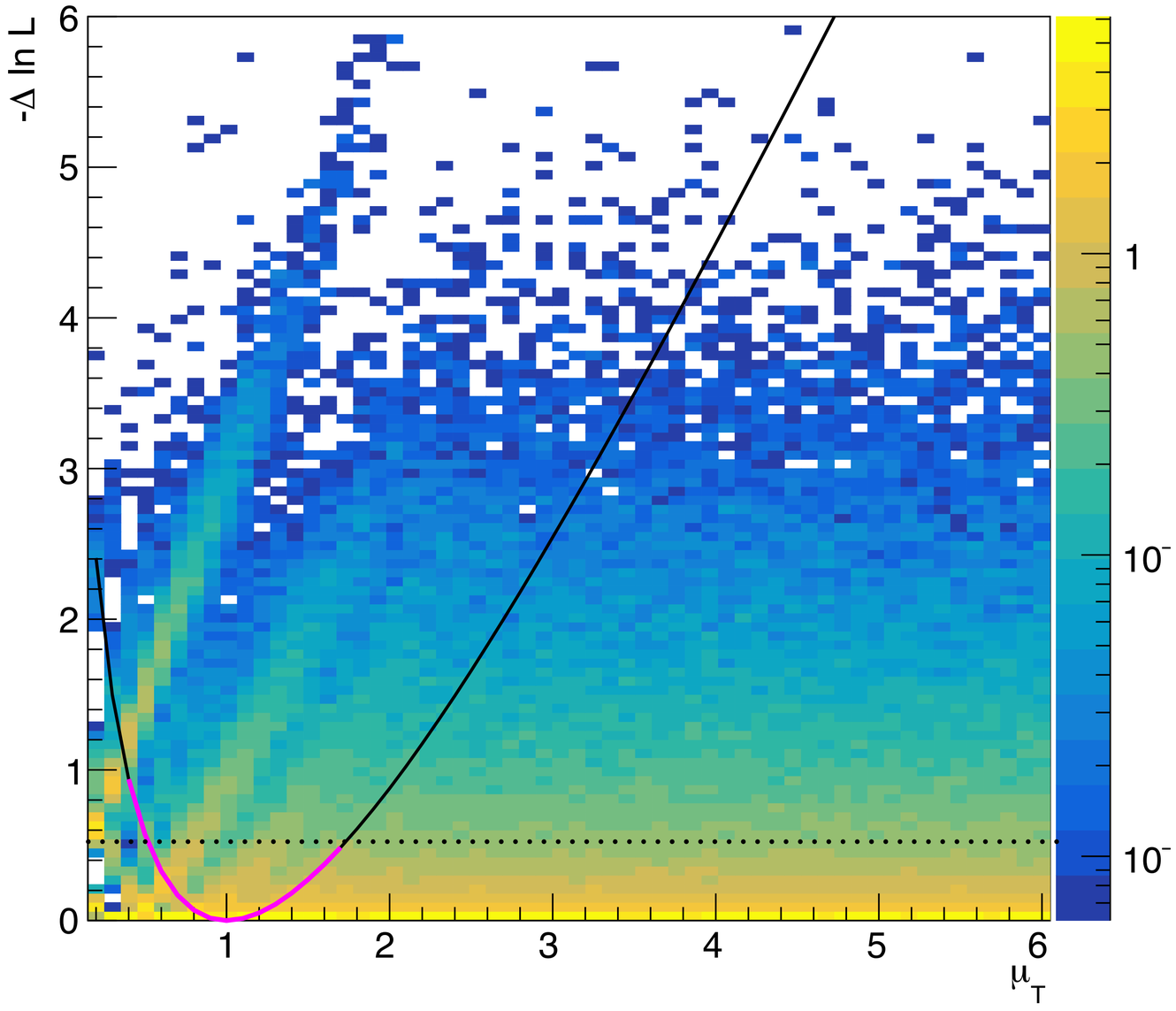
Frequentist intervals



The magenta curve shows the points for which $p < 1 - 0.68$, i.e the 68% confidence interval given our observation.

You can see its actually not so far off from what we got using the minos method which would just pick points for which q < 0.5

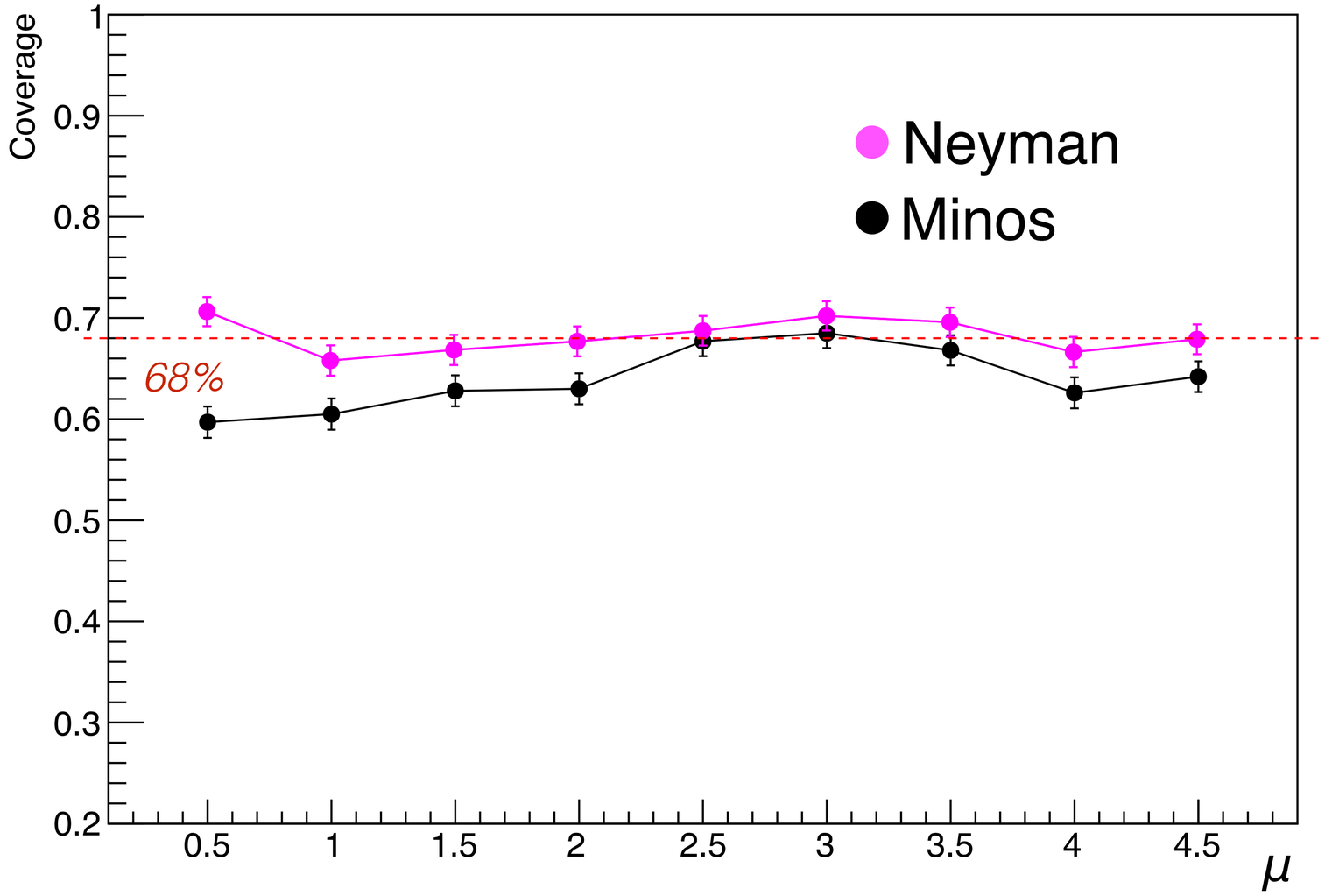
Frequentist intervals



This is not always the case however. In this example the interval is wider than what we would have gotten from the minos method!

Frequentist intervals

What is the coverage as a function of μ ?



The Neyman construction indeed does better in terms of coverage (by design) but of course it is more computationally intensive to run.

Frequentist intervals

Both Bayesian ***credible intervals*** and frequentist ***confidence intervals*** can be used as hypothesis tests.

Very simply - "*if a parameter value is not contained in the interval, that hypothesis is excluded*"

However, in practise, we often perform hypothesis tests slightly differently depending on what we are testing (eg discovery vs limits) and whether or not the hypotheses are nested (eg specified by a continuous parameter μ , or discrete, eg - Spin-0 vs Spin-2)

The next few slides are a quick run through of limit setting and discovery statistics that we use at CMS

Calculating Limits - Frequentist

Remember that in HEP, we commonly use the CLs criterion for exclusion…

The null hypothesis (signal + background in the exclusion case) is excluded at 95% CL when CLs = CLs+b/CLb <= **0.05 ,** where CLs+b is

$$p_\mu \;=\; P(\,\tilde{q}_\mu \geq \tilde{q}_\mu^{obs}\,|\,\text{signal+background}) \;=\; \int_{\tilde{q}_\mu^{\text{obs}}}^{\infty} f(\tilde{q}_\mu|\mu,\hat{\theta}_\mu^{\text{obs}})\,d\tilde{q}_\mu$$

and CLb is

$$1-p_b \;=\; P(\,\tilde{q}_\mu \geq \tilde{q}_\mu^{obs}\,|\,\text{background-only}) \;=\; \int_{q_0^{\text{obs}}}^{\infty} f(\tilde{q}_\mu|0,\hat{\theta}_0^{\text{obs}})\,d\tilde{q}_\mu$$

for some test statistic $\boldsymbol{q_\mu}$

Calculating Limits - Frequentist

At the LHC, we use the following definition of q_r ($== q_\mu$)

$$q_r = -2\ln[\mathcal{L}(\text{data}|r, \hat{\theta}_r)/\mathcal{L}(\text{data}|r = \hat{r}, \hat{\theta}])$$

where we also set $q_r = 0$ if $\hat{r} > r$

$$q_r = -2\ln[\mathcal{L}(\text{data}|r, \hat{\theta}_r)/\mathcal{L}(\text{data}|r = 0, \hat{\theta}_0)$$ if $\hat{r} < 0$

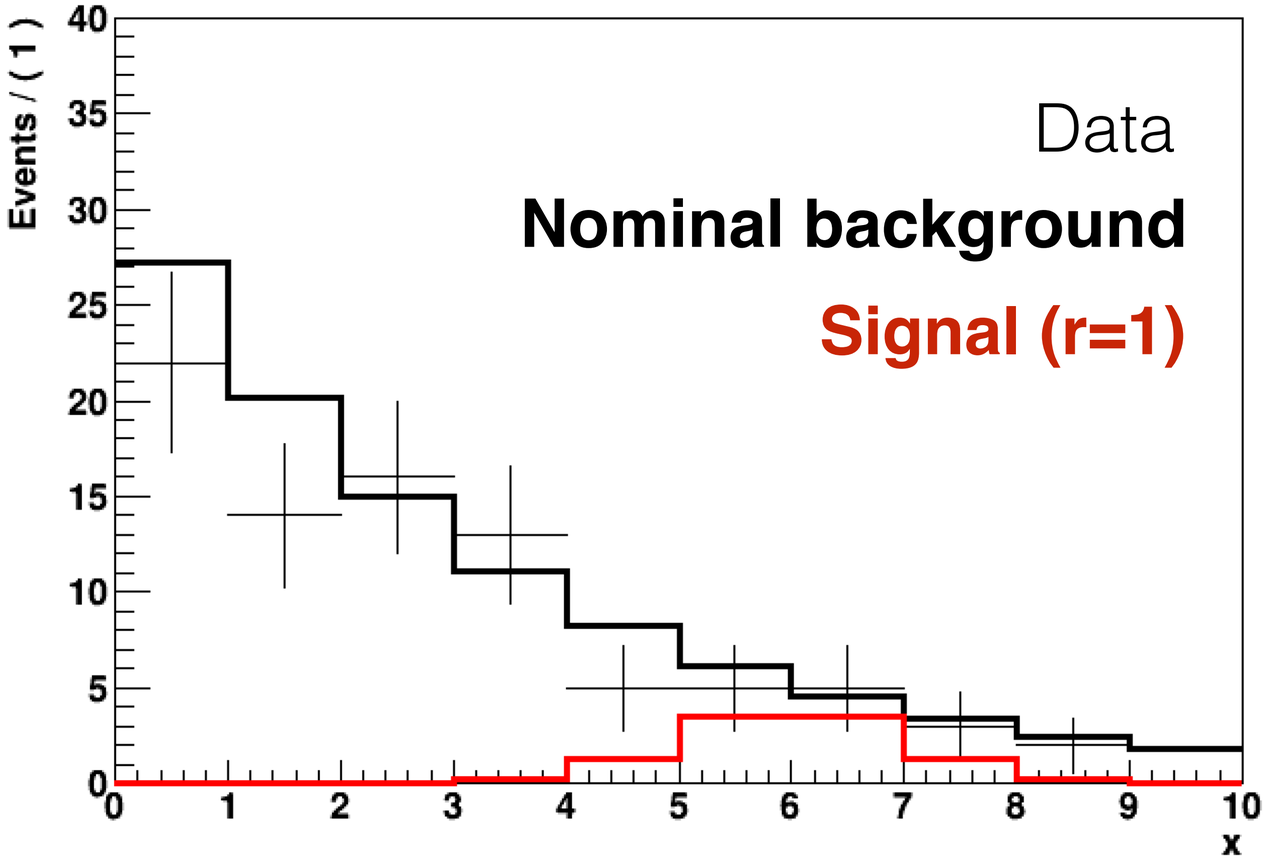
Remember that the ^ notation means, “maximum likelihood estimator”, so this test-statistic requires 2 fits, one for a fixed value of “*r*” and one floating it.

Calculating Limits - Frequentist

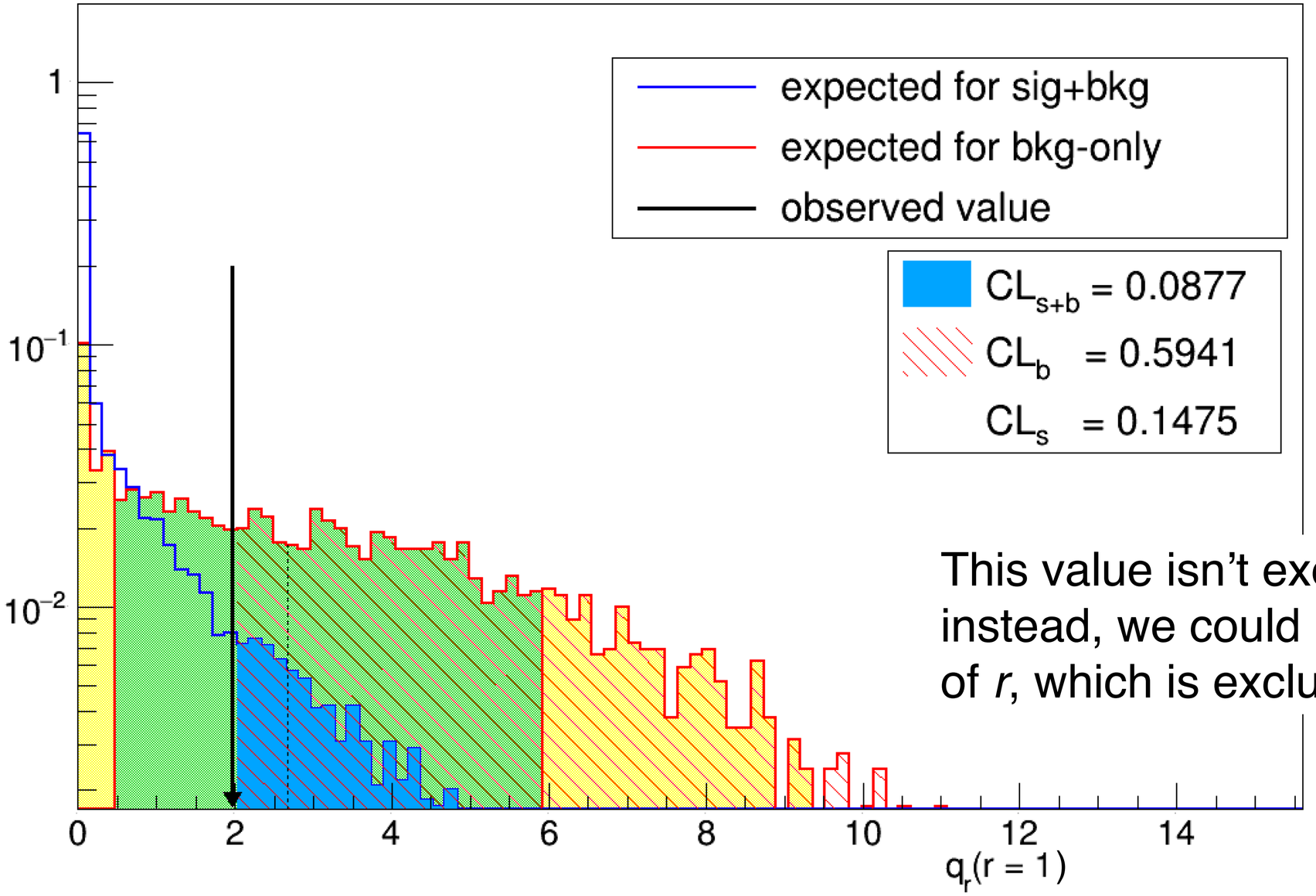
Take a multi-binned analysis

This time we have two contributing processes, the signal and the background. Only the signal will scale with the POI “*r*”

We can calculate the value of CLs for r=1. If CLs is < 0.05, then we can say the signal is excluded (at the predicted rate) at the 95% CL

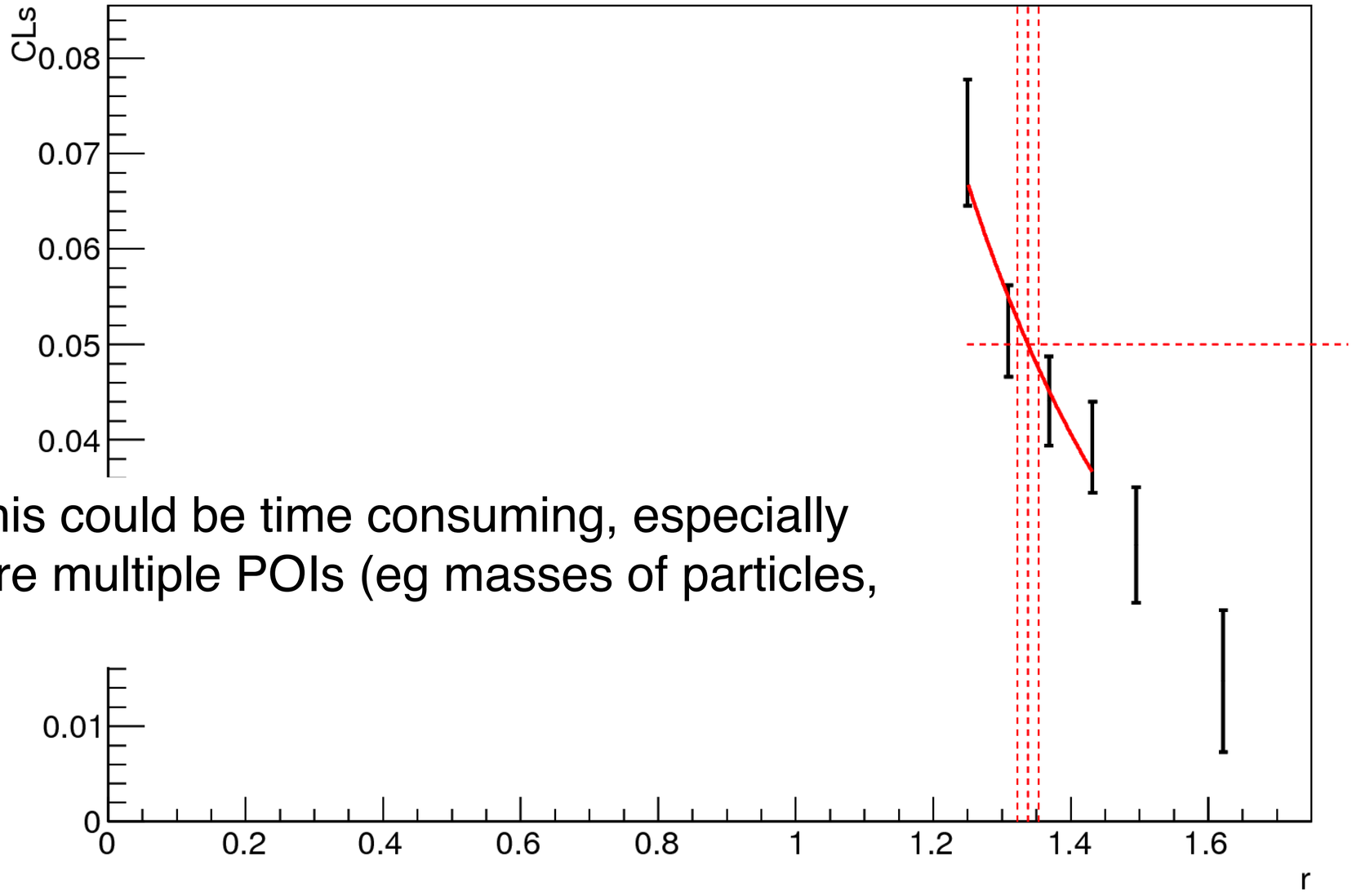


Calculating Limits - Frequentist



This value isn't excluded at the 95% CL, instead, we could look for the smallest value of *r*, which is excluded at the 95% CL

Calculating Limits - Frequentist



Clearly this could be time consuming, especially if there are multiple POIs (eg masses of particles, etc…)

Significances

Similarly, for discovery, we want to ***exclude*** the background only hypothesis.

We can define a similar test-statistic

$$q_0 = -2 \ln \frac{L(r = 0, \hat{\boldsymbol{\theta}}_0)}{L(\hat{r}, \hat{\boldsymbol{\theta}})}$$

And set $q_0 = 0$ when $\hat{r} < 0$

The p-value for rejecting the background hypothesis (r=0) is defined as

$$P_0 = \int_{q_0^{obs}}^{+\inf} f(q_0|r = 0) dq_0$$

For discovery we usually want $P_0 = 0.287 \times 10^{-6}$ (5σ!). Again, this will take a lot of computation with toys to fill the tails of the distributions

Asymptotics

Fortunately, when we use the profile likelihood (the LHC style), we get some nice properties, namely if the distribution of the estimator of the signal strength ($\hat{\mu}$ = best fit)

$$-2\Delta \ln \mathcal{L}(\mu) = \frac{(\mu - \hat{\mu})^2}{\sigma_\mu^2} + \mathcal{O}(1/\sqrt{N})$$

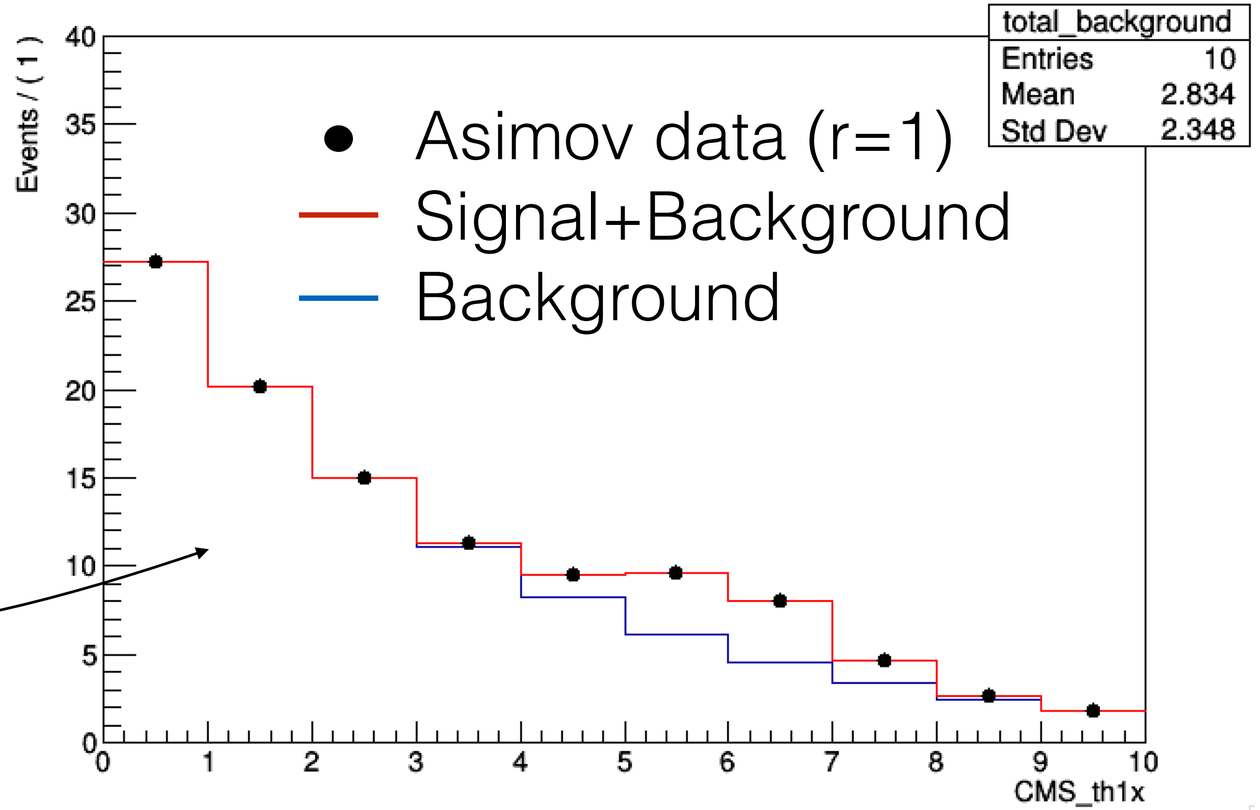
Meaning we can determine the distribution of the test-statistics in the "Asymptotic limit" * (large events in the poisson terms ***and*** lots of small nuisances)

* https://arxiv.org/pdf/1007.1727.pdf

Asymptotics

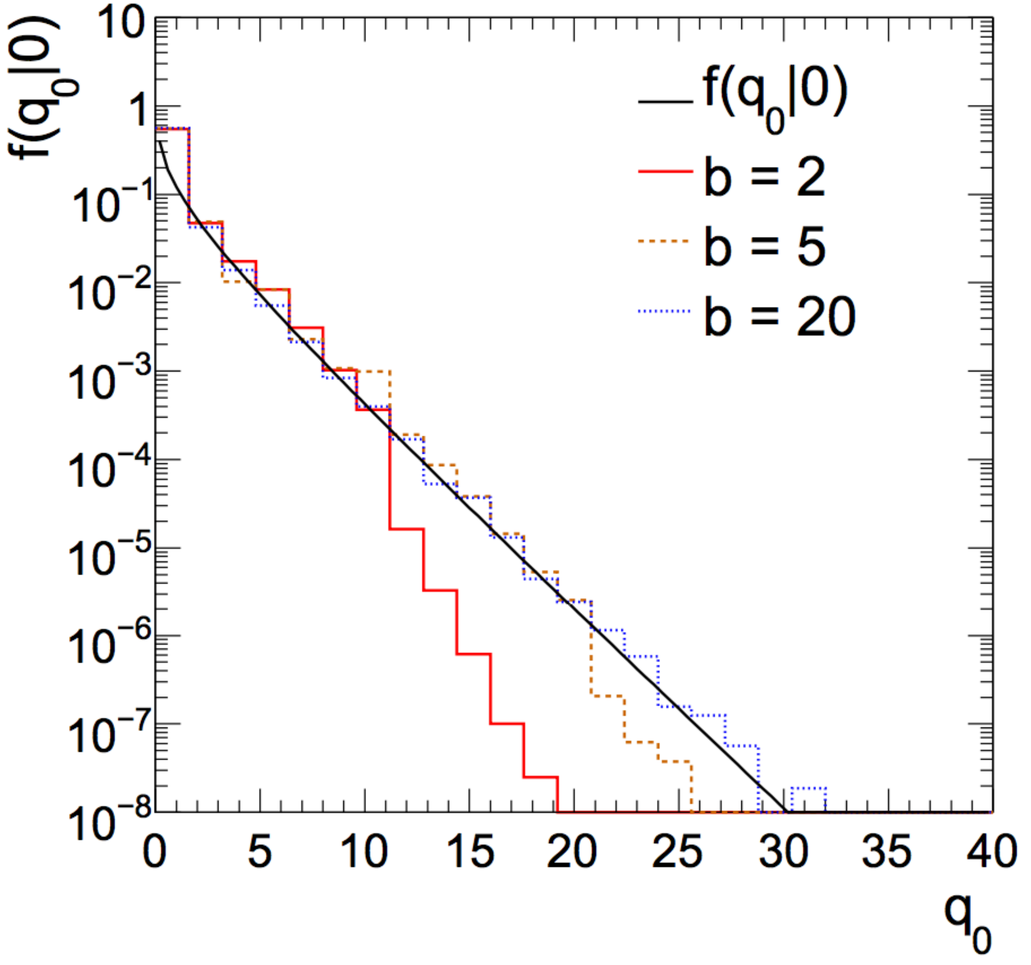
The formula make use of the Asimov dataset (to estimate σ/μ), a dataset constructed from the maximum likelihood estimates (^ values) of the POIs (and nuisances), with statistical fluctuations suppressed

Example, for a multi-binned analysis, with the Asimov for r=1

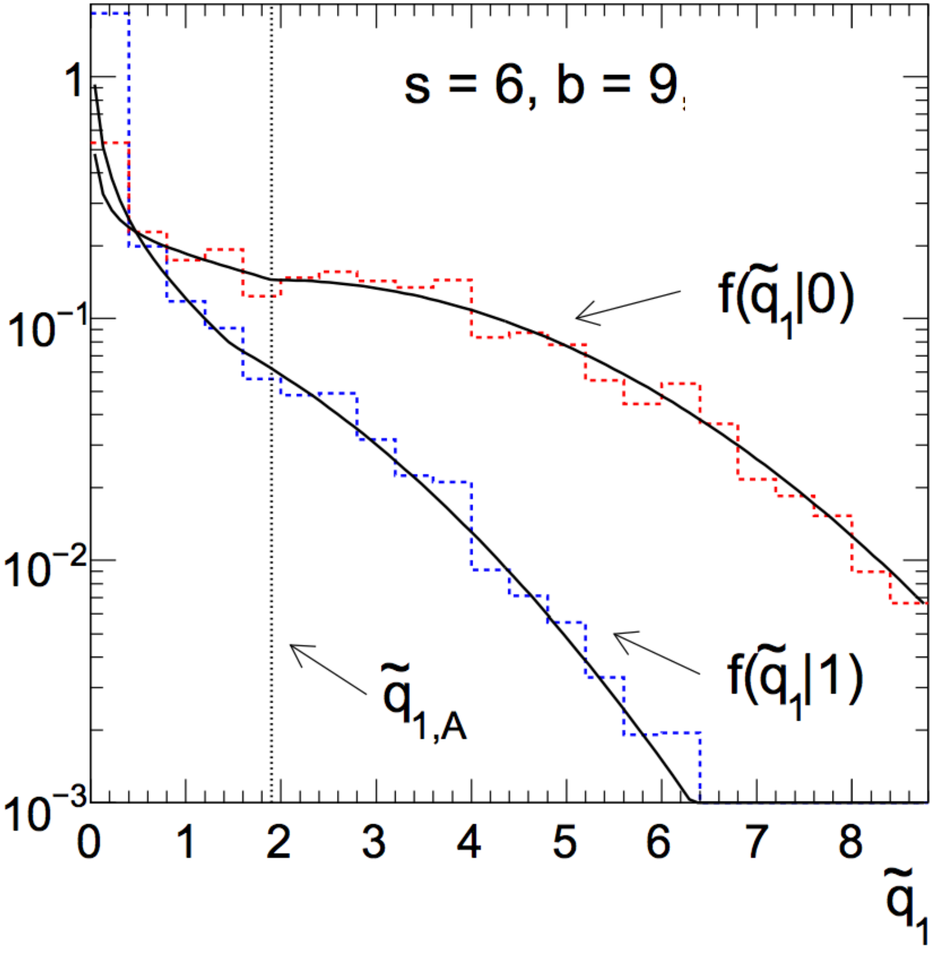


Asymptotics

Discovery



Limits



Asymptotic distributions agree rather well with MC toys for discovery and limit-setting test-statistics!

* https://arxiv.org/pdf/1007.1727.pdf