# **Statistics**

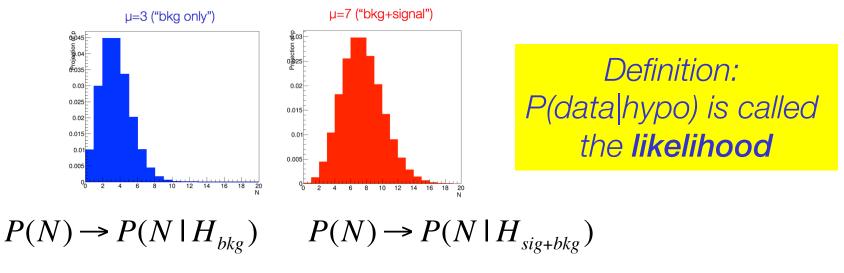
W. Verkerke

Short recap of yesterday



## Probabilities vs conditional probabilities

 Note that probability models strictly give conditional probabilities (with the condition being that the underlying hypothesis is true)



Suppose we measure N=7 then can calculate

$$L(N=7|H_{bkg})=2.2\%$$
  $L(N=7|H_{sig+bkg})=14.9\%$ 

- Data is more likely under sig+bkg hypothesis than bkg-only hypo
- Is this what we want to know? Or do we want to know  $L(H_{s+b}|N=7)$ ?



## Interpreting probabilities

#### Frequentist:

Constants of nature are fixed – you cannot assign a probability to these. Probability are restricted to observable experimental results

- "The Higgs either exists, or it doesn't" you can't assign a probability to that
- Definition of P(data|hypo) is objective (and technical)

## Bayesian:

Probabilities can be assigned to constants of nature

- Quantify your belief in the existence of the Higgs can assign a probablity
- But is can very difficult to assign a meaningful number (e.g. Higgs)

## Example of weather forecast

Bayesian: "The probability it will rain tomorrow is 95%"

Assigns probability to constant of nature ("rain tomorrow")
 P(rain-tomorrow|satellite-data) = 95%

Frequentist: "If it rains tomorrow, 95% of time satellite data looks like what we observe now"

Only states P(satellite-data|rain-tomorrow)



# Formulating evidence for discovery

- In the frequentist school you restrict yourself to P(data|theory) and there is no concept of 'priors'
  - But given that you consider (exactly) 2 competing hypothesis, very low probability for data under Hb lends credence to 'discovery' of Hsb (since Hb is 'ruled out'). Example

$$P(data|H_b)=10^{-7}$$
  
  $P(data|H_{sb})=0.5$ 



"H<sub>b</sub> ruled out" → "Discovery of H<sub>sb</sub>"

- Given importance to interpretation of the lower probability, it is customary to quote it in "physics intuitive" form: Gaussian σ.
  - E.g. '5 sigma' → probability of 5 sigma Gaussian fluctuation =2.87x10<sup>-7</sup>
- No formal rules for 'discovery threshold'
  - Discovery also assumes data is not too unlikely under H<sub>sb</sub>. If not, no discovery, but again no formal rules ("your good physics judgment")
  - NB: In Bayesian case, both likelihoods low reduces Bayes factor K to O(1)



## Working with Likelihood functions for distributions

- How do the statistical inference procedures change for Likelihoods describing distributions?
- Bayesian calculation of P(theo data) they are exactly the same.
  - Simply substitute counting model with binned distribution model

$$P(H_{s+b} | \vec{N}) = \frac{L(\vec{N} | H_{s+b})P(H_{s+b})}{L(\vec{N} | H_{s+b})P(H_{s+b}) + L(\vec{N} | H_b)P(H_b)}$$



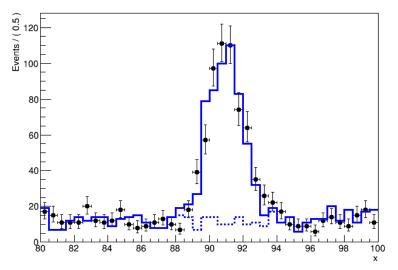
Simply fill in new Likelihood function Calculation otherwise unchanged

$$P(H_{s+b} \mid \vec{N}) = \frac{\prod_{i} Poisson(N_{i} \mid \tilde{s}_{i} + \tilde{b}_{i})P(H_{s+b})}{\prod_{i} Poisson(N_{i} \mid \tilde{s}_{i} + \tilde{b}_{i})P(H_{s+b}) + \prod_{i} Poisson(N_{i} \mid \tilde{b}_{i})P(H_{b})}$$



## Working with Likelihood functions for distributions

 Frequentist calculation of P(data|hypo) also unchanged, but question arises if P(data|hypo) is still relevant?



$$L(\vec{N} \mid H_b) = \prod_{i} Poisson(N_i \mid \tilde{b}_i)$$

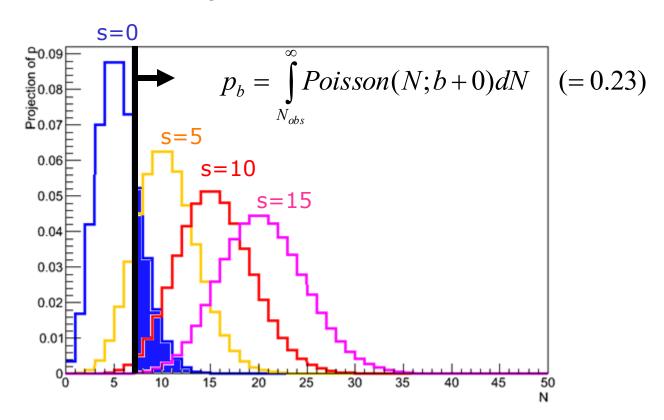
$$L(\vec{N} \mid H_{s+b}) = \prod_{i} Poisson(N_i \mid \tilde{s}_i + \tilde{b}_i)$$

- L(N|H) is probability to obtain exactly the histogram observed.
- Is that what we want to know? Not really. We are interested in probability to observe any 'similar' dataset to given dataset, or in practice dataset 'similar or more extreme' that observed data
- Need a way to quantify 'similarity' or 'extremity' of observed data



# P-values for counting experiments

- Now make a measurement N=N<sub>obs</sub> (example N<sub>obs</sub>=7)
- Definition: p-value: probability to obtain the observed data, or more extreme in future repeated identical experiments
  - Example: p-value for background-only hypothesis





## The Likelihood Ratio as a test statistic

 Given two hypothesis H<sub>b</sub> and H<sub>s+b</sub> the ratio of likelihoods is a useful test statistic

$$\lambda(\vec{N}) = \frac{L(\vec{N} \mid H_{s+b})}{L(\vec{N} \mid H_b)}$$

- Intuitive picture:
  - → If data is likely under H<sub>b</sub>, L(N|H<sub>b</sub>) is large, L(N|H<sub>s+b</sub>) is smaller

$$\lambda(\vec{N}) = \frac{\text{small}}{\text{large}} = \text{small}$$

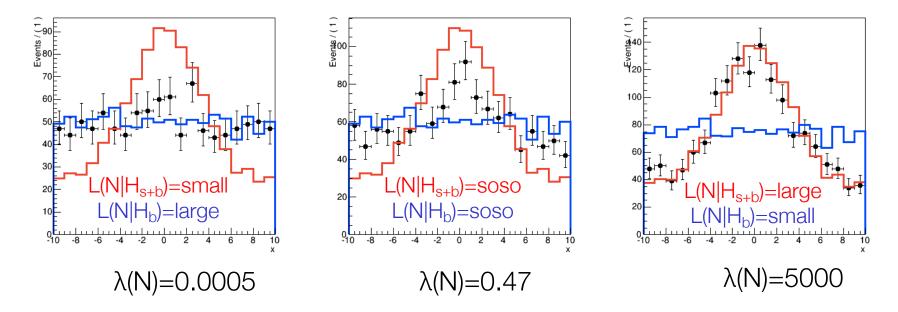
→ If data is likely under H<sub>s+b</sub> L(N|H<sub>s+b</sub>) is large, L(N|H<sub>b</sub>) is smaller

$$\lambda(\vec{N}) = \frac{\text{large}}{\text{small}} = \text{large}$$



# Visualizing the Likelihood Ratio as ordering principle

The Likelihood ratio as ordering principle

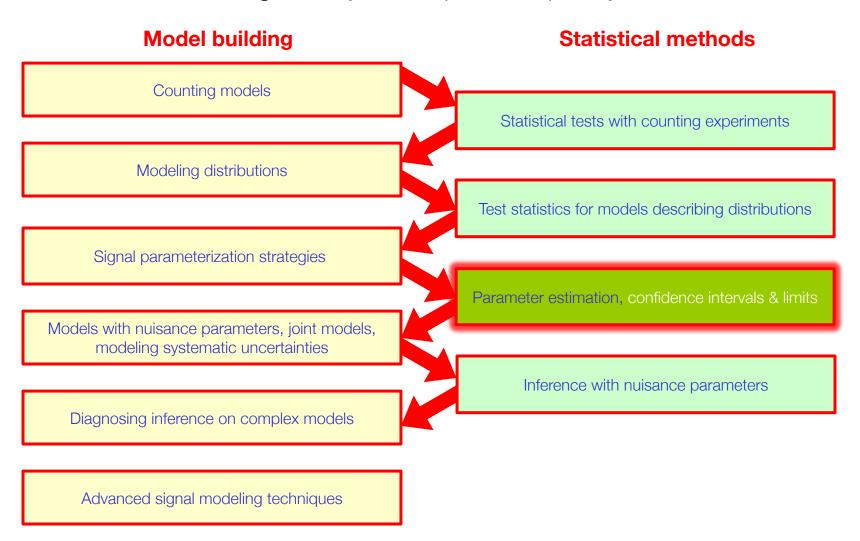


- Frequentist solution to 'relevance of P(data|theory') is to order all observed data samples using a (Likelihood Ratio) test statistic
  - Probability to observe 'similar data or more extreme' then amounts to calculating 'probability to observe test statistic λ(N) as large or larger than the observed test statistic λ(N<sub>obs</sub>)



## Roadmap of this course

Start with basics, gradually build up to complexity





## Parameter estimation – Maximum likelihood

 Practical estimation of maximum likelihood performed by minimizing the negative log-Likelihood

$$L(\vec{p}) = \prod_{i} f(\vec{x}_{i}; \vec{p})$$

$$-\ln L(\vec{p}) = -\sum_{i} \ln F(\vec{x}_{i}; \vec{p})$$

- Advantage of log-Likelihood is that contributions from events can be summed, rather than multiplied (computationally easier)
- In practice, find point where derivative of –logL is zero

$$\left. \frac{d \ln L(\vec{p})}{d\vec{p}} \right|_{p_i = \hat{p}_i} = 0$$

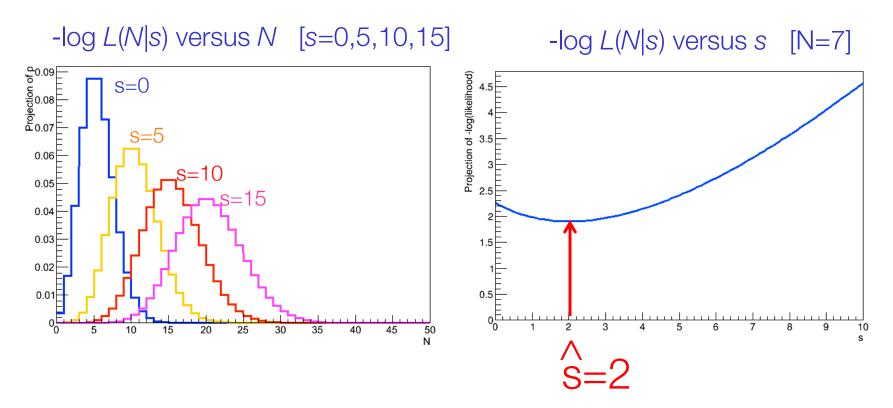
• Standard notation for ML estimation of p is  $\hat{p}$ 



# Example of Maximum Likelihood estimation

Illustration of ML estimate on Poisson counting model

$$L(N \mid s) = Poisson(N \mid s + \tilde{b})$$



Note that Poisson model is discrete in N, but continuous in s!



## Estimating variance on parameters

Variance on of parameter can also be estimated from Likelihood using the variance estimator

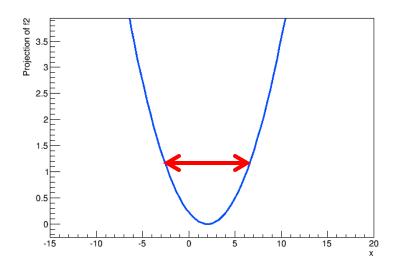
$$\hat{\sigma}(p)^2 = \hat{V}(p) = \left(\frac{d^2 \ln L}{d^2 p}\right)^{-1}$$
From Rao-Cramer-Frechet inequality
$$V(\hat{p}) \ge 1 + \frac{db}{dp} \left(\frac{d^2 \ln L}{d^2 p}\right)$$

From Rao-Cramer-Frechet

b = bias as function of p, inequality becomes equality in limit of efficient estimator

Valid if estimator is efficient and unbiased!

Illustration of Likelihood Variance estimate on a Gaussian distribution



$$f(x \mid \mu, \sigma) = \frac{1}{\sigma \sqrt{2\pi}} \exp\left[-\frac{1}{2} \left(\frac{x - \mu}{\sigma}\right)^{2}\right]$$

$$\ln f(x \mid \mu, \sigma) = -\ln \sigma - \ln \sqrt{2\pi} + \frac{1}{2} \left(\frac{x - \mu}{\sigma}\right)^{2}$$

$$\frac{d \ln f}{d\sigma}\Big|_{x = \mu} = \frac{-1}{\sigma} \implies \frac{d^{2} \ln f}{d^{2} \sigma}\Big|_{x = \mu} = \frac{1}{\sigma^{2}}$$



## What can we do with composite hypothesis

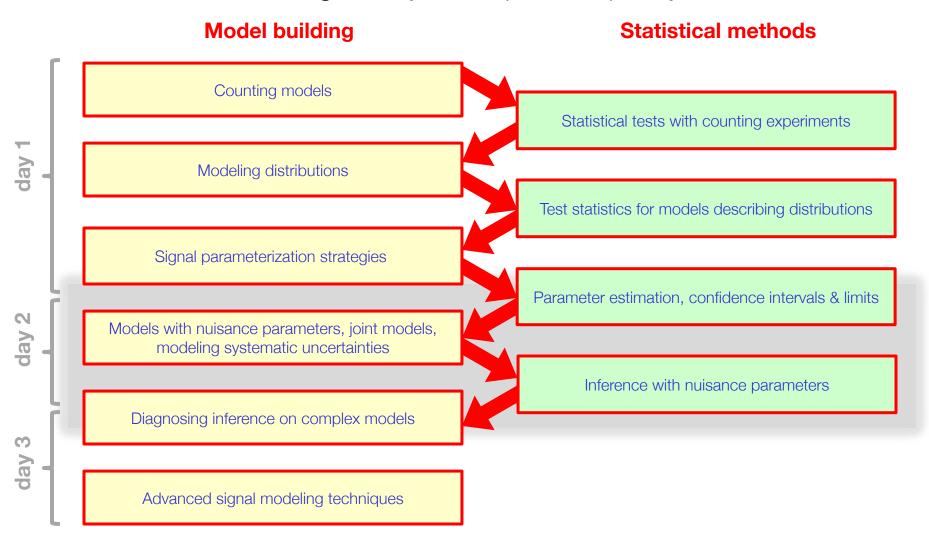
- With simple hypotheses inference is restricted to making statements about P(D|hypo) or P(hypo|D)
- With composite hypotheses many more options
- 1 Parameter estimation and variance estimation
  - What is value of s for which the observed data is most probable?
  - What is the variance (std deviation squared) in the estimate of s?

#### $s=5.5 \pm 1.3$

- 2 Confidence intervals
  - Statements about model parameters using frequentist concept of probability
  - s<12.7 at 95% confidence level</li>
  - 4.5 < s < 6.8 at 68% confidence level</li>
- 3 Bayesian credible intervals
  - Bayesian statements about model parameters
  - s<12.7 at 95% credibility

## Roadmap of this course

Start with basics, gradually build up to complexity

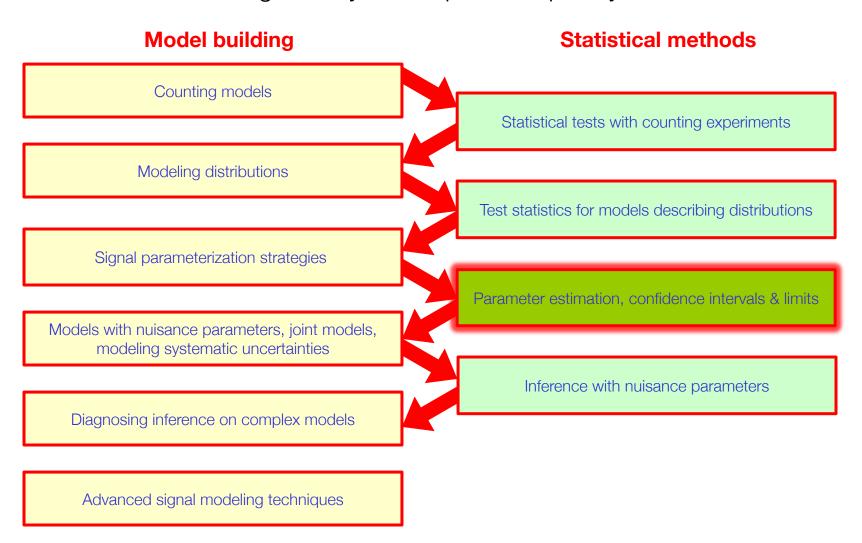


# Statistical methods 3 (continued)

Inference with parameters:
maximum likelihood, confidence
intervals, upper limits, likelihood
ratio and asymptotic formulae

## Roadmap of this course

• Start with basics, gradually build up to complexity



## What can we do with composite hypothesis

- With simple hypotheses inference is restricted to making statements about P(D|hypo) or P(hypo|D)
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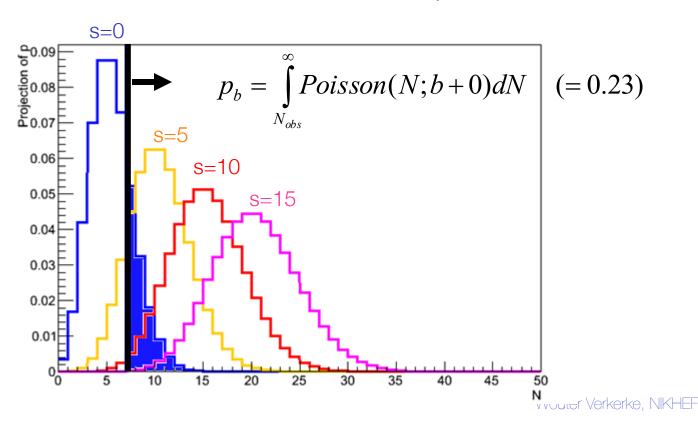
## Interval estimation with fundamental methods

- Can also construct parameters intervals using 'fundamental' methods explored earlier (Bayesian or Frequentist)
- Construct Confidence Intervals or Credible Intervals with defined probabilistic meaning, independent of assumptions on normality of distribution (Central Limit Theorem) → "95% C.L."
- With fundamental methods you greater flexibility in types of interval. E.g when no signal observed 

  upper limit (construct 'upper limit interval')

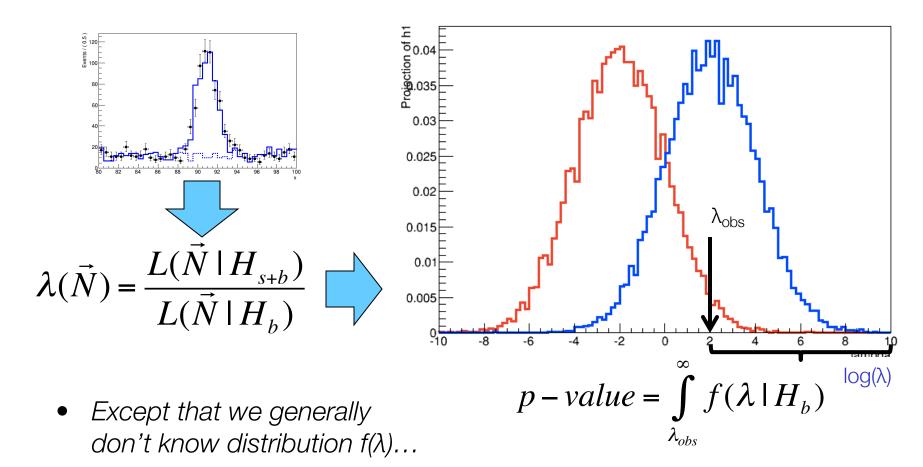
## Reminder - Frequentist test statistics and p-values

- Definition of 'p-value': Probability to observe this outcome or more extreme in future repeated measurements is x%, if hypothesis is true
- Note that the definition of p-value assumes an explicit ordering of possible outcomes in the 'or more extreme' part



## P-values with a likelihood ratio test statistic

 With the introduction of a (likelihood ratio) test statistic, hypothesis testing of models of arbitrary complexity is now reduced to the same procedure as the Poisson example



# A different Likelihood ratio for composite hypothesis testing

 On composite hypotheses, where both null and alternate hypothesis map to values of µ, we can define an alternative likelihood-ratio test statistics that has better properties

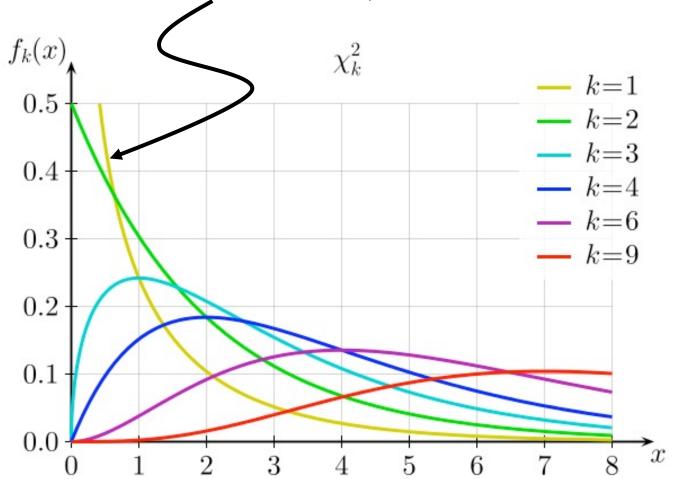
- Advantage: distribution of new λ<sub>μ</sub> has known asymptotic form
- Wilks theorem: distribution of  $-log(\lambda_{\mu})$  is asymptotically distribution as a  $\chi^2$  with  $N_{param}$  degrees of freedom\*

\*Some regularity conditions apply

•  $\rightarrow$  Asymptotically, we can *directly* calculate p-value from  $\lambda_{\mu}^{\text{obs}}$ 

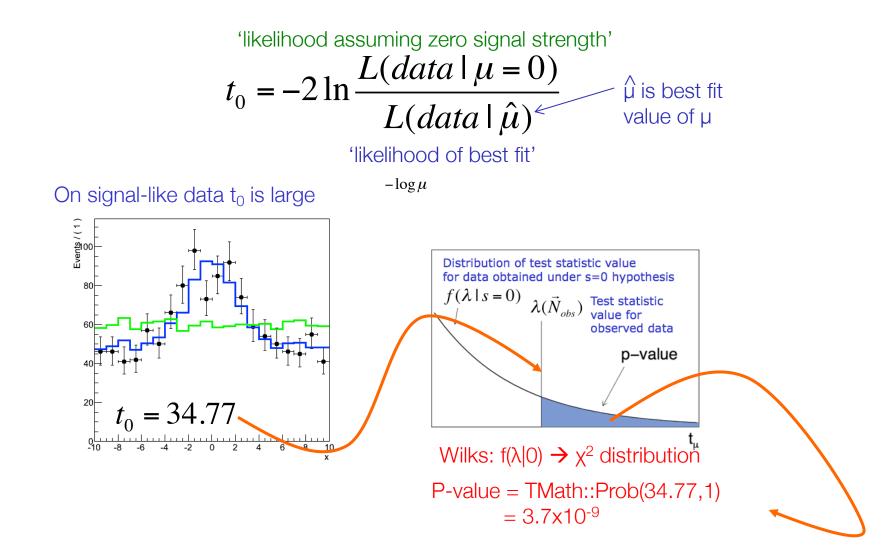
# What does a $\chi^2$ distribution look like for n=1?

Note that it for n=1, it does not peak at 1, but rather at 0...



## Composite hypothesis testing in the asymptotic regime

For 'histogram example': what is p-value of null-hypothesis



## Composite hypothesis testing in the asymptotic regime

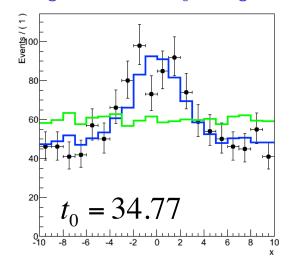
For 'histogram example': what is p-value of null-hypothesis

'likelihood assuming zero signal strength'

$$t_0 = -2 \ln \frac{L(data \mid \mu = 0)}{L(data \mid \hat{\mu})} \qquad \text{$\stackrel{\hat{\mu}$ is best fit value of $\mu$}{}}$$

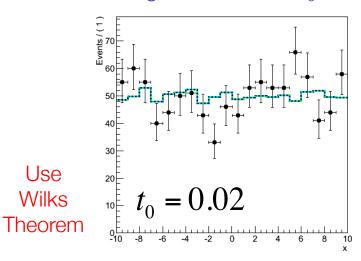
'likelihood of best fit'

#### On signal-like data to is large



P-value = TMath::Prob(34.77,1) =  $3.7 \times 10^{-9}$ 

#### On background-like data to is small



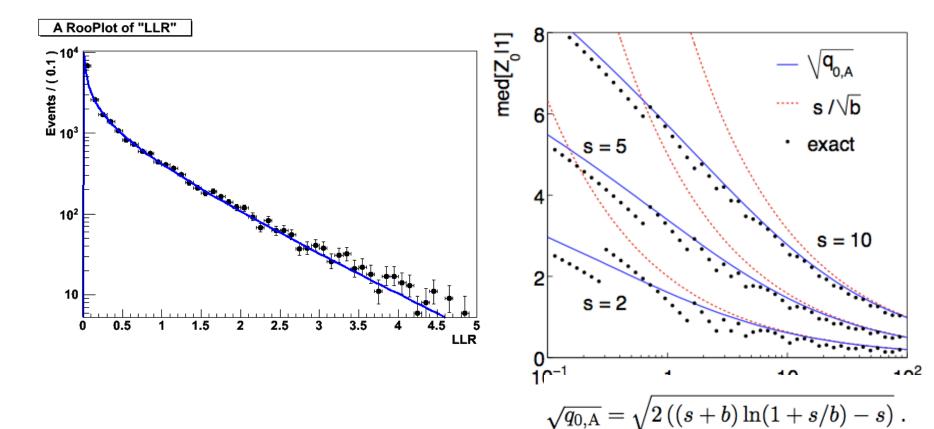
P-value = TMath::Prob(0.02,1) = 0.88

# How quickly does $f(\lambda_{\mu}|\mu)$ converge to its asymptotic form

Pretty quickly –

Here is an example of likelihood function for 10-bin distribution with 200 events

Here is an example for event counting at various s,b

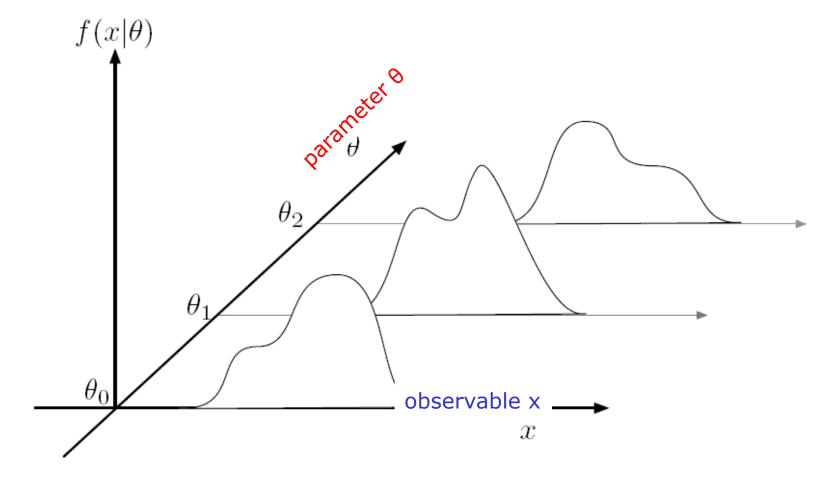


## From hypothesis testing to confidence intervals

- Next step for composite hypothesis is to go from p-values for a hypothesis defined by fixed value of μ to an interval statement on μ
- Definition: A interval on  $\mu$  at X% confidence level is defined such that the true of value of  $\mu$  is contained X% of the time in the interval.
  - Note that the output is not a probabilistic statement on the true s value
  - The true μ is fixed but unknown each observation will result in an estimated interval [μ<sub>-</sub>,μ<sub>+</sub>]. X% of those intervals will contain the true value of μ
  - Coverage = guarantee that probabilistic statements is true (i.e. repeated future experiments do reproduce results in X% of cases)
- Definition of confidence intervals does not make any assumption on shape of interval
  - → Can choose one-sided intervals ('limits'), two-sided intervals ('measurements'), or even disjoint intervals ('complicated measurements')

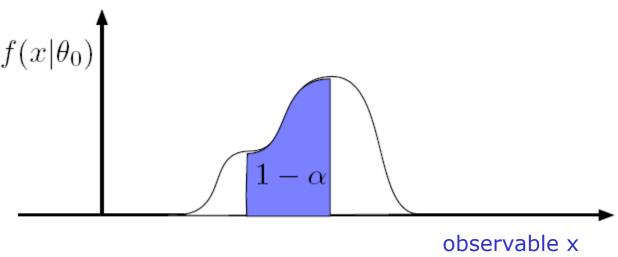
## Exact confidence intervals – the Neyman construction

- Simplest experiment: one measurement (x), one theory parameter  $(\theta)$
- For each value of parameter θ, determine distribution in in observable

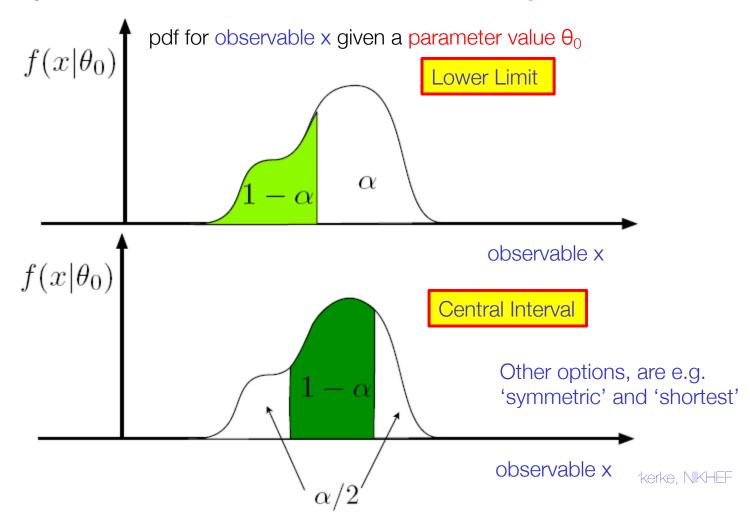


- Focus on a slice in θ
  - For a 1- $\alpha$ % confidence Interval, define *acceptance interval* that contains 100%- $\alpha$ % of the distribution

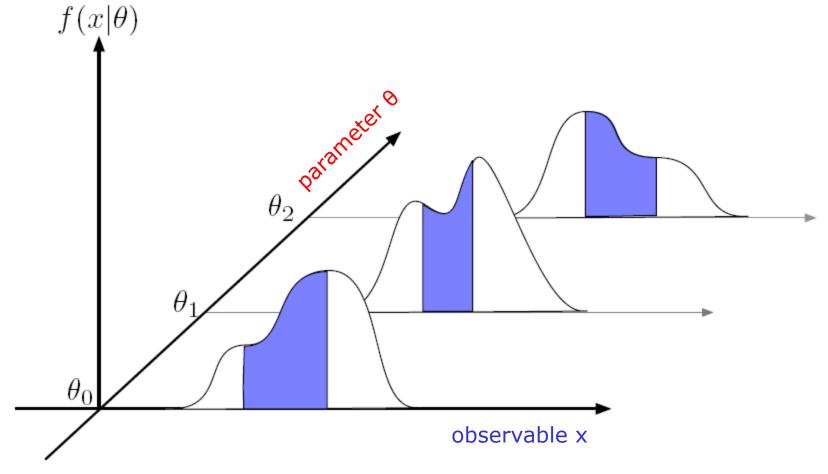
pdf for observable x given a parameter value  $\theta_0$ 



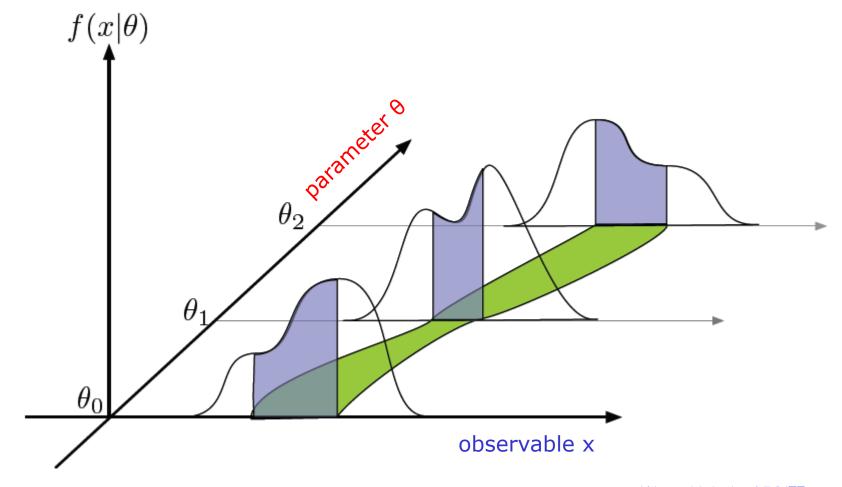
- Definition of acceptance interval is not unique
  - → Choose shape of interval you want to set here.
    - Algorithm to define acceptance interval is called 'ordering rule'



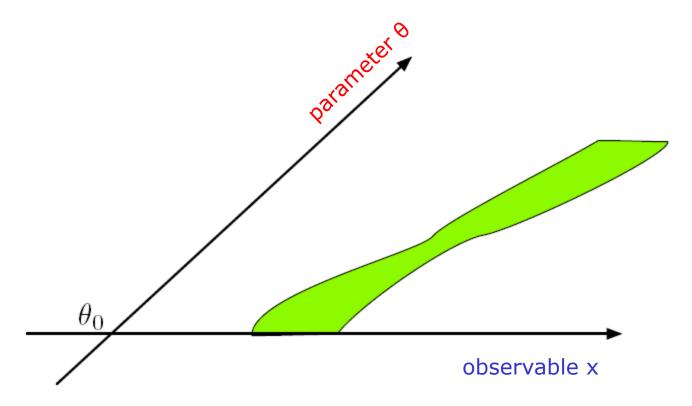
 Now make an acceptance interval in observable x for each value of parameter θ



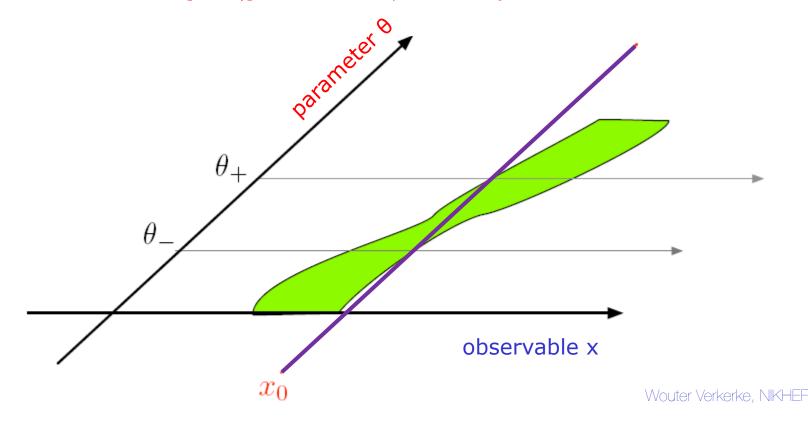
This makes the confidence belt



This makes the confidence belt



- The confidence belt can constructed in advance of any measurement, it is a property of the model, not the data
- Given a measurement  $x_0$ , a confidence interval  $[\theta_+, \theta_-]$  can be constructed as follows
- The interval  $[\theta_{-},\theta_{+}]$  has a 68% probability to cover the true value



## What confidence interval means & concept of coverage

- A confidence interval is an interval on a parameter that contains the true value X% of the time
- This is a property of the procedure, and should be interpreted in the concept of repeated identical measurements:

Each future measurement will result a confidence interval that has somewhat different limits every time ('confidence interval limits are a random variable')

But procedure is constructed such that true value is in X% of the intervals in a series of repeated measurements (this calibration concept is called 'coverage'. The Neyman constructions guarantees coverage)

 It is explicitly <u>not</u> a probability statement on the true value you are trying to measure. In the frequentist the true value is fixed (but unknown)

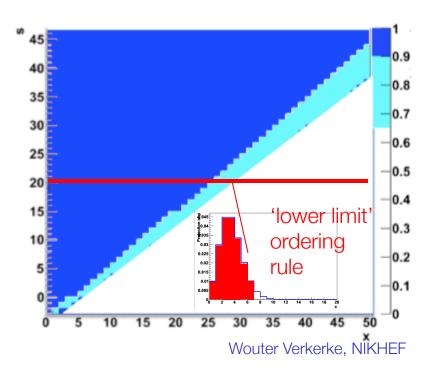
# The confidence interval – Poisson counting example

 Given the probability model for Poisson counting example: for every hypothesized value of s, plot the expected distribution N



'central' ordering 0.9 rule 0.8 35 0.7 30 -0.6 25 0.5 20 0.4 15 0.3 10 0.2 0.1

# Confidence belt for 68% and 90% lower limit

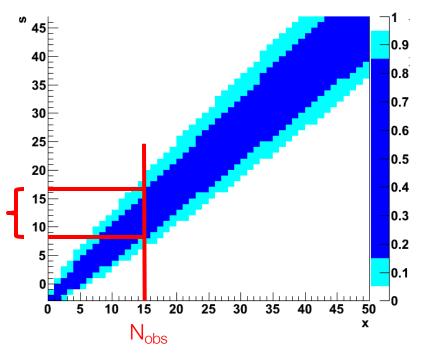


## The confidence interval – Poisson counting example

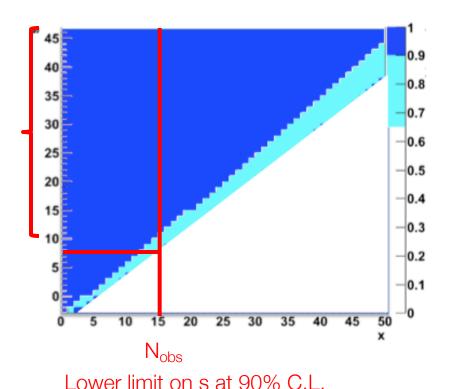
 Given confidence belt and observed data, confidence interval on parameter is defined by belt intersection

Confidence belt for 68% and 90% central intervals

Confidence belt for 68% and 90% lower limit

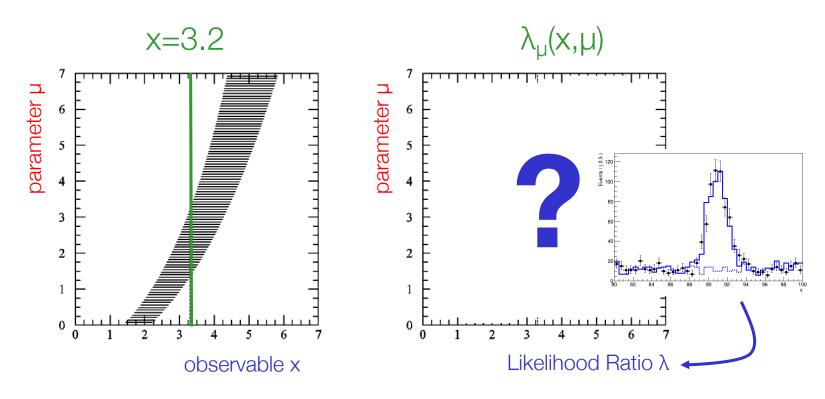


Central interval on s at 68% C.L.



#### Confidence intervals using the Likelihood Ratio test statistic

- Neyman Construction on Poisson counting looks like 'textbook' belt.
- In practice we'll use the <u>Likelihood Ratio test statistic</u> to summarize the measurement of a (multivariate) distribution for the purpose of hypothesis testing.
- Procedure to construct belt with LR is identical:
   obtain distribution of λ for every value of μ to construct confidence belt



#### The asymptotic distribution of the likelihood ratio test statistic

Given the likelihood ratio

$$t_{\mu} = -2\log \lambda_{\mu}(x) = -2\log \frac{L(x \mid \mu)}{L(x \mid \hat{\mu})}$$

Q: What do we know about asymptotic distribution of  $\lambda(\mu)$ ?

• A: Wilks theorem  $\rightarrow$  Asymptotic form of  $f(t|\mu)$  is a  $\chi^2$  distribution

$$f(t_{\mu}|\mu) = \chi^2(t_{\mu},n)$$

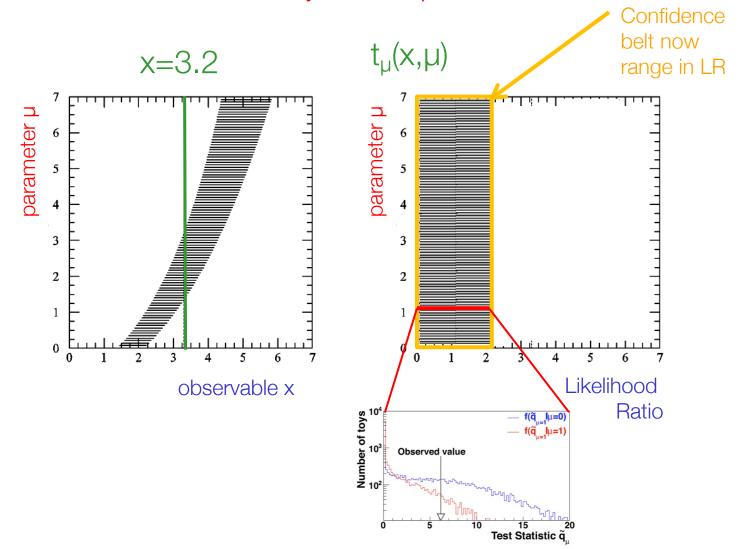
Where

 $\mu$  is the hypothesis being tested and n is the number of parameters (here 1:  $\mu$ )

- Note that f(t<sub>μ</sub>|μ) is independent of μ!
  - $\rightarrow$  Distribution of  $t_{\mu}$  is the same for every 'horizontal slice' of the belt

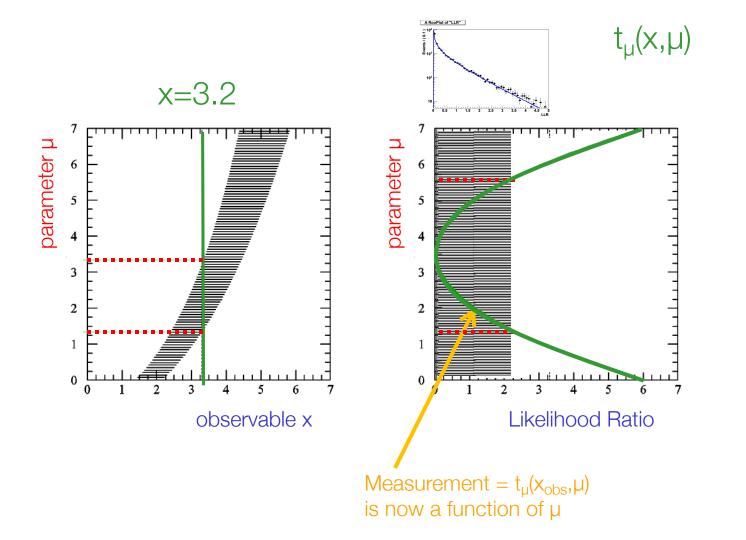
## Confidence intervals using the Likelihood Ratio test statistic

Procedure to construct belt with LR is identical:
 obtain distribution of λ for every value of μ to construct belt



#### What does the observed data look like with a LR?

 Note that while belt is (asymptotically) independent of parameter μ, observed quantity now is dependent of the assumed μ



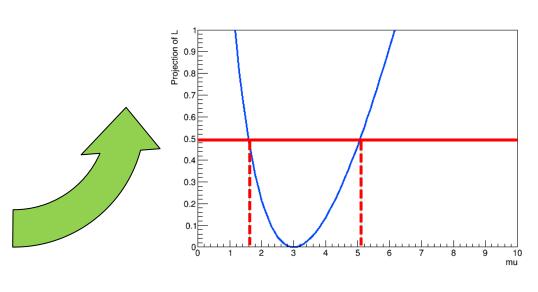
#### Connection with likelihood ratio intervals

- If you assume the asymptotic distribution for t<sub>µ</sub>,
  - Then the confidence belt is exactly a box
  - And the constructed confidence interval can be simplified to finding the range in μ where t<sub>u</sub>=½·Z²
  - → This is exactly the MINOS error

#### FC interval with Wilks Theorem

# 7 6 3 2 1 0 0 1 2 3 4 5 6 7

#### MINOS / Likelihood ratio interval



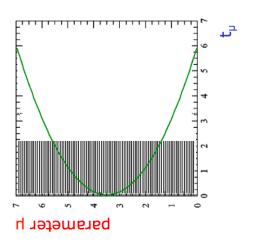
Wouter Verkerke, NIKHEF

## Recap on confidence intervals

- Confidence intervals on parameters are constructed to have precisely defined probabilistic meaning
  - This calibration is called "coverage"
     The Neyman Construction has coverage by construction
  - This is different from parameter variance estimates
     (or Bayesian methods) that don't have (a guaranteed) coverage
  - For most realistic models confidence intervals are calculated using (Likelihood Ratio) test statistics to define the confidence belt

#### Asymptotic properties

- In the asymptotic limit (Wilks theorem),
   Likelihood Ratio interval converges to a
   Neyman Construction interval
   (with guaranteed coverage) "Minos Error"
   NB: the likelihood does not need to be parabolic for Wilks theorem to hold
- Separately, in the limit of normal distributions the likelihood becomes exactly parabolic and the ML Variance estimate converges to the Likelihood Ratio interval



## Bayesian inference with composite hypothesis

 With change L→L(µ) the prior and posterior model probabilities become probability density functions

$$P(H_{s+b} \mid \vec{N}) = \frac{L(\vec{N} \mid H_{s+b})P(H_{s+b})}{L(\vec{N} \mid H_{s+b})P(H_{s+b}) + L(\vec{N} \mid H_{b})P(H_{b})}$$

$$P(\mu \mid \vec{N}) = \frac{L(\vec{N} \mid \mu)P(\mu)}{\int L(\vec{N} \mid \mu)P(\mu)d\mu}$$

$$Posterior$$

$$Prior$$

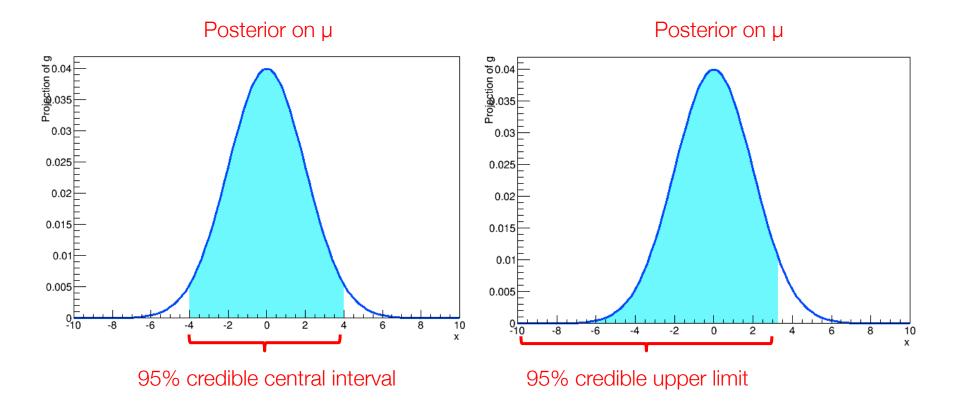
$$probability density$$

$$P(\mu \mid \vec{N}) \propto L(\vec{N} \mid \mu)P(\mu)$$

NB: Likelihood is not a probability density

## Bayesian credible intervals

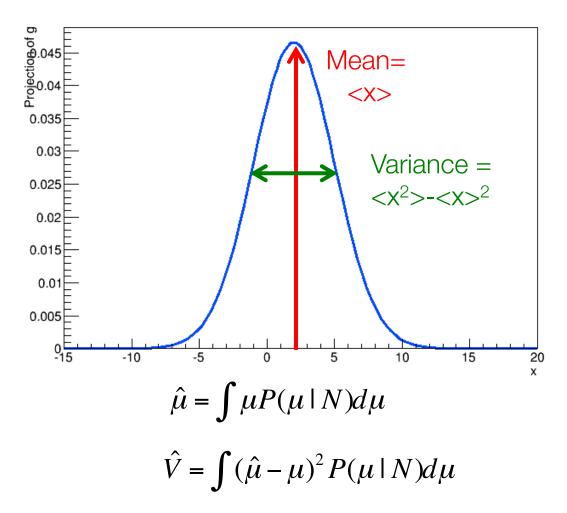
 From the posterior density function, a credible interval can be constructed through integration



Note that Bayesian interval estimation require no minimization
 of –logL, just integration

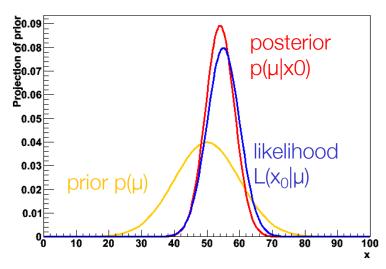
## Bayesian parameter estimation

- Bayesian parameter estimate is the posterior mean
- Bayesian variance is the posterior variance



# **Choosing Priors**

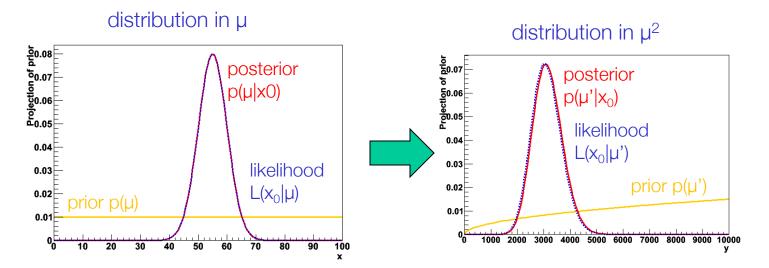
- As for simple models, Bayesian inference always in involves a prior
   now a prior probability density on your parameter
- When there is clear prior knowledge, it is usually straightforward to express that knowledge as prior density function
  - Example: prior measurement of  $\mu = 50 \pm 10$



- Posterior represents updated belief → It incorporates information from measurement and prior belief
- But sometimes we only want to publish result of this experiment, or there is no prior information. What to do?

# **Choosing Priors**

- Common but thoughtless choice: a flat prior
  - Flat implies choice of metric. Flat in x, is not flat in  $x^2$



- Flat prior implies choice on of metric
  - A prior that is flat in  $\mu$  is not flat in  $\mu^2$
  - 'Preferred metric' has often no clear-cut answer.
     (E.g. when measuring neutrino-mass-squared, state answer in m or m²)
  - In multiple dimensions even complicated (prior flat in x,y or is prior flat in r, $\phi$ ?)

# Is it possible to formulate an 'objective' prior?

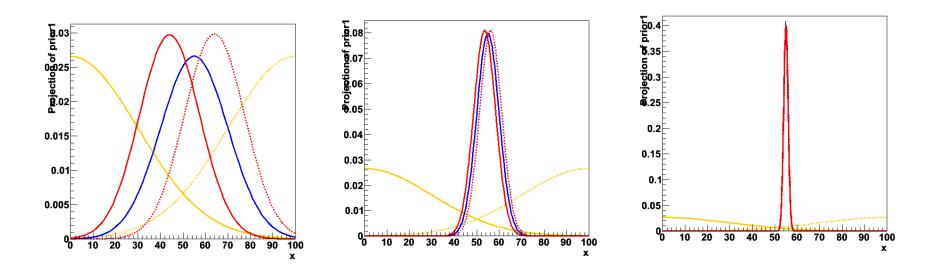
- Can one define a prior p(µ) which contains as little information as possible, so that the posterior pdf is dominated by the likelihood?
  - A bright idea, vigorously pursued by physicist Harold Jeffreys in in mid-20thcentury:
  - This is a really really thoughtless idea, recognized by Jeffreys as such, but dismayingly common in HEP: just choose p(μ) uniform in whatever metric you happen to be using!
- "Jeffreys Prior" answers the question using a prior uniform in a metric related to the Fisher information.

$$I(\theta) = -E \left[ \frac{\partial^2}{\partial \theta^2} \log f(x \mid \theta) \middle| \theta \right]$$

- Unbounded mean  $\mu$  of gaussian:  $p(\mu) = 1$
- Poisson signal mean  $\mu$ , no background:  $p(\mu) = 1/\sqrt{\mu}$
- Many ideas and names around on non-subjective priors
  - Advanced subject well beyond scope of this course.
  - Many ideas (see e.g. summary by Kass & Wasserman),
     but very much an open/active in area of research

# Sensitivity Analysis

- Since a Bayesian result depends on the prior probabilities, which are either personalistic or with elements of arbitrariness, it is widely recommended by Bayesian statisticians to study the sensitivity of the result to varying the prior.
- Sensitivity generally decreases with precision of experiment



 Some level of arbitrariness – what variations to consider in sensitivity analysis

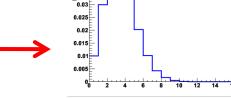
## Likelihood Principle

- As noted above, in both Bayesian methods and likelihood-ratio based methods, the probability (density) for obtaining the data at hand is used (via the likelihood function), but probabilities for obtaining other data are not used!
- In contrast, in typical frequentist calculations (e.g., a p-value which
  is the probability of obtaining a value as extreme or more extreme
  than that observed), one uses probabilities of data not seen.
- This difference is captured by the Likelihood Principle\*:

If two experiments yield likelihood functions which are proportional, then Your inferences from the two experiments should be identical.

#### The "Karmen Problem"

- Simple counting experiment:
  - You expected precisely 2.8 background events with a Poisson distribution



A RooPlot of "x"

- You count the total number of observed events N=s+b
- You make a statement on s, given N<sub>obs</sub> and b=2.8
- You observe N=0!
  - Likelihood:  $L(s) = (s+b)^0 \exp(-s-b) / 0! = \exp(-s) \exp(-b)$
- Likelihood –based intervals
  - $LR(s) = exp(-s) exp(-b)/exp(-b) = exp(-s) \rightarrow Independent of b!$
  - Bayesian integral also independent of factorizing exp(-b) term
- So for zero events observed, likelihood-based inference about signal mean **s** is independent of expected b.
- For essentially all frequentist confidence interval constructions, the fact that n=0 is less likely for b=2.8 than for b=0 results in narrower confidence intervals for μ as b increases.
  - Clear violation of the L.P.

## Likelihood Principle Example #2

- Binomial problem famous among statisticians
- Translated to HEP: You want to know the trigger efficiency e.
  - You count until reaching n=400 zero-bias events, and note that of these, m=1 passed trigger.
    - Estimate e = 1/400, compute binomial confidence interval for e.
  - Your colleague (in a different sample!) counts zero-bias events until m=1 have passed the trigger. She notes that this requires n=400 events.
    - Intuitively, e=1/400 *over-estimates* e because she stopped *just* upon reaching 1 passed event. (The relevant distribution is the negative binomial.)
- Each experiment had a different stopping rule. Frequentist confidence intervals depend on the stopping rule.
  - It turns out that the likelihood functions for the binomial problem and the negative binomial problem differ only by a constant!
  - So with same n and m, (the strong version of) the L.P. demands same inference about e from the two stopping rules!

# Summary

#### Maximum Likelihood

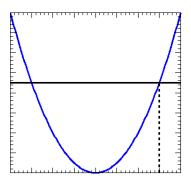
- Point and variance estimation
- Variance estimate assumes normal distribution. No upper/lower limits

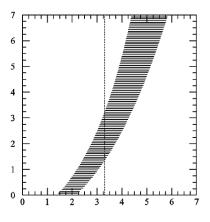
#### Frequentist confidence intervals

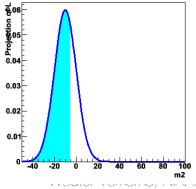
- Extend hypothesis testing to composite hypothesis
- Neyman construction provides exact "coverage"
   = calibration of quoted probabilities
- Strictly p(data|theory)
- Asymptotically identical to likelihood ratio intervals (MINOS errors, does not assume parabolic L)

#### Bayesian credible intervals

- Extend P(theo) to p.d.f. in model parameters
- Integrals over posterior density → credible intervals
- Always involves prior density function in parameter space







# Statistical methods 3b (continued)

Expected results, upper limits and asymptotic formulae