Bayesian Data Analysis

and some other things

A. Caldwell

Max Planck Institute for Physics

1. Some fundamentals
2. The Poisson Distribution
3. Bayesian Analysis with the Poisson distribution
4. Poisson distribution for signal and background
5. Examples

$\Delta p \cdot \Delta q \geq \frac{1}{2}\hbar$

Max-Planck-Institut für Physik
(Werner-Heisenberg-Institut)

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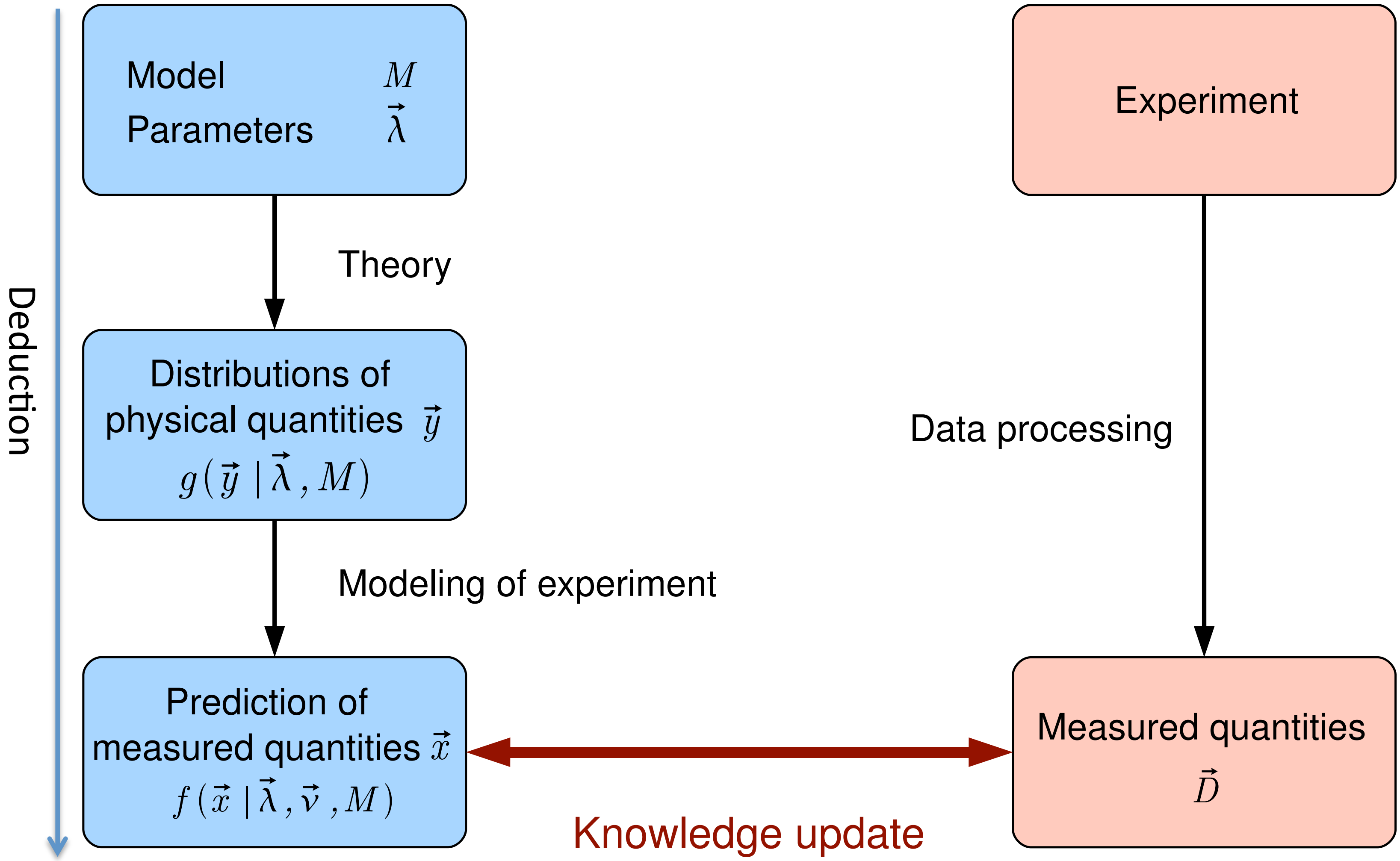
How we learn



Model M

Parameters $\vec{\lambda}$

Theory

Distributions of physical quantities $\vec{y}$

$g(\vec{y}\,|\,\vec{\lambda}, M)$

Modeling of experiment

Prediction of measured quantities $\vec{x}$

$f(\vec{x}\,|\,\vec{\lambda}, \vec{\nu}, M)$

Experiment

Data processing

Measured quantities

$\vec{D}$

Knowledge update

Deduction

Logical Basis

Model building and making predictions from models follows deductive reasoning:

Given A➔B (major premise)
Given B➔C (major premise)
Then, given A you can conclude that C is true

etc.

Everything is clear, we can make frequency distributions of possible outcomes within the model, etc. This is math, so it is correct …

Logical Basis

However, in physics what we want to know is the validity of the model given the data. i.e., logic of the form:

Given $A \rightarrow C$ with some ‘probability’
Measure C, what can we say about A ?

Well, maybe $A_1 \rightarrow C$, $A_2 \rightarrow C$, …

We can only disprove (C not possible in A, then A invalid).

We are only capable of expressing a ‘degree of belief’ in A. And since we can never say anything is true, the question is – is it good enough ? Are we willing to bet on A providing the right answer to the next question ? Under what odds ?

Logical basis

Instead of truth, we consider knowledge

Knowledge = **justified ~~true~~ belief**

Justification comes from the data.

Start with some knowledge or maybe plain belief

Build a model

Make some predictions

Do the experiment

Data analysis gives updated knowledge (belief in possible parameter values)

Which probability ?

Data analysis is based on building a ‘probability’ for the data. But is this well defined ?

Imagine we flip a coin 10 times, and get the following result:

T H T H H T H T T H

We now repeat the process with and get

T T T T T T T T T T

Which outcome has higher probability ?

Take a model where H, T are equally likely. Then, probability of the sequence is

outcome 1

And

outcome 2

Something seem wrong with this result ?

Given a fair coin, we could also calculate the chance of getting n times H:

And we find the following result:

n	p
0	$1\cdot 2^{-10}$
1	$10\cdot 2^{-10}$
2	$45\cdot 2^{-10}$
3	$120\cdot 2^{-10}$
4	$210\ \cdot 2^{-10}$
5	$252\ \cdot 2^{-10}$
6	$210\ \cdot 2^{-10}$
7	$120\ \cdot 2^{-10}$
8	$45\ \cdot 2^{-10}$
9	$10\ \cdot 2^{-10}$
10	$1\ \cdot 2^{-10}$

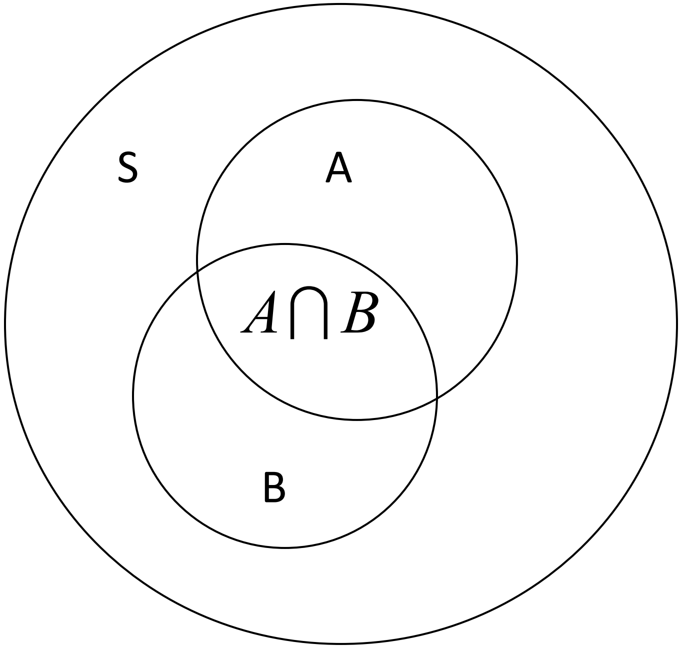
There are typically an infinite number of choices you can make for the ‘probability of the data’ or likelihood.

If someone claims to have an optimal definition, ask them ‘based on what criterion ?’ There is no one best answer !

Choosing a probability of your data is a critical component of the analysis process. Get the most out of your data !

Mathematical Definitions

Consider a set, S, the sample space, which can be divided into subsets.



Probability is a real-valued function defined by the Axioms of Probability (Kolmogorov):

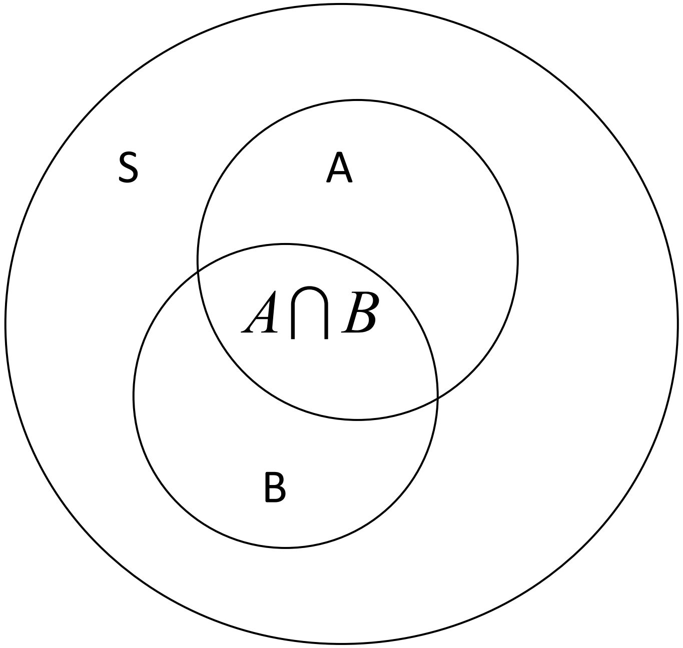
1. For every subset A in S, P(A)≥0.
2. For disjoint subsets

$$A \cap B = \phi,$$

$$P(A \cup B) = P(A) + P(B)$$

3. P(S)=1

Mathematical Definitions



Definition of conditional probability:

$$P(A \mid B) = \frac{P(A \bigcap B)}{P(B)}$$

Since $P(A \bigcap B) = P(B \bigcap A)$, Bayes' Theorem follows

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

Law of Total Probability

$$P(B) = \sum_i P(B \mid A_i) P(A_i)$$

for any subset B and for disjoint A_i such that $\bigcup_i A_i = S$

Combining with Bayes' Theorem gives

$$\boxed{P(A|B) = \frac{P(B|A)P(A)}{\sum_i P(B|A_i)P(A_i)}}$$

If you want to make a statement about how much ‘probability’ to assign to A, there is only one way – Bayes’ Theorem.

Why isn't everyone a Bayesian ?

My suspicion: it is because most people do not understand the frequentist approach. Frequentist statements and Bayesian statements are thought to be about the same logical concept, and the frequentist statement does not require a prior, so …

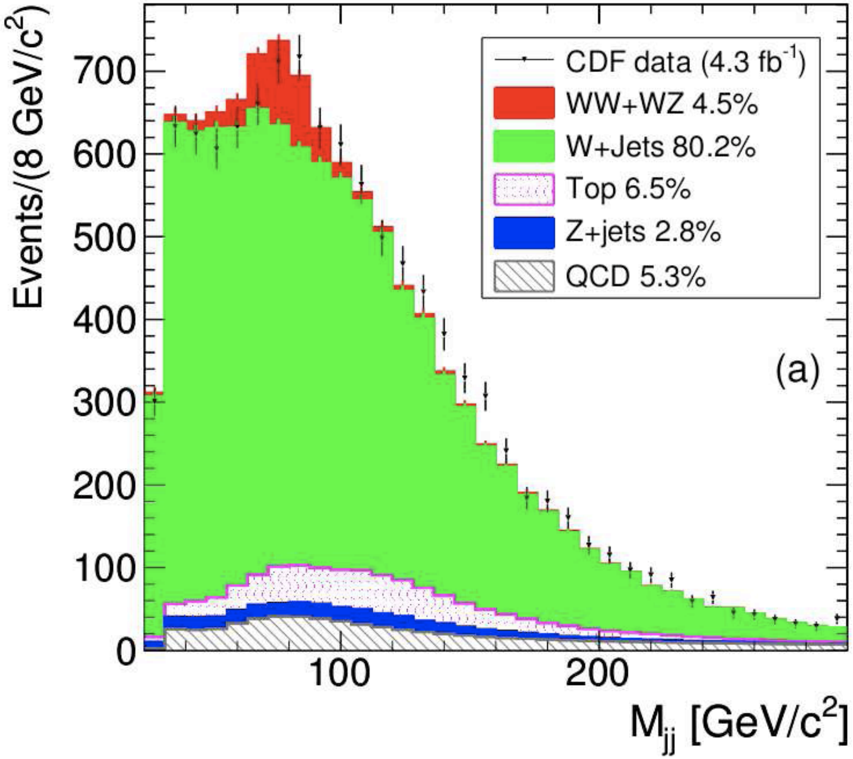
A. L. Read, *Presentation of search results: the CL_S technique,* J. Phys. G: Nucl. Part. Phys. **28** (2002) 2693-2704.

nearly all physicists tend to misinterpret frequentist results as statements about the theory given the data.

Frequentist statements are not statements about the model – only about the data in the context of the model. This is not what we wanted to know … At least not the ultimate statement.

Why isn’t everyone a Bayesian ?

G. D’Agostini, Probably a discovery: Bad mathematics means rough scientific communication, arXiv:1112.3620v2 [physics.data-an]



Quoting a Discovery article:
It is what is known as a ``three-sigma event,” and this refers to the statistical certainty of a given result. In this case, this result has a 99.7 percent chance of being correct (and a 0.3 percent chance of being wrong).”

$$1 - P(D|H_0) = P(H_1|D)$$

This is nonsense !

The Higgs announcement

Gemeinsame Presseerklärung des
Komitee für Elementarteilchenphysik KET
Forschungsschwerpunkt ATLAS (BMBF-FSP 101 ATLAS)
Forschungsschwerpunkt CMS (BMBF-FSP 102 CMS)
Deutsches Elektronen-Synchrotron DESY
Max-Planck-Institut für Physik
Helmholtz-Allianz „Physik an der Teraskala“

Der Nachweis eines neuen Teilchens wird in der Teilchenphysik klassischerweise auf zwei Stufen gestellt: Die Messungen, die die Wissenschaftler an ihren Experimenten durchführen, beruhen auf Statistik. Sie geben daher zu jedem ihrer Ergebnisse die Sicherheit als so genannte Signifikanz an. Die Einheit, die sie dafür verwenden ist sigma, dargestellt durch den griechischen Buchstaben σ. Die erste Stufe eines Teilchenfunds („evidence“) ist erreicht, wenn sich das Signal des Teilchens mit einer Deutlichkeit zeigt, dass die Physiker mit 99,75 Prozent Sicherheit von seiner Echtheit ausgehen. Dies entspricht einer Signifikanz von 3σ. Von einer „Entdeckung“ und damit der zweiten Stufe sprechen die Forscher bei einer Signifikanz von 5σ, das entspricht einer Fehlerwahrscheinlichkeit von 0,000057%.

Translation - Probability of error is 0,000057%

Error on what ????? That the Higgs is found - not correct

What happened

equated

$$1 - P(D|H_0) = P(H_1|D)$$

Probability of observing the data or something more extreme given the background only hypothesis

Probability that the Higgs exists

This is logical nonsense …

Who's fault is this confusion ? I would say – physicists should know better ! In the Bayesian approach, we state our prior assumptions and show how they lead to the conclusions.

Poisson Distribution

A Poisson distribution applies when we do not know the number of trials (it is a large number), but we know that there is a fixed probability of 'success' per trial, and the trials occur independently of each other.

Alternatively – a continuous time process with a constant rate will produce a Poisson distributed number of events in a fixed time interval.

High energy physics example: beams collide at a high frequency (10 MHz, say), and the chance of a 'good event' is very small. The resulting number of events in a fixed time will follow a Poisson distribution. A single trial is one crossing of the beams.

Nuclear physics example: a large sample of radioactive atoms will produce a Poisson distributed number of events in a fixed time interval (assuming a $\tau >> T$)

Poisson Distribution

The Poisson distribution can be derived from the Binomial distribution in the limit when N →∞ and p →0, but Np fixed and finite. Then

$$P(r|N,p) \to P(n|\nu)$$

The expected number of events is calculated from a rate, or from a luminosity and cross section or some other way

$$\nu = R \cdot T \text{ or } \nu = \mathcal{L} \cdot \sigma \text{ or...}$$

Poisson Distribution - derivation

$$P(n|N,p) = \frac{N!}{n!(N-n)!}p^n(1-p)^{N-n}$$

$$P(n|N,\frac{\nu}{N}) = \frac{N!}{n!(N-n)!}\frac{\nu^n}{N^n}\left(1-\frac{\nu}{N}\right)^{N-n}$$

$N \rightarrow \infty$

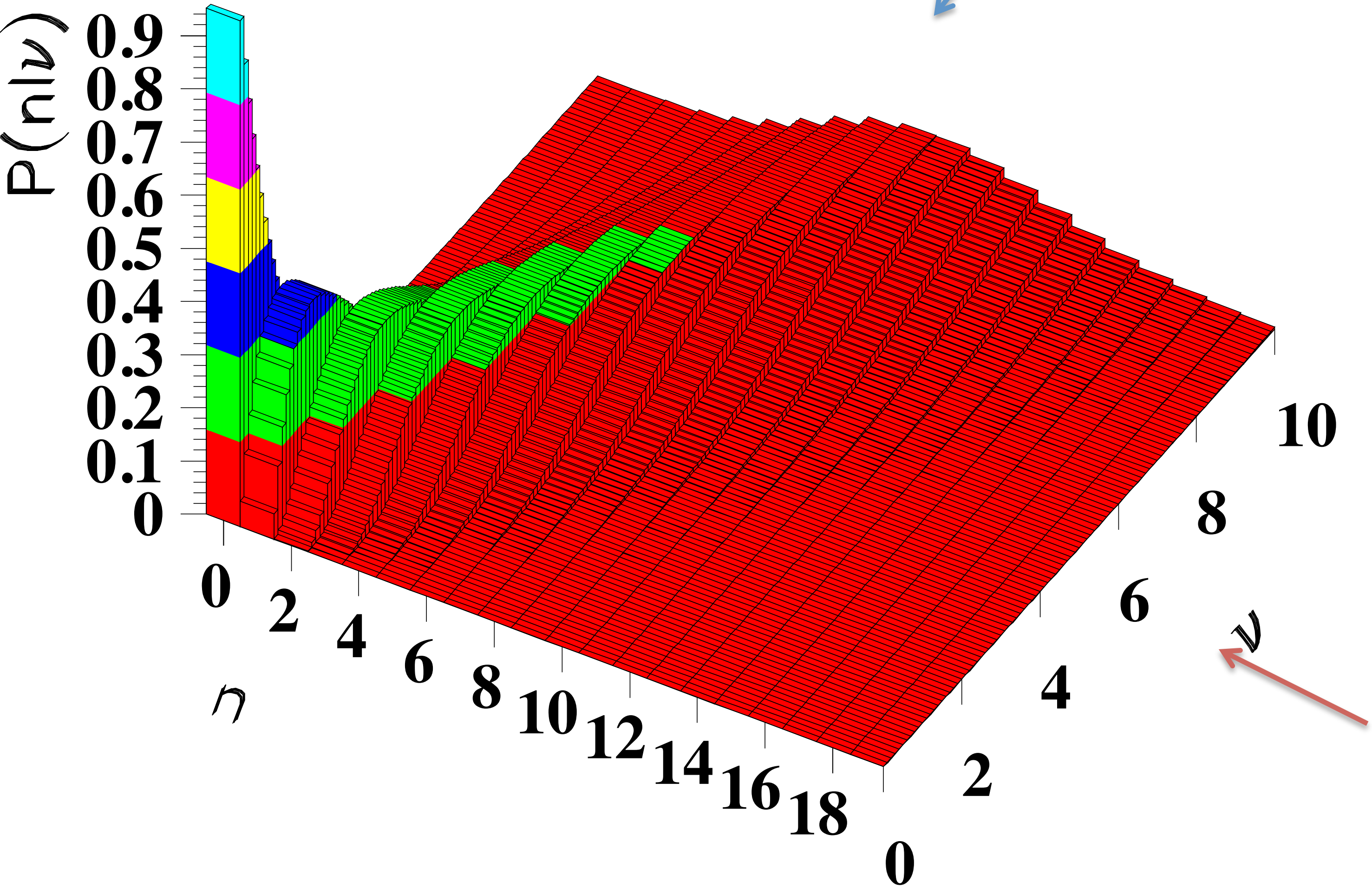
$$\frac{N!}{(N-n)!} = N\cdot(N-1)\cdot\ldots\cdot(N-n+1) \approx N^n$$

$$\left(1-\frac{\nu}{N}\right)^{N-n} \rightarrow \left(1-\frac{\nu}{N}\right)^{N} \rightarrow e^{-\nu}$$

$$\boxed{P(n|\nu) = \frac{e^{-\nu}\nu^n}{n!}}$$

Poisson Distribution

Poisson Example



Quantity used in likelihood analysis

Probability of the data used in confidence level setting

Poisson Distribution-cont.

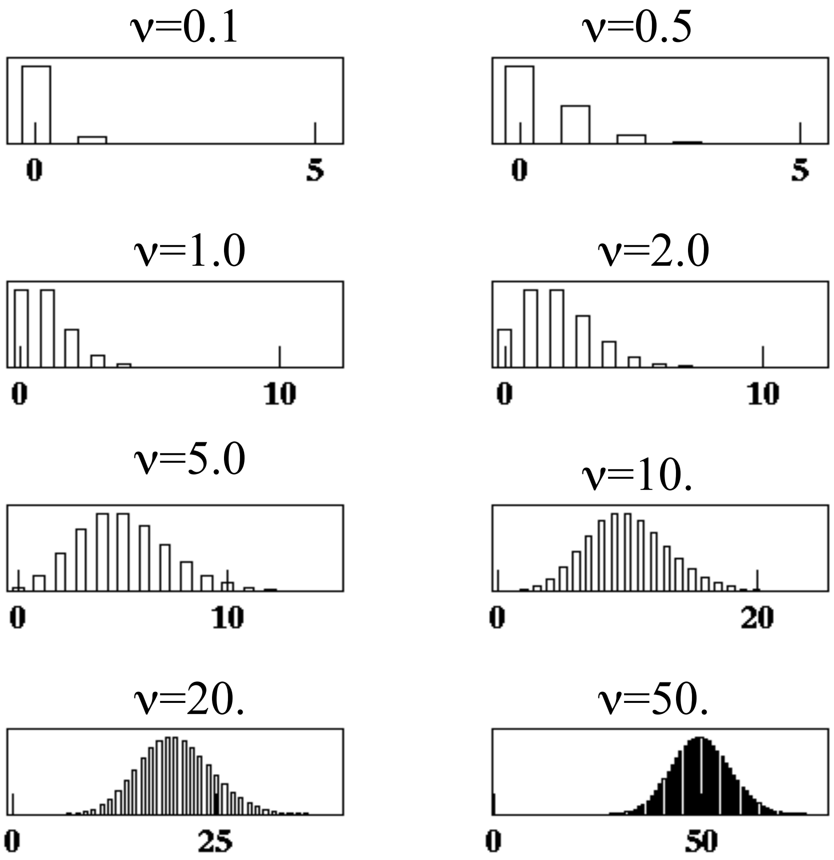
$$\boxed{P(n\,|\,\nu) = \frac{\nu^{n} e^{-\nu}}{n!}}$$

$$n^* = \lfloor \nu \rfloor$$

$$n^* = \lceil \nu \rceil - 1$$

$$E[n] = \nu$$

$$\mathrm{V}[\mathrm{n}] = \nu$$



Notes:

- As ν increases, the distribution becomes more symmetric
- Approximately Gaussian for large ν

Bayesian Data Analysis-Poisson Distribution

Typical examples – counting experiments, failure rates, cross sections,…

$$P(\nu|n) = \frac{P(n|\nu)P_0(\nu)}{\int_0^\infty P(n|\nu)P_0(\nu)d\nu} = \frac{\frac{\nu^n e^{-\nu}}{n!}P_0(\nu)}{\int_0^\infty \frac{\nu^n e^{-\nu}}{n!}P_0(\nu)d\nu}$$

This is our master formula. Result in general will depend on choice of prior. *In general, we need to go straight to the numerical solution.*

Why not – computing is cheap today. Avoid the simplifications and approximations. You can do the full calculation given the right tool.

Poisson - cont.

This is a lecture, so you expect some formulae.

If we assume a flat prior starting at 0 and extending up to some maximum of ν much larger than *n*.

$$P(\nu|n) = \frac{\frac{\nu^n e^{-\nu}}{n!} P_0(\nu)}{\int_0^\infty \frac{\nu^n e^{-\nu}}{n!} P_0(\nu) d\nu} = \frac{\frac{\nu^n e^{-\nu}}{n!}}{\int_0^{\nu_{max}} \frac{\nu^n e^{-\nu}}{n!} d\nu}$$

$$\int_0^{\nu_{max}} \frac{\nu^n e^{-\nu}}{n!} d\nu \approx \frac{1}{n!} \int_0^\infty \nu^n e^{-\nu} d\nu = \frac{1}{n!} n! = 1$$

$$P(\nu|n) = \frac{e^{-\nu} \nu^n}{n!} \qquad \nu^* = n$$

Poisson - cont.

The expectation value:

$$< \nu >= \int_0^\infty P(\nu|n)\nu d\nu = \int_0^\infty \frac{\nu^n e^{-\nu}}{n!}\nu d\nu = \frac{(n+1)!}{n!} = n+1$$

The variance:

$$\begin{aligned}
\sigma^2 &= \int_0^\infty P(\nu|n)(\nu - < \nu >)^2 d\nu \\
&= \int_0^\infty \frac{\nu^n e^{-\nu}}{n!}\nu^2 d\nu - < \nu >^2 \overbrace{\int_0^\infty \frac{\nu^n e^{-\nu}}{n!} d\nu}^{1} \\
&= \frac{(n+2)!}{n!} - (n+1)^2 = n+1
\end{aligned}$$

Poisson - cont.

Note: $n=0 \quad <\nu>=1 \quad ???$

From prior, expect

$$< \nu > \; = \int_0^{\nu_{max}} P_0(\nu)\nu d\nu = \int_0^{\nu_{max}} \frac{\nu}{\nu_{max}} d\nu$$

$$= \left[\frac{\nu^2}{2(\nu_{max})}\right]_0^{\nu_{max}}$$

$$= \frac{\nu_{max}}{2}$$

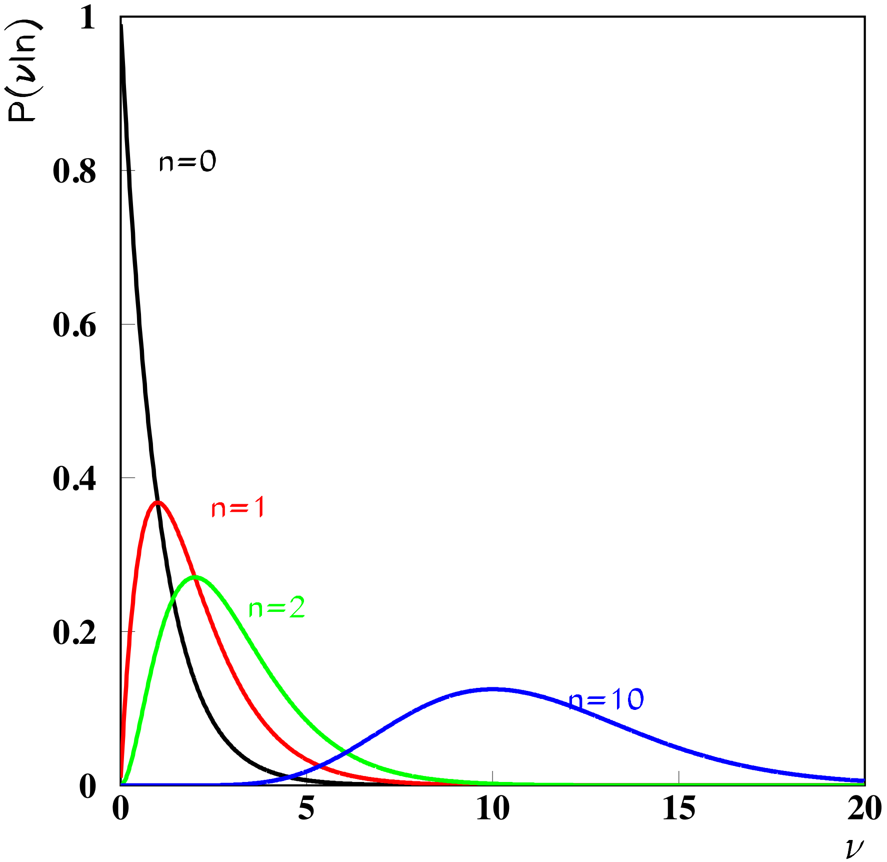
What happened ?

n=0 is a measurement !

$$P(\nu|0) = e^{-\nu}$$

Poisson – cont.

Some examples



Comments:

If you decide to quote the mode as your nominal result, you would use $\nu^*=n$. For large enough n, the 68% probability region is then approximately

$$n - \sqrt{n} \to n + \sqrt{n}$$

Poisson - cont.

The cumulative distribution function:

$$\begin{aligned} F(\nu|n) &= \int_0^\nu \frac{\nu'^n e^{-\nu'}}{n!} d\nu' \\ &= \frac{1}{n!}\left[-\nu'^n e^{-\nu'}|_0^\nu + n\int_0^\nu \nu'^{n-1} e^{-\nu' d\nu'} \right] \\ &= 1 - e^{-\nu}\sum_{i=0}^{n} \frac{\nu^i}{i!} \end{aligned}$$

Poisson – Examples

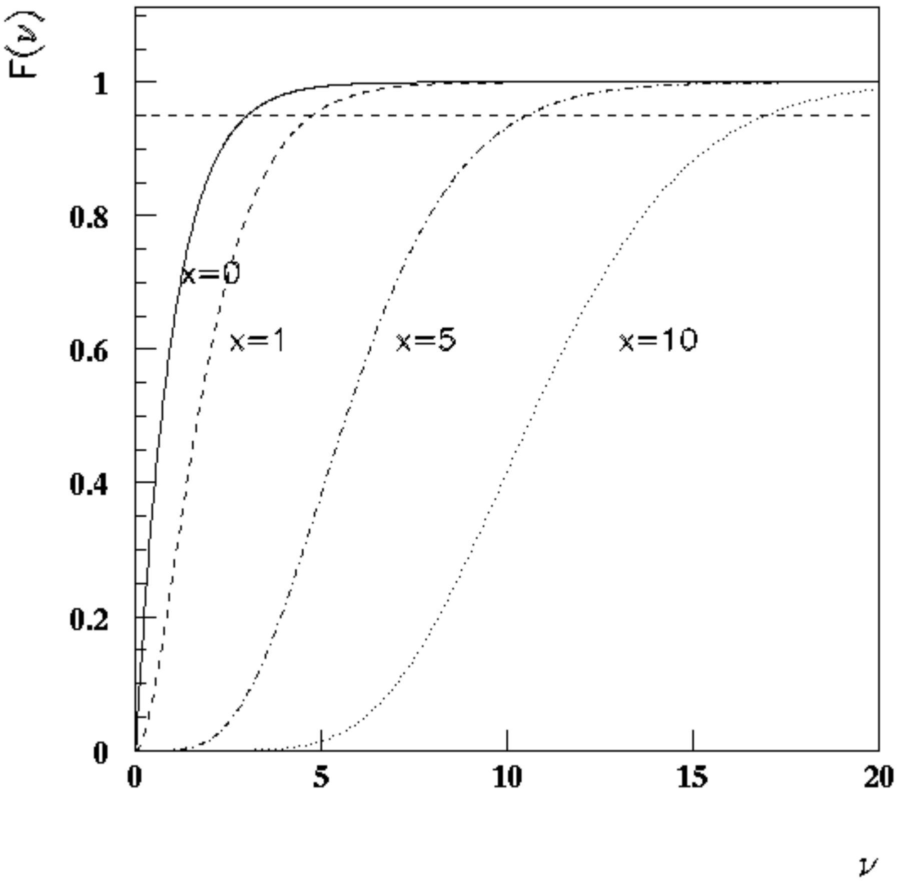
Assume measure zero counts.

With flat prior assumption

$$\begin{aligned} P(\nu|n=0) &= e^{-\nu} \\ F(\nu|n=0) &= 1-e^{-\nu} \end{aligned}$$

For a 95% credibility upper limit

$$\begin{aligned} 0.95 &= 1-e^{-\nu} \\ \nu &\approx 3 \end{aligned}$$



Poisson – cont.

What if we cannot (or do not want to) take a flat prior

Suppose we can model the prior belief as $P_0(\nu) = \frac{1}{10} e^{-\nu/10}$

Now Bayes tells us $P(\nu \mid x = 0) = \dfrac{P(0 \mid \nu) P_0(\nu)}{\int_0^\infty P(0 \mid \nu) P_0(\nu) d\nu} = \dfrac{e^{-\nu} \; \frac{1}{10} e^{-\nu/10}}{\int_0^\infty \frac{1}{10} e^{-11\nu/10} d\nu} = \frac{11}{10} e^{-11\nu/10}$

$$< \nu >= \int_0^\infty \frac{11}{10} e^{-11\nu/10} \nu d\nu = 0.91$$

$P(\nu \le 2.7) = 95\%$, i.e., $\nu \le 2.7$ with 95% probability

Exercises

1. paper and pencil
   a) Find the distribution of the waiting time for the kth event in a process with a constant rate λ.
   b) For a Poisson with mean 1.5, what is the probability to see 6 or more events ? What is the probability to see exactly 0 events ?
   c) Prove that for a Poisson distribution

$$n^* = \lfloor \nu \rfloor = \lceil \nu \rceil - 1$$

Poisson Distribution-cont.

We often have to deal with a superposition of two Poisson processes – the signal and the background, which are indistinguishable in the experiment. Usually we know the background expectations and want to know the probability of a signal in addition.

Example, the signal for large extra dimensions may be the observation of events where momentum balance is (apparently) strongly violated. However this can be mimicked by neutrinos, energy leakage from the detector, etc.

Use the subscripts B for background, s for signal,

and assume n events are observed

$$P(n) = \sum_{n_s=0}^{n} P(n_s \,|\, \nu_s) P(n - n_s \,|\, \nu_B)$$

$$= e^{-(\nu_B + \nu_s)} \sum_{n_s=0}^{n} \frac{\nu_s^{\;n_s} \nu_B^{\;n-n_s}}{n_s!(n-n_s)!}$$

$$= e^{-(\nu_B + \nu_s)} \frac{(\nu_s + \nu_B)^n}{n!} \underbrace{\overbrace{\sum_{n_s=0}^{n} \frac{n!}{n_s!(n-n_s)!} \left(\frac{\nu_s}{\nu_s + \nu_B}\right)^{n_s} \left(\frac{\nu_B}{\nu_s + \nu_B}\right)^{n-n_s}}^{\text{Binomial formula with } p = \left(\frac{\nu_s}{\nu_s + \nu_B}\right)}}_{=1 \text{ by normalization}}$$

$$= e^{-(\nu_B + \nu_s)} \frac{(\nu_s + \nu_B)^n}{n!}$$

The Bayesian Way

$$\mu = \lambda + \nu \qquad P(n|\mu) = \frac{e^{-\mu}\mu^n}{n!}$$

Assuming that the background is perfectly known:

$$P(\nu|n,\lambda) = \frac{P(n|\nu,\lambda)P_0(\nu)}{\int P(n|\nu,\lambda)P_0(\nu)d\nu}$$

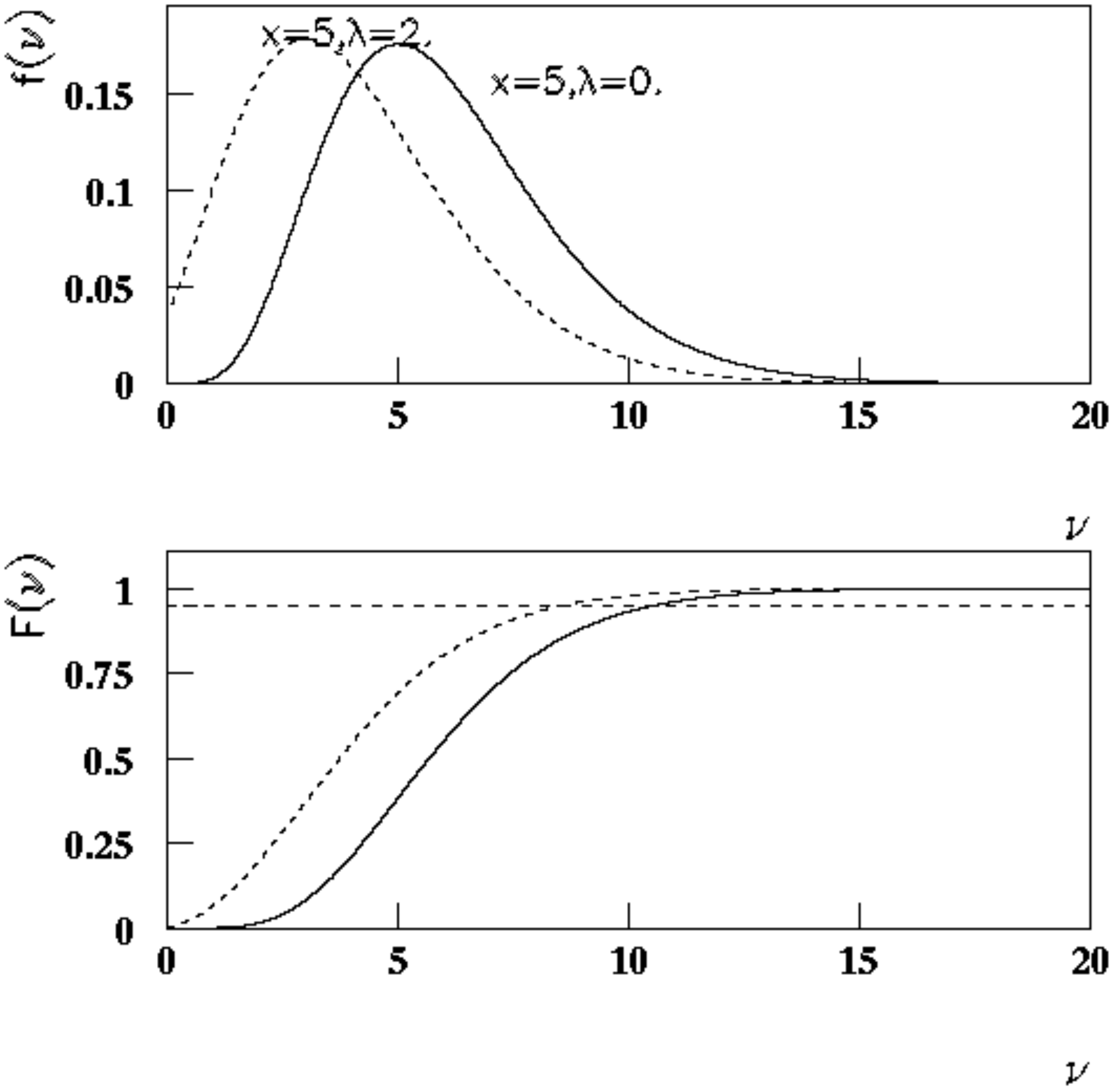
assuming a flat $P_0(\nu)$ and integrating by parts.

$$\boxed{P(\nu|n,\lambda) = \frac{e^{-\nu}(\lambda+\nu)^n}{n!\sum_{i=0}^{n}\frac{\lambda^i}{i!}}}$$

The cumulative pdf is

$$\boxed{F(\nu|n,\lambda) = 1 - \frac{e^{-\nu}\sum_{i=0}^{n}\frac{(\lambda+\nu)^i}{i!}}{\sum_{i=0}^{n}\frac{\lambda^i}{i!}}}$$

Poisson – cont.



Comment:

For n=0, $P(\nu|n, \lambda)=e^{-\nu}$. It does not matter how much background you have, you get the same probability distribution for the signal.

Example

Want to test a new theory – Large Extra Dimensions. If this hypothesis is correct, we expect events with certain characteristics in (let's say) proton-proton collisions. We design an experiment to look for this process.

There will also be indistinguishable events from 'known' physics. The analysis has been designed to reduce these, but there will be some background left.

Background expectation: $\lambda = \sigma_{SM} \cdot \mathcal{L} \cdot a_{SM}$

Signal expectation: $\nu = \sigma_{LED} \cdot \mathcal{L} \cdot a_{LED}$

Have a nearly infinite number of collisions of protons with very small probability to generate an event per bunch crossing: Poisson process

Example

Probabilistic model:

$$P(n_B|\lambda) = \frac{e^{-\lambda}\lambda^{n_B}}{n_B!}$$

$$P(n_S|\nu) = \frac{e^{-\nu}\nu^{n_S}}{n_S!}$$

$$P(n|\lambda,\nu) = \frac{e^{-\mu}\mu^{n}}{n!}$$

$$\mu = \lambda + \nu$$

Example

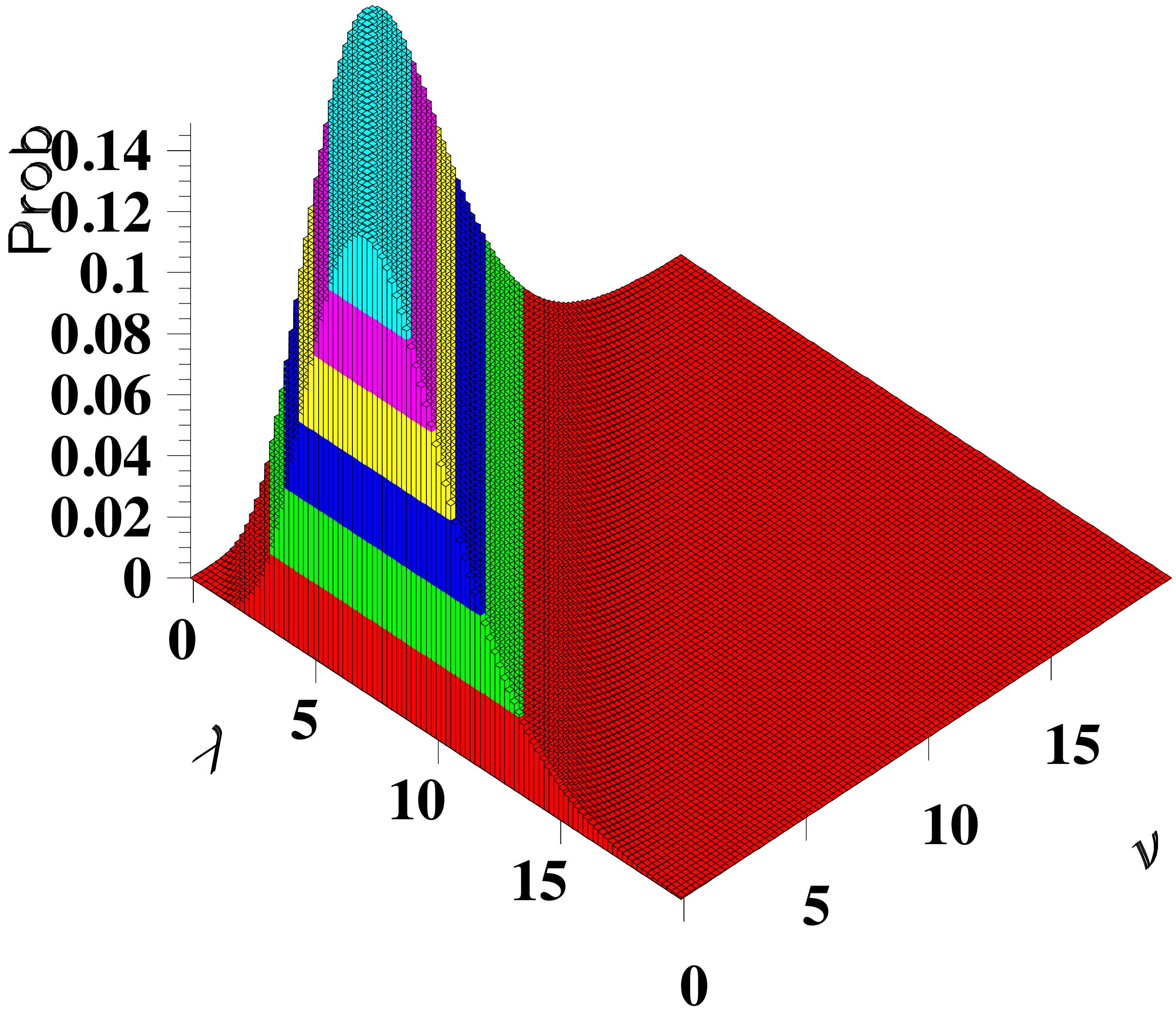
Compare two situations:

1) no knowledge on the background

2) Separate data help us constrain the background

Suppose we measure *n*=7 events, what can we say ?

n=7 Poisson



With Background knowledge - Bayes

$$P(\nu, \lambda|n) = \frac{P(n|\nu, \lambda)P(\lambda)P(\nu)}{\int P(n|\nu, \lambda)P(\lambda)P(\nu)d\lambda d\nu}$$

$$P(n|\lambda, \nu) = \frac{e^{-(\lambda+\nu)}(\lambda + \nu)^n}{n!}$$

$$P(\lambda) = \frac{1}{\sqrt{2\pi}\sigma_\lambda} e^{-\frac{1}{2}\frac{(\lambda-\lambda_0)^2}{\sigma_\lambda^2}}$$

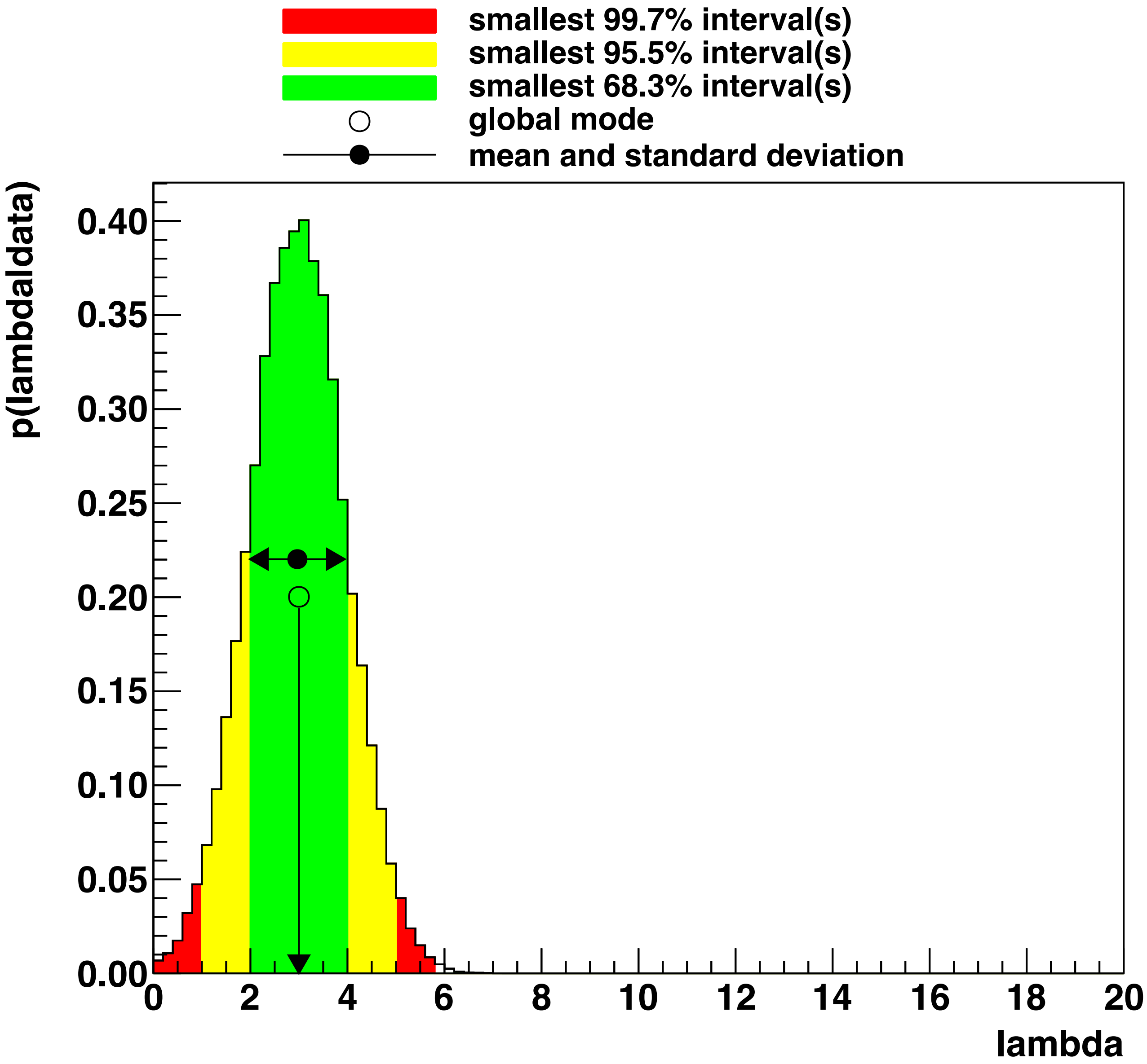
$$P_0(\nu) = \mathrm{constant}$$

We solve this numerically (here with the BAT package) https://www.mpp.mpg.de/bat/

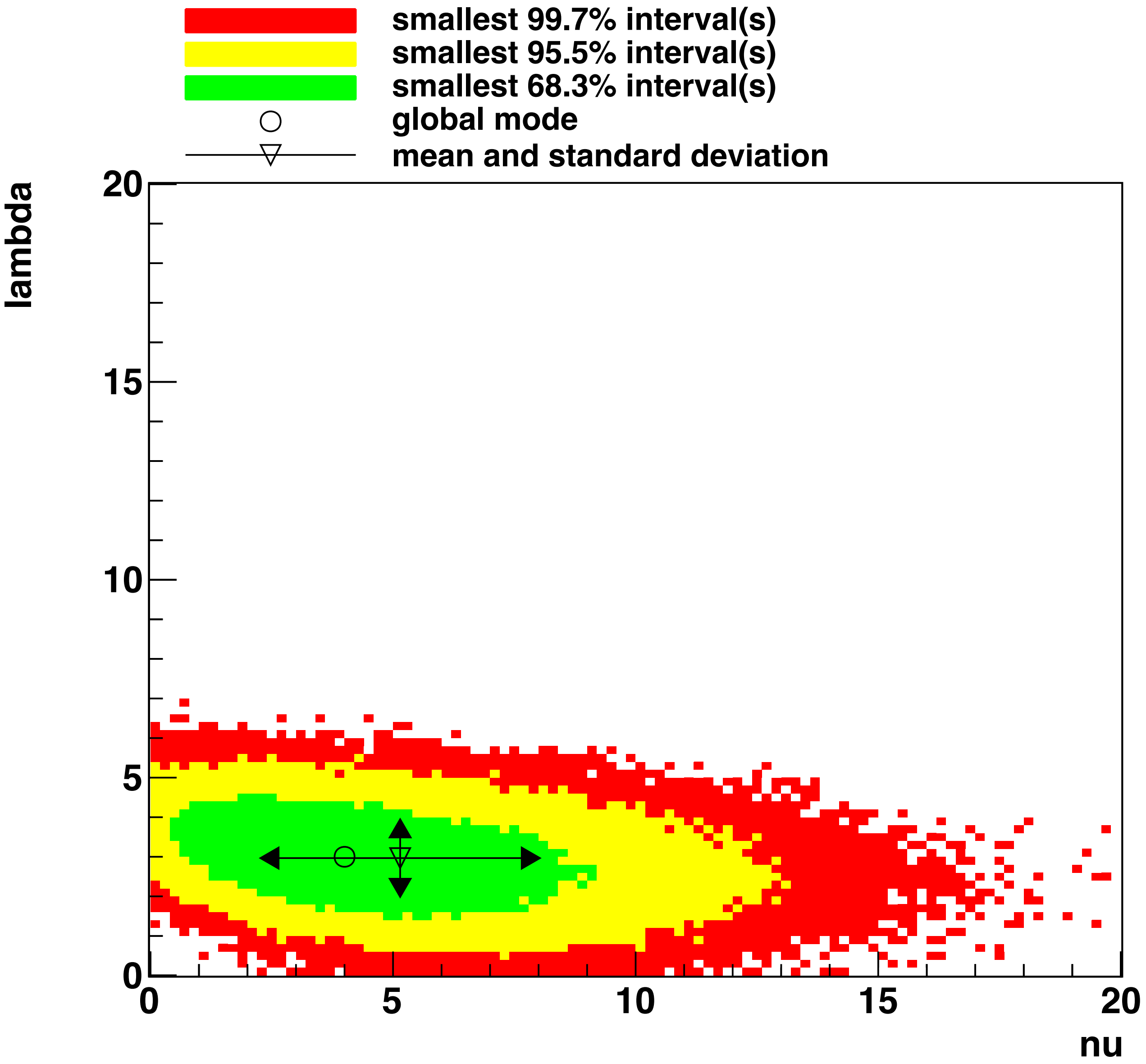
To get a probability distribution for the physics parameter, we marginalize

$$P(\nu|n) = \int P(\nu, \lambda|n)d\lambda$$

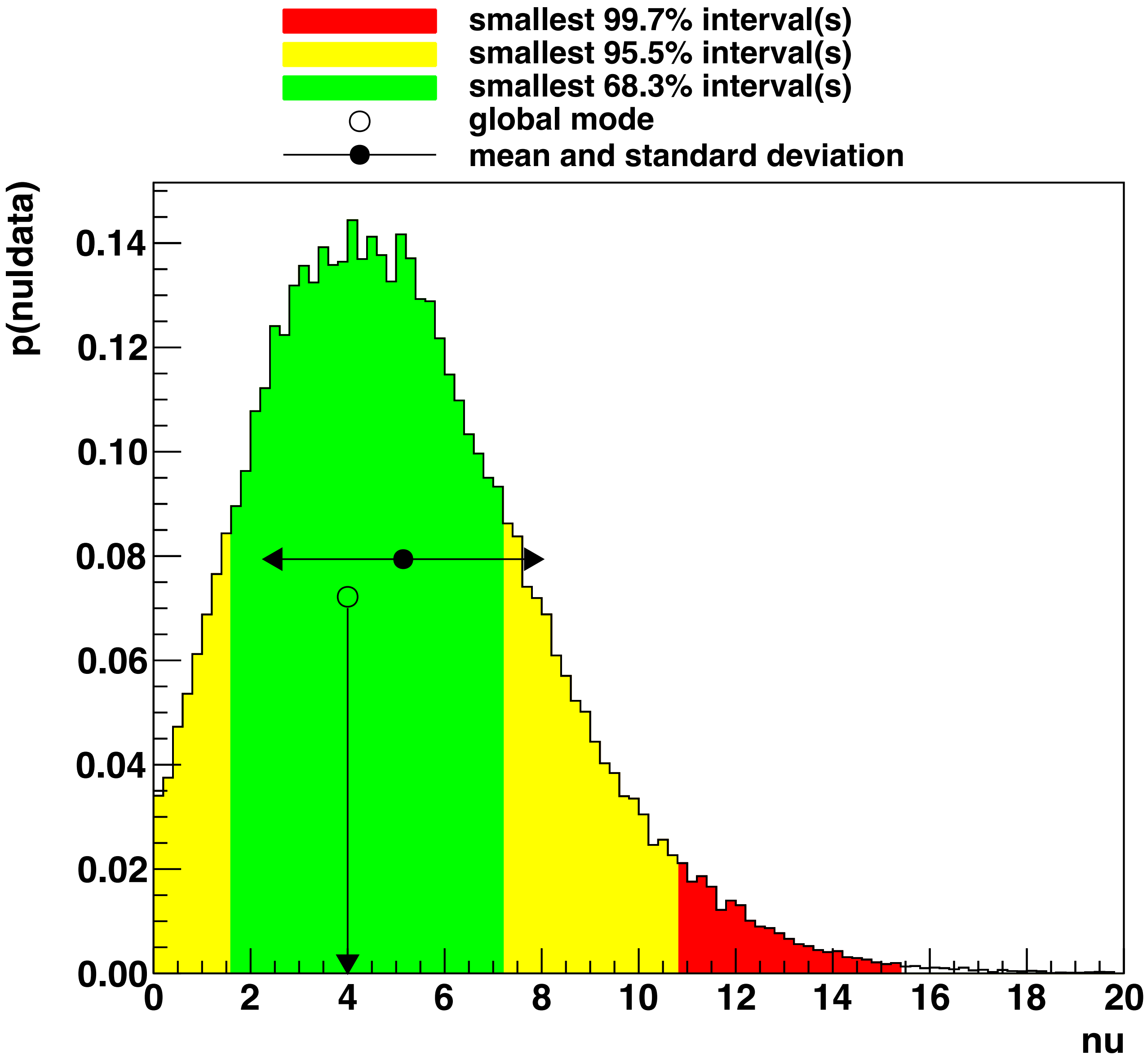
n=7 Constrained Background



n=7 Constrained Background



n=7 Constrained Background



Example: Double Beta Decay

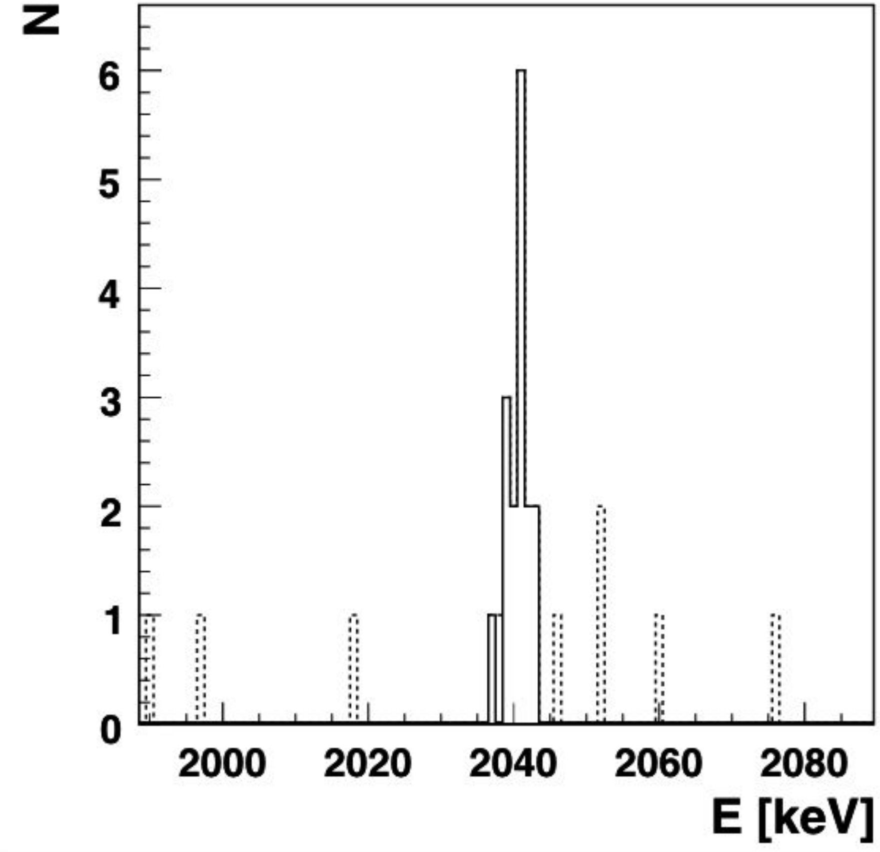
One of the outstanding questions in Particle Physics is whether the neutrino is its own antiparticle (so-called Majorana particle).

The only practical way which has been found to search for the Majorana nature of neutrinos (particle same as antiparticle) is double beta decay (because of the light mass of neutrinos, helicity flip is very unlikely unless the neutrinos have very low energy).

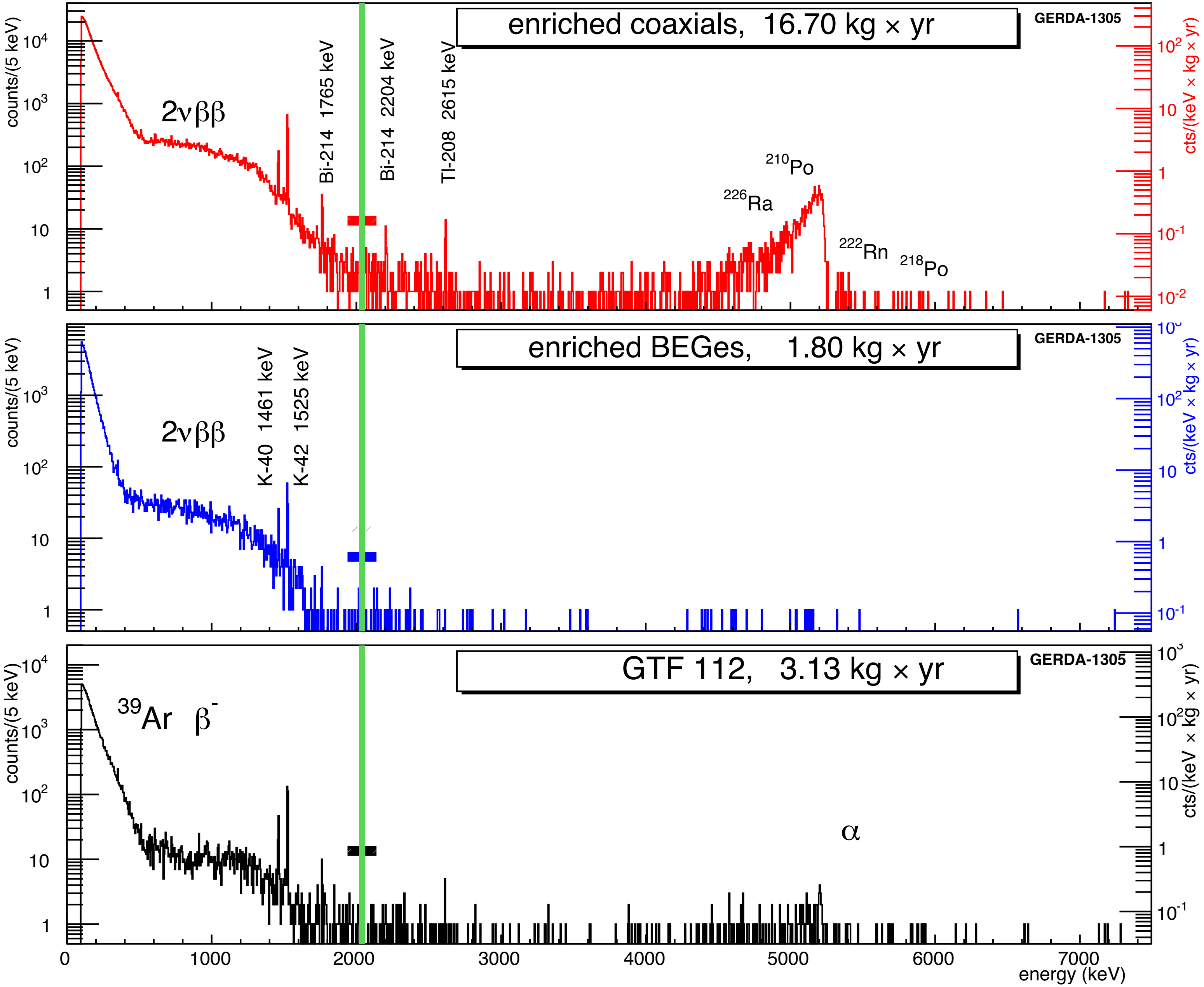
For us, what is interesting is that we are looking for a peak at a well-defined energy in a sparse spectrum.

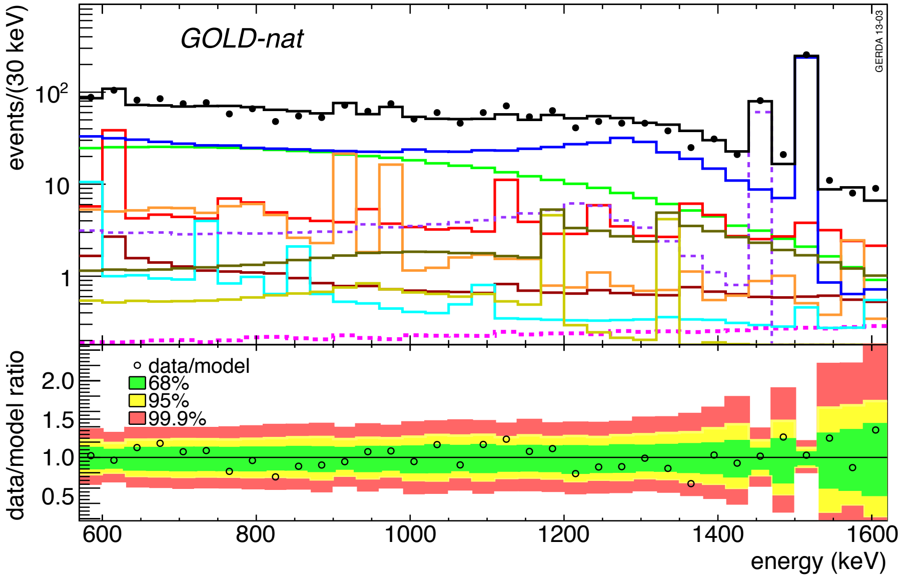
A. Caldwell, K. Kröninger, Phys. Rev. D 74 (2006) 092003

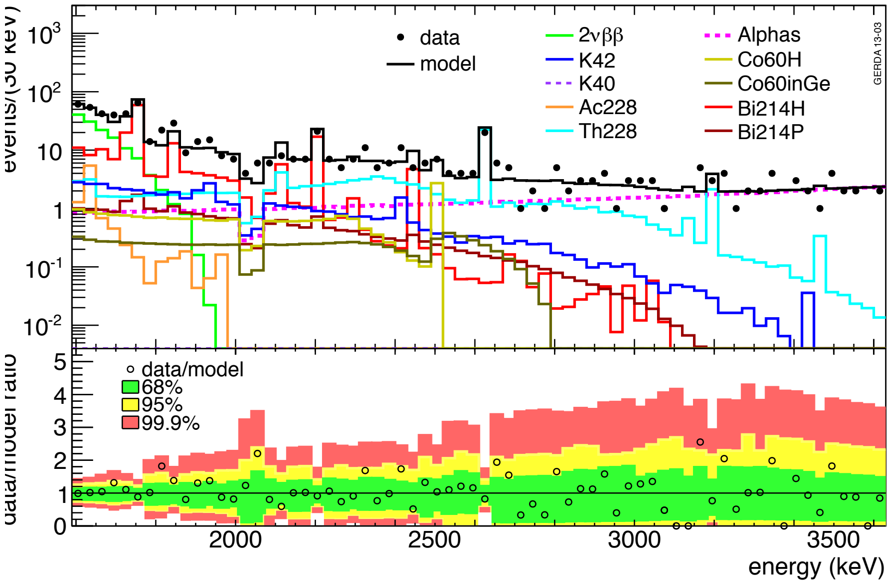
Discovery or not ?



Analyze energy spectrum and decide if there is evidence for a signal. Counting experiment – Poisson statistics.

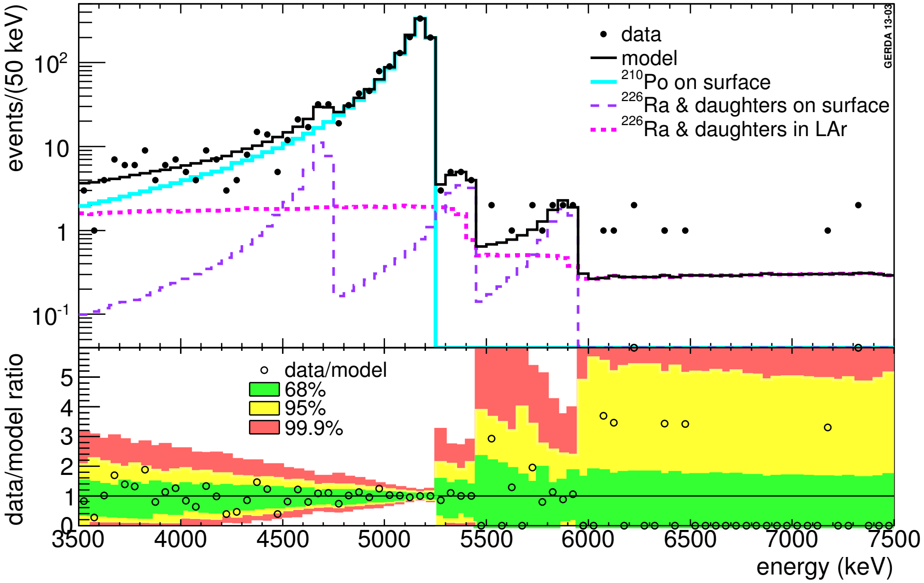

enriched coaxials, 16.70 kg × yr
GERDA-1305
counts/(5 keV)
cts/(keV × kg × yr)
2νββ
Bi-214 1765 keV
Bi-214 2204 keV
Tl-208 2615 keV
226Ra
210Po
222Rn
218Po
enriched BEGes, 1.80 kg × yr
GERDA-1305
K-40 1461 keV
K-42 1525 keV
2νββ
GTF 112, 3.13 kg × yr
GERDA-1305
39Ar β-
α
0
1000
2000
3000
4000
5000
6000
7000
energy (keV)





$$P(\vec{D}|\vec{N}) = \prod_i \frac{e^{-\nu_i}\nu_i^{n_i}}{n_i!}$$

$$\nu_i(\vec{N}) = \sum_j \epsilon_j N_j \int_{\Delta E_i} f_j(E)dE$$



Error Bars for Distributions of Numbers of Events

Ritu Aggarwal, Allen Caldwell

European Physical Journal Plus

Do not put error bars on event counts !

Exercises

1. For the following data set:

Data Set	Source in/out	Run Time	Events
1	Out	1000 s	100
2	In	2000 s	250

a) Plot the probability distribution for the background rate from Data set 1 only

b) Analyze the two data sets simultaneously; plot the 2D probability density for the background and signal rates.

c) Find the 68% central credibility interval for the decay rate. If your sample had a mass of one gram, and the isotope in the sample has an atomic mass of m_A=110 gm/mole, what is the lifetime of the isotope (value with uncertainty) ?

Bayesian Data Analysis

and some other things

A. Caldwell
Max Planck Institute for Physics

1. Another example – fitting an energy spectrum
2. Frequentist intervals and Bayesian intervals for Poisson process
3. P-values; definitions and pitfalls
4. BAT

Max-Planck-Institut für Physik
(Werner-Heisenberg-Institut)

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Example-energy spectrum

Suppose we make a measurement of an energy with a calorimeter. What can we say about the 'true' value ? If we assume a flat prior, we get

$$P(E_0|E) = P(E|E_0) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(E_0-E)^2}{2\sigma^2}}$$

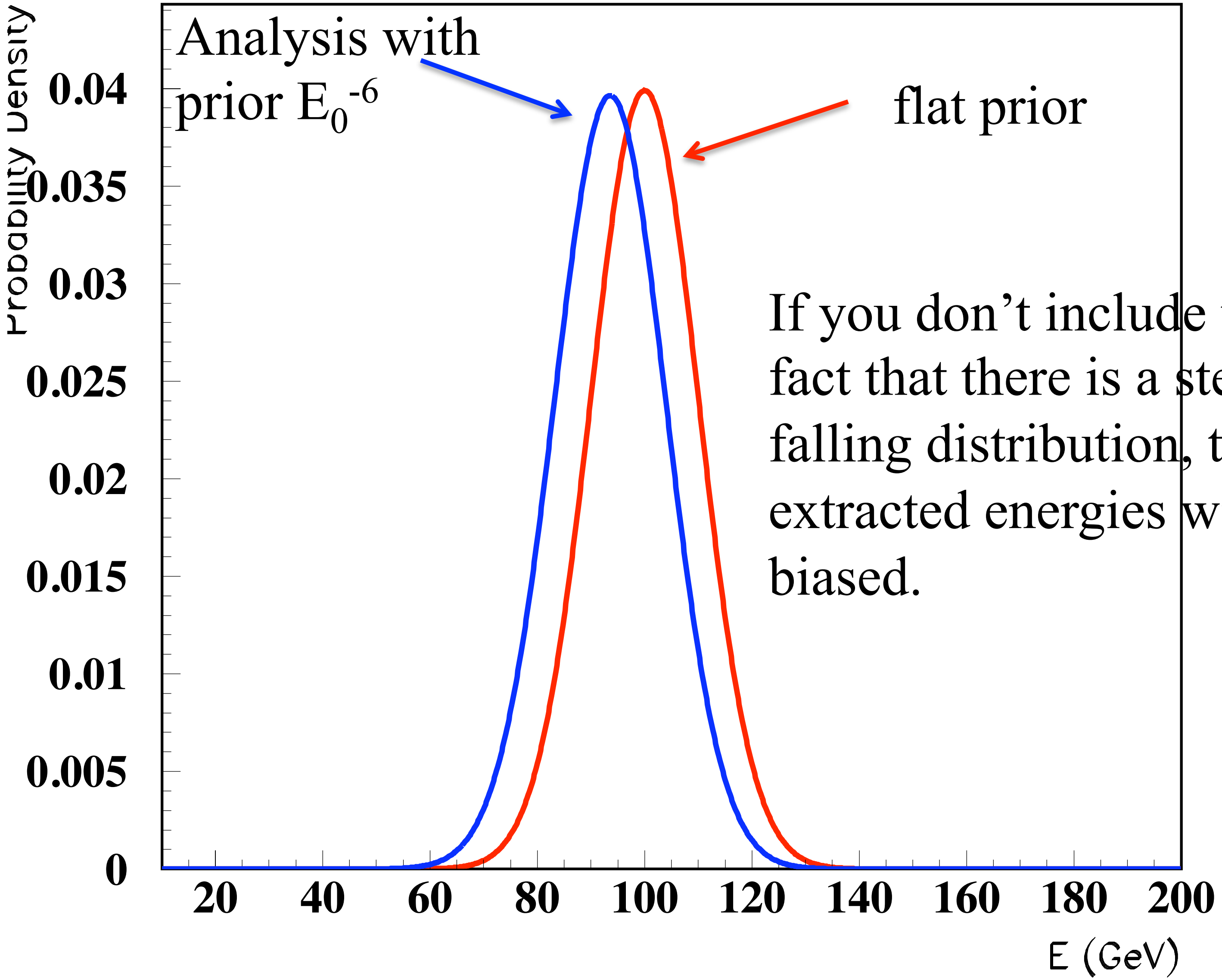
The probability distribution for the true energy is a Gaussian centered on the measured value. However, energy distributions often have a steep distribution. Suppose the starting distribution was

$$f(E_0) \propto E_0^{-6}$$

then

$$f(E) \propto \int \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(E_0-E)^2}{2\sigma^2}} E_0^{-6} dE_0$$

one measurement of the energy, resolution 10 GeV, measured 100 GeV



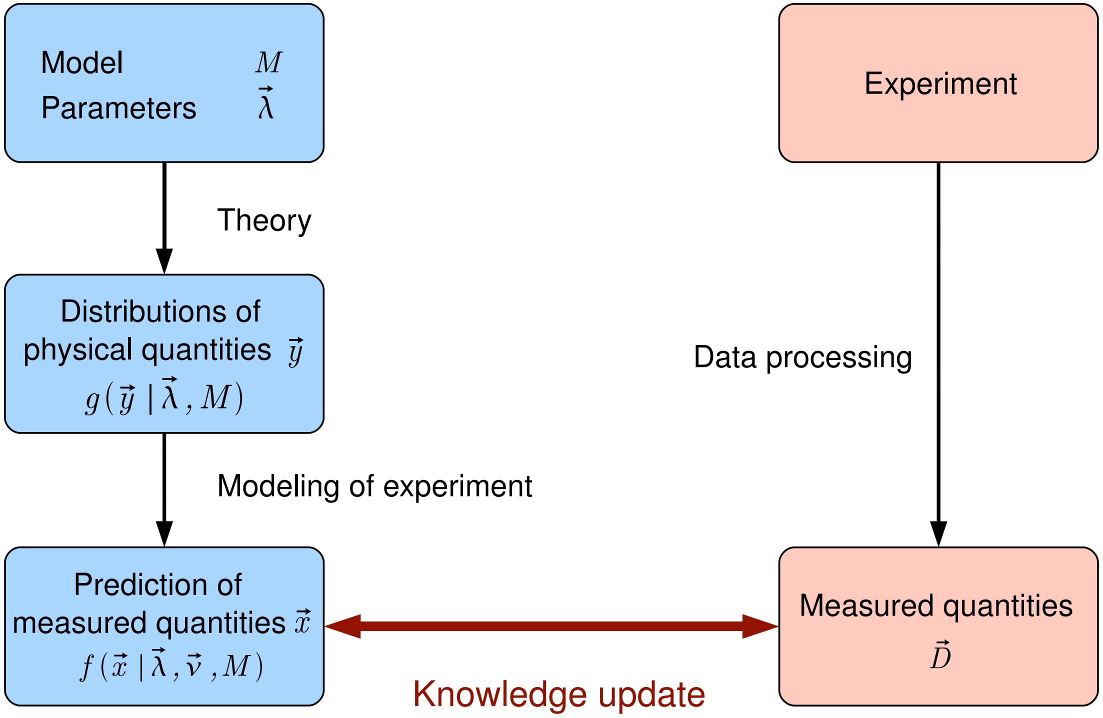
Analysis with prior E_0^{-6}

flat prior

If you don’t include the fact that there is a steeply falling distribution, the extracted energies will be biased.

Power for Energy Spectrum

Suppose what we are trying to extract is the power of the underlying energy distribution. How would we proceed ?


Model M
Parameters $\vec{\lambda}$
Theory
Distributions of physical quantities $\vec{y}$
$g(\vec{y}\,|\,\vec{\lambda}, M)$
Modeling of experiment
Prediction of measured quantities $\vec{x}$
$f(\vec{x}\,|\,\vec{\lambda}, \vec{\nu}, M)$
Experiment
Data processing
Measured quantities
$\vec{D}$
Knowledge update

In this case, assume $g(E_0|\lambda, M) \propto E_0^{-\lambda}$

Power example

We assume the measured values are related to the true as:

$$P(E|E_0) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(E_0 - E)^2}{2\sigma^2}}$$

Now apply the ‘law of total probability’

$$P(E|\lambda) = \int P(E|E_0) P(E_0|\lambda) dE_0$$

And Bayes’ equation yields $P(\lambda|E) \propto \prod_i P(E_i|\lambda) P_0(\lambda)$

$$P(\lambda|E) \propto \left[\prod_i \int \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(E_i - E_0)^2}{2\sigma^2}} E_0^{-\lambda} dE_0 \right] P_0(\lambda)$$

Power example

$$P(\lambda|E) \propto \left[\prod_i \int \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(E_i - E_0)^2}{2\sigma^2}} E_0^{-\lambda} dE_0\right] P_0(\lambda)$$

Need numerical approach.

1. Either integrate numerically many many times during parameter scan.

2. Make a histogram of expected number of entries in measured energy bins from your event simulation, then reweight the distribution for different values of λ and see how the agreement between expected and measured varies (Poisson statistics). Note that this does not use the equation above – in this case

$$P(E|\lambda) = \prod_{i=1}^{Nbins} \frac{e^{-\nu_i}\nu_i^{n_i}}{n_i!}$$

n_i Number of events in energy bin *i*

$\nu_i = \nu_i(\lambda)$ Expectation based on λ

Reweighting a Simulated Distribution

1. Generate events according to a reasonable pdf. In this case, interested in $f(E_0) \propto E_0^{-\lambda}$.

2. Smear the true energy to account for the apparatus resolution. Can also apply other constraints, e.g. lower thresholds on energy measurement, etc.

$$E = E_0 + \delta \qquad P(\delta|E_0) = \frac{1}{\sqrt{2\pi}\sigma(E_0)} e^{-\frac{1}{2}(\frac{\delta}{\sigma(E_0)})^2}$$

$$\sigma(E_0) = \sqrt{a^2 \cdot E_0 + b^2 \cdot E_0^2 + \sigma_n^2}$$

Reweighting Simulated Spectrum

Suppose now you wanted to simulate a distribution with a different power of λ. Can give the simulated events a weight

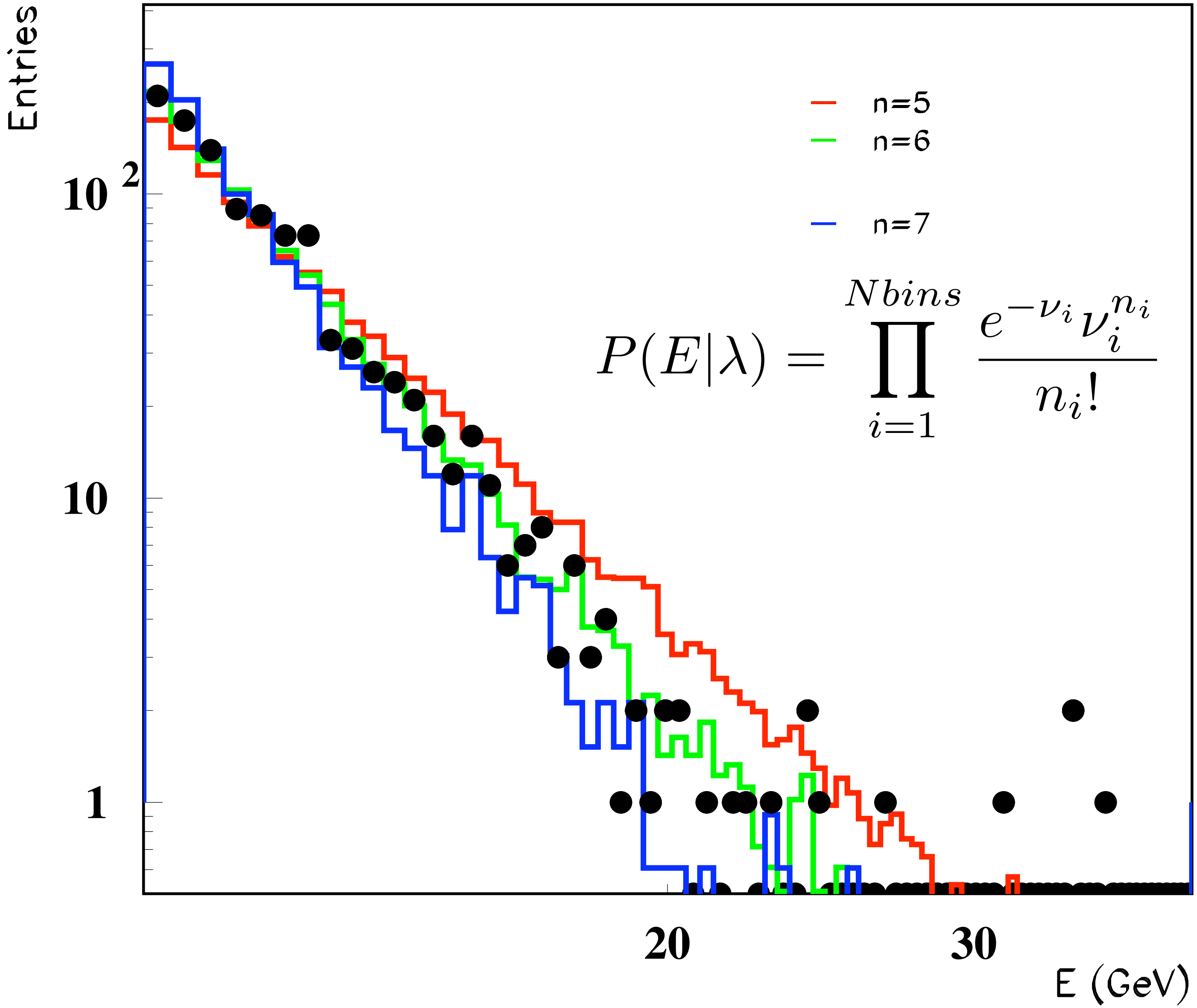
$$w(E_0) = \frac{f(E_0|\lambda')}{f(E_0|\lambda_{\mathrm{gen}})}$$

Statistical uncertainty (in the limit of a large number of events) behaves as

$$\sqrt{\sum_i w(E_{0i})^2}$$

Rule of thumb: avoid large weights (here, initial λ should not be too big) and make sure you have plenty of simulated events !

Power example



$$P(E|\lambda) = \prod_{i=1}^{Nbins} \frac{e^{-\nu_i} \nu_i^{n_i}}{n_i!}$$

Assumes no uncertainty on ν_i

Comparison of Bayesian Credible Intervals & Frequentist Confidence Level Intervals

Bayesian interval from cumulative of the Posterior pdf

Neymann Classical Interval – for each value of the parameter, find set of possible outcomes that contain at least 1-α probability. For the central interval and Poisson distribution:

$$n_1 = \sup_{n \in 0, \ldots, \infty} \left\{ \sum_{i=0}^{n} P(i|\nu) \leq \alpha/2 \right\} + 1$$

$$P(n=0|\nu) > \alpha/2 \rightarrow n_1 = 0$$

$$n_2 = \inf_{n \in 0, \ldots, \infty} \left\{ \sum_{i=n}^{\infty} P(i|\nu) \leq \alpha/2 \right\} - 1$$

$$\mathcal{O}^C_{1-\alpha} = \{n_1, \ldots, n_2\}$$

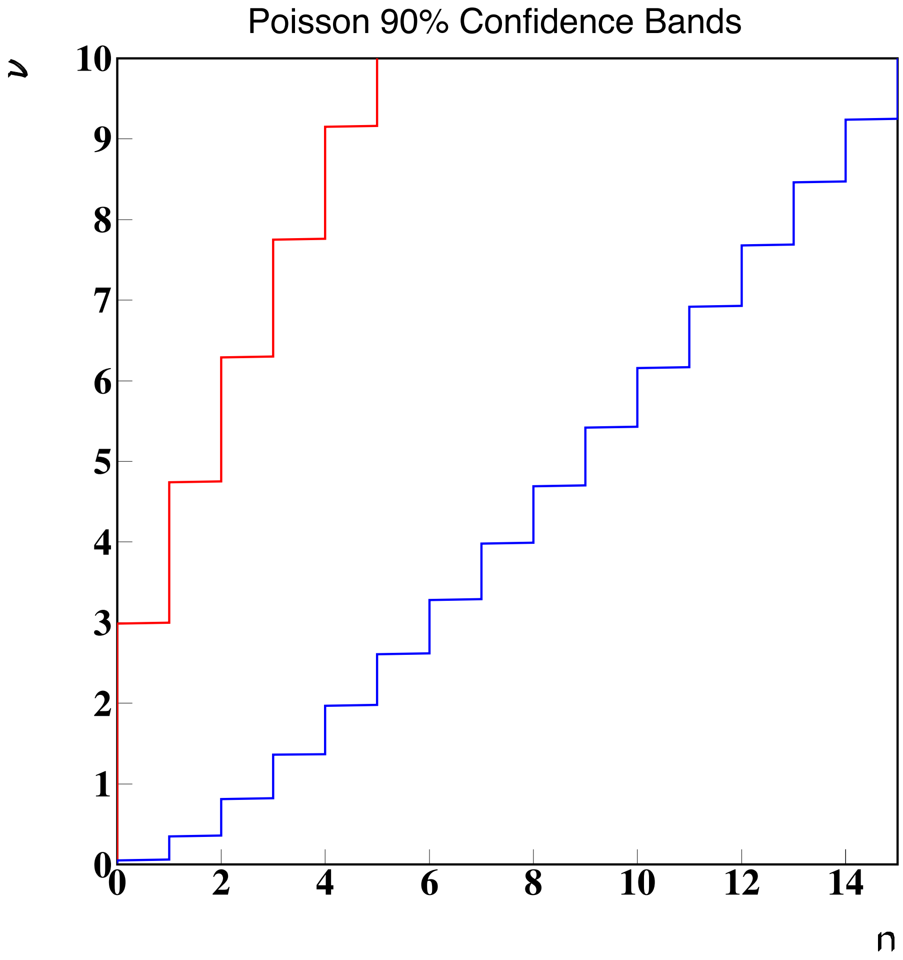
Poisson Example

Example for ν=10/3

n	$P(n\|\nu)$	$F(n\|\nu)$	R	$F_R(n\|\nu)$
0	0.0357	0.0357	7	0.9468
1	0.1189	0.1546	5	0.8431
2	0.1982	0.3528	2	0.4184
3	0.2202	0.5730	1	0.2202
4	0.1835	0.7565	3	0.6019
5	0.1223	0.8788	4	0.7242
6	0.0680	0.9468	6	0.9111
7	0.0324	0.9792	8	0.9792
8	0.0135	0.9927	9	0.9927
9	0.0050	0.9976	10	0.9976
10	0.0017	0.9993	11	0.9993
11	0.0005	0.9998	12	0.9998
12	0.0001	1.0000	13	1.0000

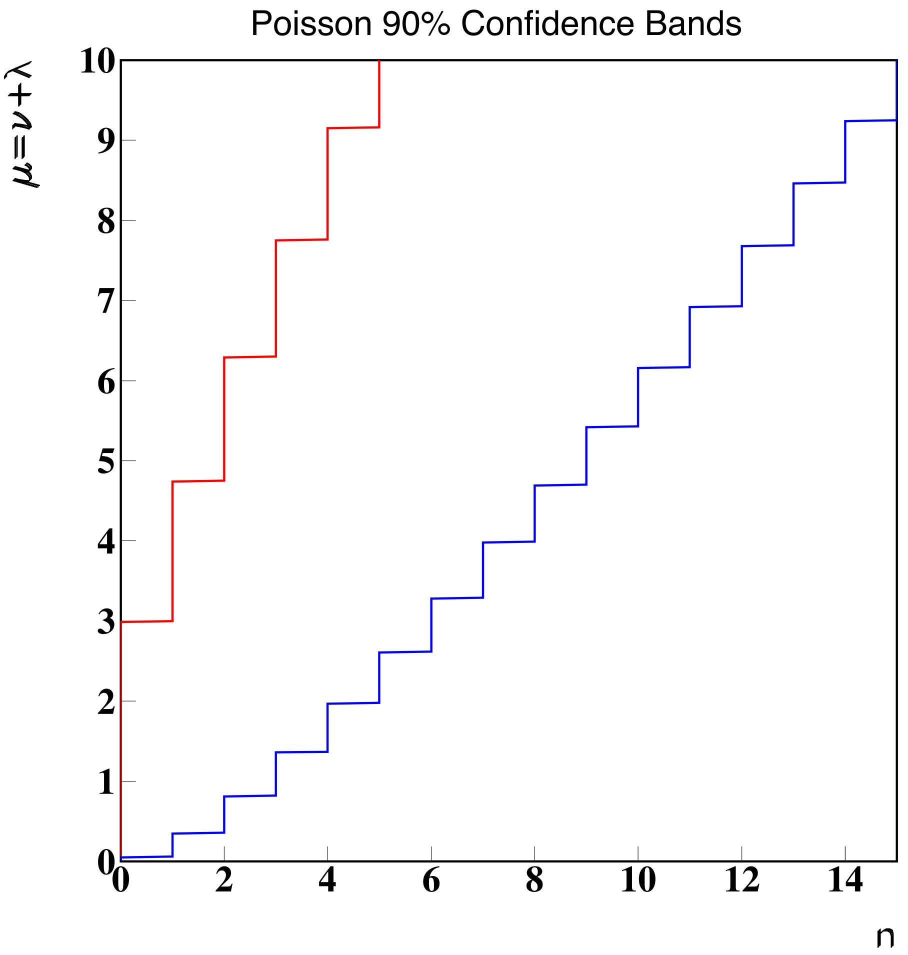
Confidence Level Calculation

We observe n events, and ask which values of ν are accepted with confidence level 1-α. For 1- α=0.9, central intervals:



Frequentist Statistics

Poisson distribution in the presence of background, with mean λ. Then we have the same curves as for signal only, but replace ν with (ν+λ).



- Traditional approach: find limit on μ, then subtract λ to get limit on ν

- limit for ν improves for a fixed n when we add background.

- can get negative limits ! For example, n=0, λ>3 gives ν<0.

Feldman-Cousins Confidence Levels

Imagine we have a Poisson process with known background expectation and unknown signal. If $\lambda \geq 3$ and $n = 0$ then the confidence interval for ν is empty (or includes unphysical values).

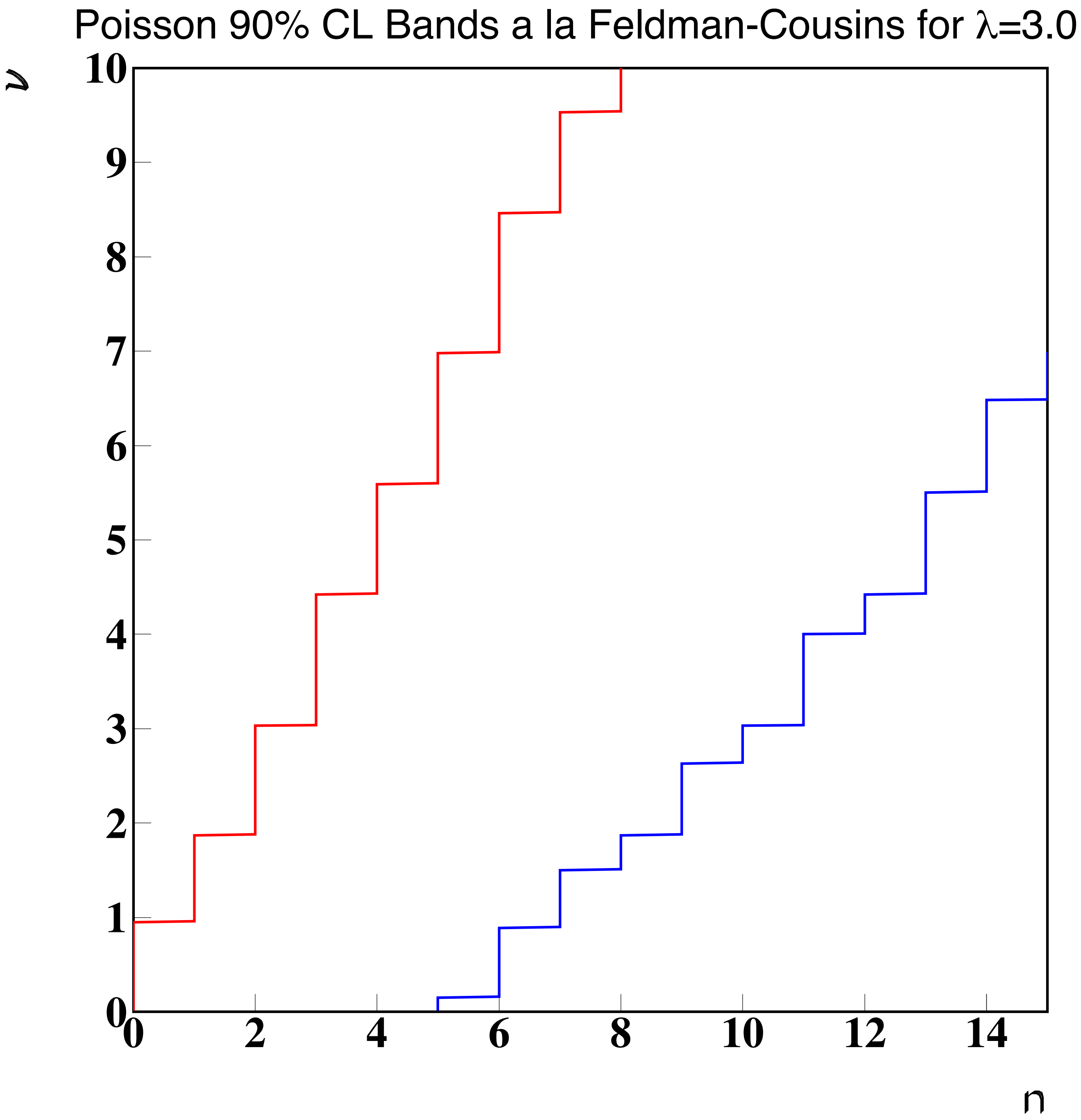
This has led to new definitions for the Confidence Intervals. The most popular (at least in particle physics) is the Feldman-Cousins construction, where a rank is assigned to possible outcomes based on

$$r = \frac{P(n|\mu = \lambda + \nu)}{P(n|\hat{\mu})}$$

Where $\hat{\mu}$ is the value of μ that maximizes $P(n|\mu)$ given the constraints.

Concrete example: $\lambda = 3.0 \quad \nu = 0.\bar{3}$

n	$P(n\|\nu)$	$\hat{\mu}$	$P(n\|\hat{\mu})$	r	Rank	$F_R(n\|\nu)$
0	0.0357	3.0	0.050	0.717	5	0.7565
1	0.1189	3.0	0.149	0.796	4	0.7208
2	0.1982	3.0	0.224	0.885	3	0.6091
3	0.2202	3.0	0.224	0.983	1	0.2202
4	0.1835	4.0	0.195	0.941	2	0.4037
5	0.1223	5.0	0.175	0.699	6	0.8788
6	0.0680	6.0	0.161	0.422	7	0.9468
7	0.0324	7.0	0.149	0.217	8	0.9792
8	0.0135	8.0	0.140	0.096	9	0.9927
9	0.0050	9.0	0.132	0.038	10	0.9976
10	0.0017	10.0	0.125	0.014	11	0.9993
11	0.0005	11.0	0.119	0.004	12	0.9998


Poisson 90% CL Bands a la Feldman-Cousins for λ=3.0
ν
10
9
8
7
6
5
4
3
2
1
0
0
2
4
6
8
10
12
14
n

Comparing Feldman-Cousins with Bayesian Analysis with same background $\lambda = 3.0$ and a flat prior.

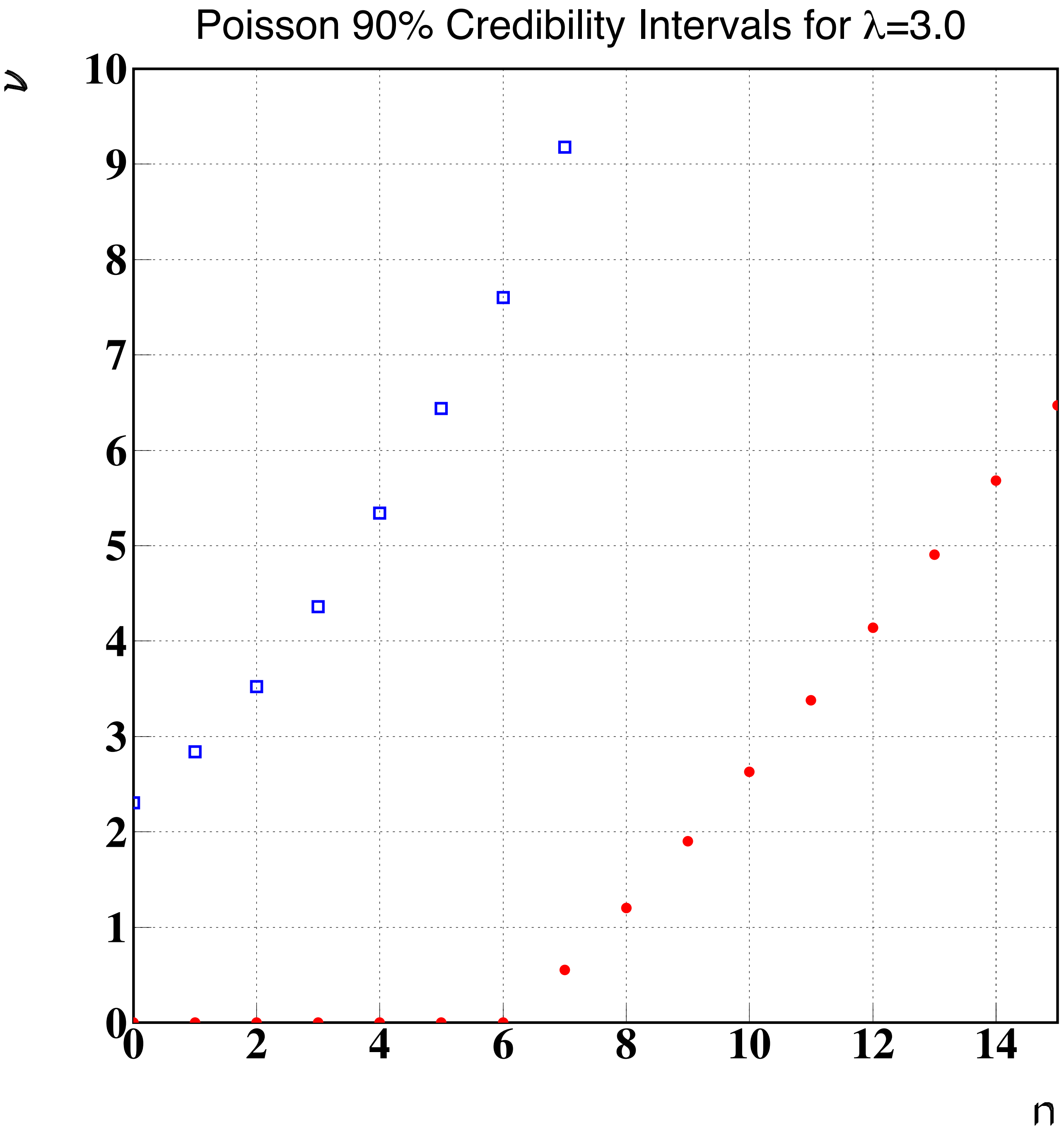
Recall: $P(\nu|n,\lambda) = \dfrac{e^{-\nu}(\lambda+\nu)^n}{n!\sum_{i=0}^{n}\frac{\lambda^i}{i!}}$

$$F(\nu|n,\lambda) = 1 - \frac{e^{-\nu}\sum_{i=0}^{n}\frac{(\lambda+\nu)^i}{i!}}{\sum_{i=0}^{n}\frac{\lambda^i}{i!}}$$

We will take the smallest interval with 90% credibility. I.e.,

$$\int_{P>C} P(\nu|n,\lambda)d\nu = 0.90$$

We find ν_{down} ν_{up} fulfilling this condition. Numerical integration.


Poisson 90% Credibility Intervals for λ=3.0
ν
10
9
8
7
6
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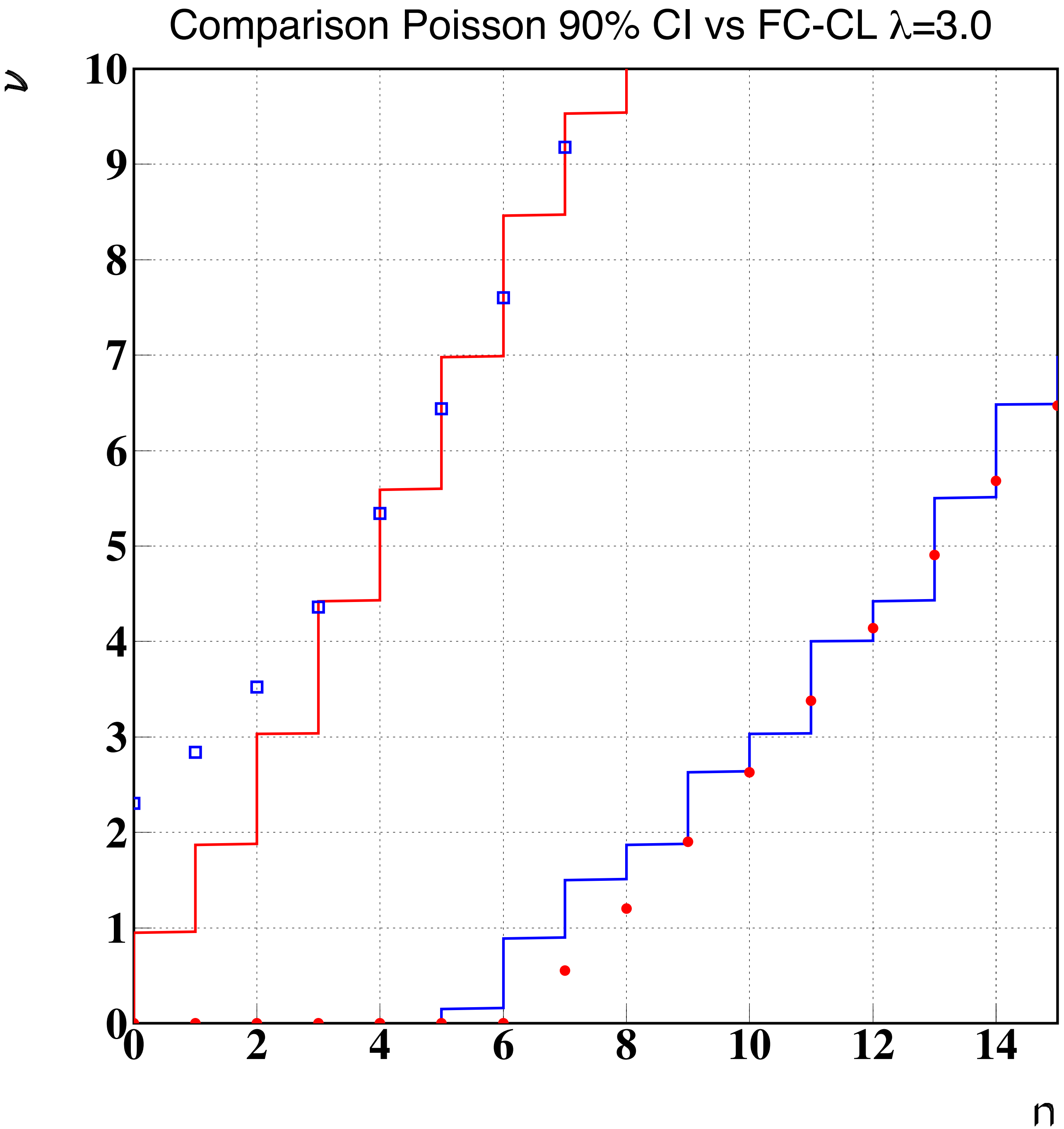
4
3
2
1
0
0
2
4
6
8
10
12
14
n


Comparison Poisson 90% CI vs FC-CL λ=3.0
ν
0
1
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10
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12
14
n

p-values and Goodness-of-fit

In general, we can think of quantities that summarize a 'distance' between the expectation and the observed. E.g., χ^2 is such a quantity. It is a test statistic (scalar function of the data, given the model).

$T(x|M,\lambda)$ Test statistic for possible data *x* given the model M and parameters λ

Create probability density for this quantity:

$$P(T(x|M,\lambda)) = P(x|M,\lambda)\frac{dx}{dT}$$

p-values and Goodness-of-fit

A p-value is a value of the cumulative pdf for the test statistic for some observed value of the data, D.

$$p = F(T(D)) = \int_{T_{\min}}^{T(D)} P(T)dT \qquad (= 1 - p)$$

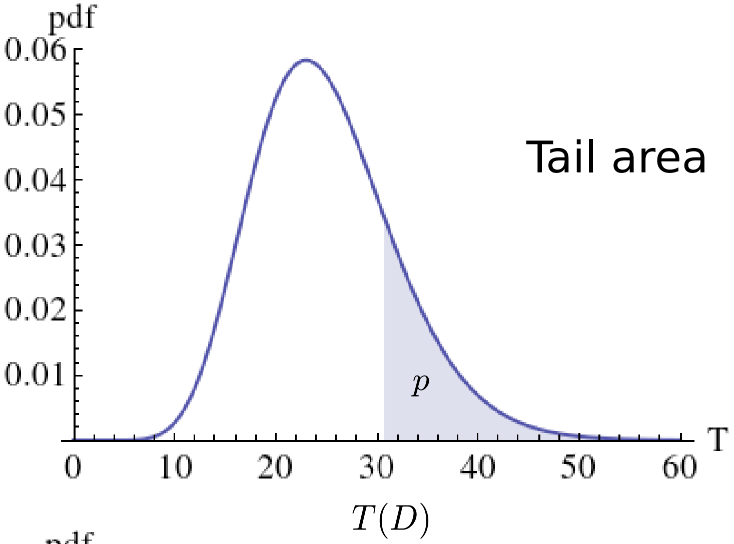
If the model is correct, we expect a flat distribution for p-values between (0,1).

$$P(F) = P(x)\frac{dx}{dF(T)} = \frac{P(x)}{d/dx \int P(T)dT} = \frac{P(x)}{d/dx \int P(x)dx} = 1$$

p-values and Goodness-of-fit

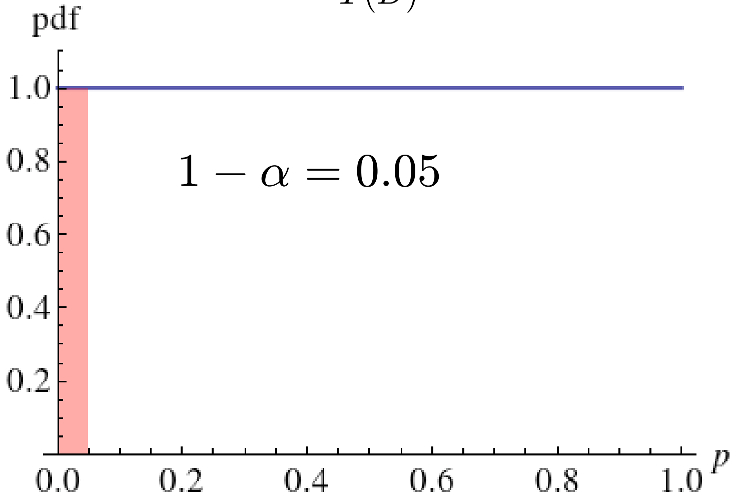
- Definition:

$$p \equiv P(T > T(D)|M)$$



Tail area

- Assuming *M* and before data is taken: *p* uniform in [0,1]



$1 - \alpha = 0.05$

- Confidence level α:

$$p < 1 - \alpha \Rightarrow \text{ reject model}$$

Why do we reject the small p-values if all are equally likely ?

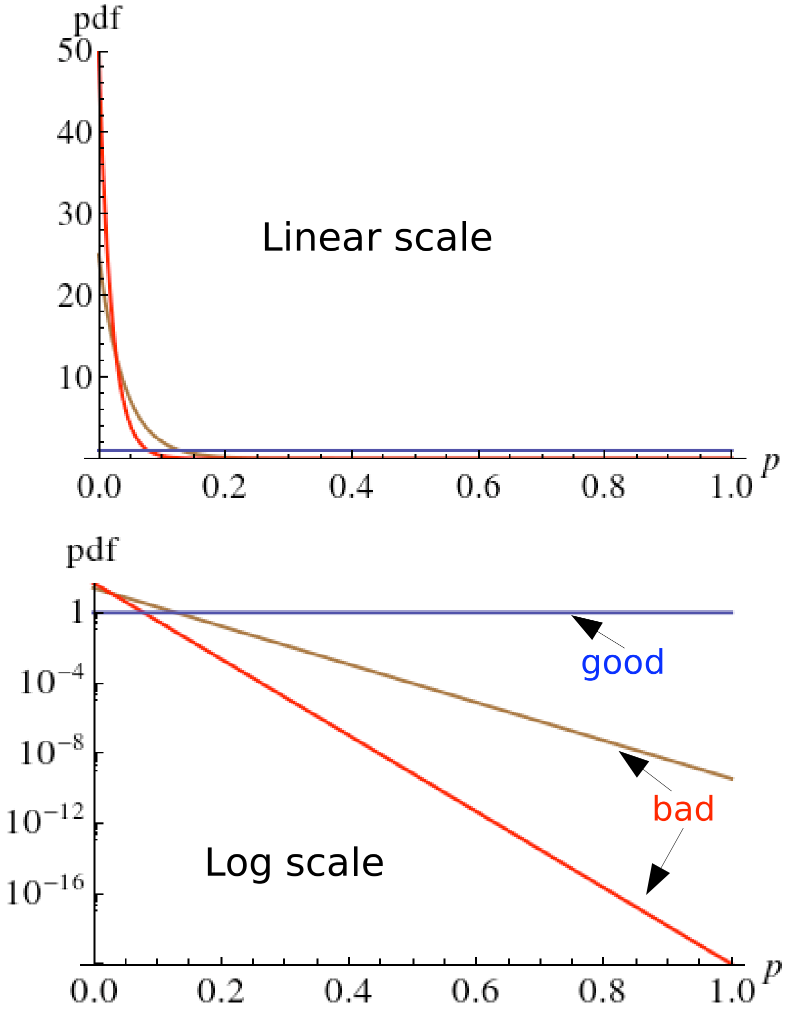
Comment on reasoning behind p-values

- Need prior knowledge about alternatives
- Good model: flat p-value

$$P(p|M_0) = 1$$

- Bad model: peak at *p*=0, sharply falling

$$P(p|M_i) \approx c_i e^{-c_i p} \ , \quad c_i \gg 1$$



Reasoning behind p-values

- Similar prior for all models $P(M_i) \approx P(M_j)$
- Bayes Theorem: $P(M_0|p) \approx \dfrac{P(p|M_0)}{\sum_{i=0}^{K} P(p|M_i)}$

Small *p*

$$P(M_0|p \approx 0) \approx \frac{1}{1 + \sum_{i=1}^{K} c_i} \ll 1$$

Large *p*

$$P(M_0|p \approx 1) \approx 1$$

Bayes Theorem gives justification to p-values

Goodness of Fit

Use χ^2 as our test statistic. The probability distribution of χ^2 is known analytically. This is one of the main reasons why this test statistic is so popular. Strictly only applicable in limited cases (data follow Gaussian distribution from expectation, resolutions are not parameter dependent, if parameters fitted, then function needs to be linear in parameters, …).

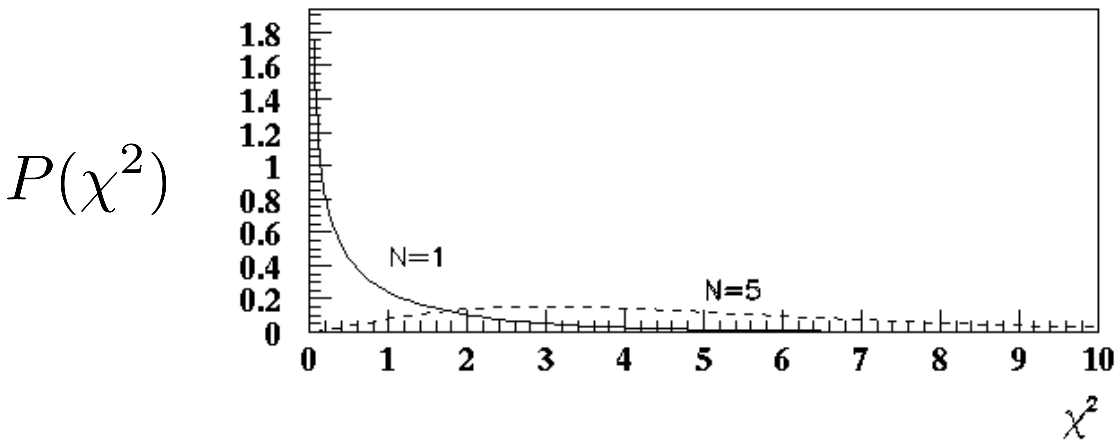
$$\boxed{P(\chi^2)d\chi^2 = \frac{1}{2^{N/2}\Gamma(N/2)} e^{-\chi^2/2}(\chi^2)^{(N/2)-1} d\chi^2}$$

$$\Gamma(n) = (n-1)! \qquad \text{n integer} > 0$$

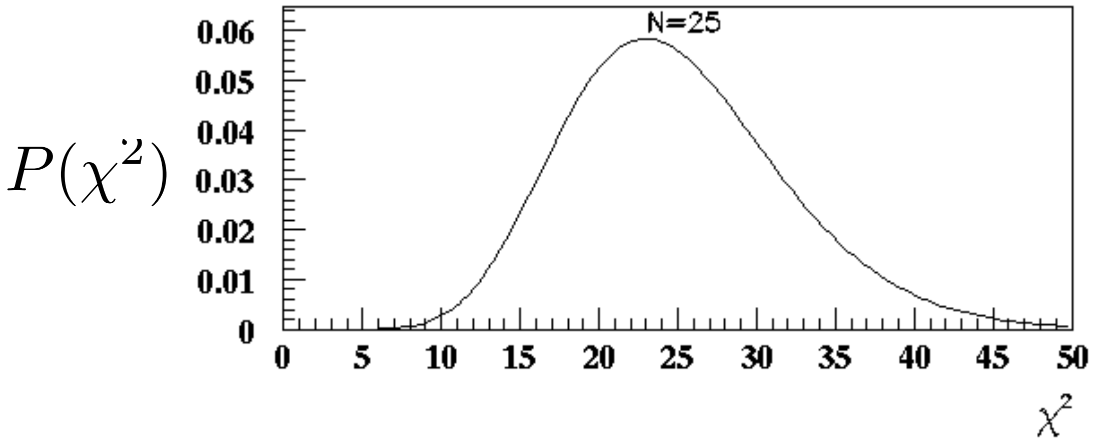
$$\Gamma(n+1/2) = \frac{(2n)!}{4^n n!}\sqrt{\pi} \qquad \text{n integer} \geq 0$$

Goodness of Fit

For a given (least-squares) fit to a set of data, a certain χ^2 value will be obtained. One can then look up in tables whether this value is reasonable by calculating, e.g.,



$$p = \int_{\chi_0^2}^{\infty} P(\chi^2) d\chi^2$$



Warning on p-values

p-values depend critically on how you have chosen the test statistic (or discrepancy variable). The same data set can have hugely varying p-values resulting from different choices of the test quantity.

E.g., consider a model where we assume an exponential decay law. We can define the following probabilities of the data:

Unbinned likelihood

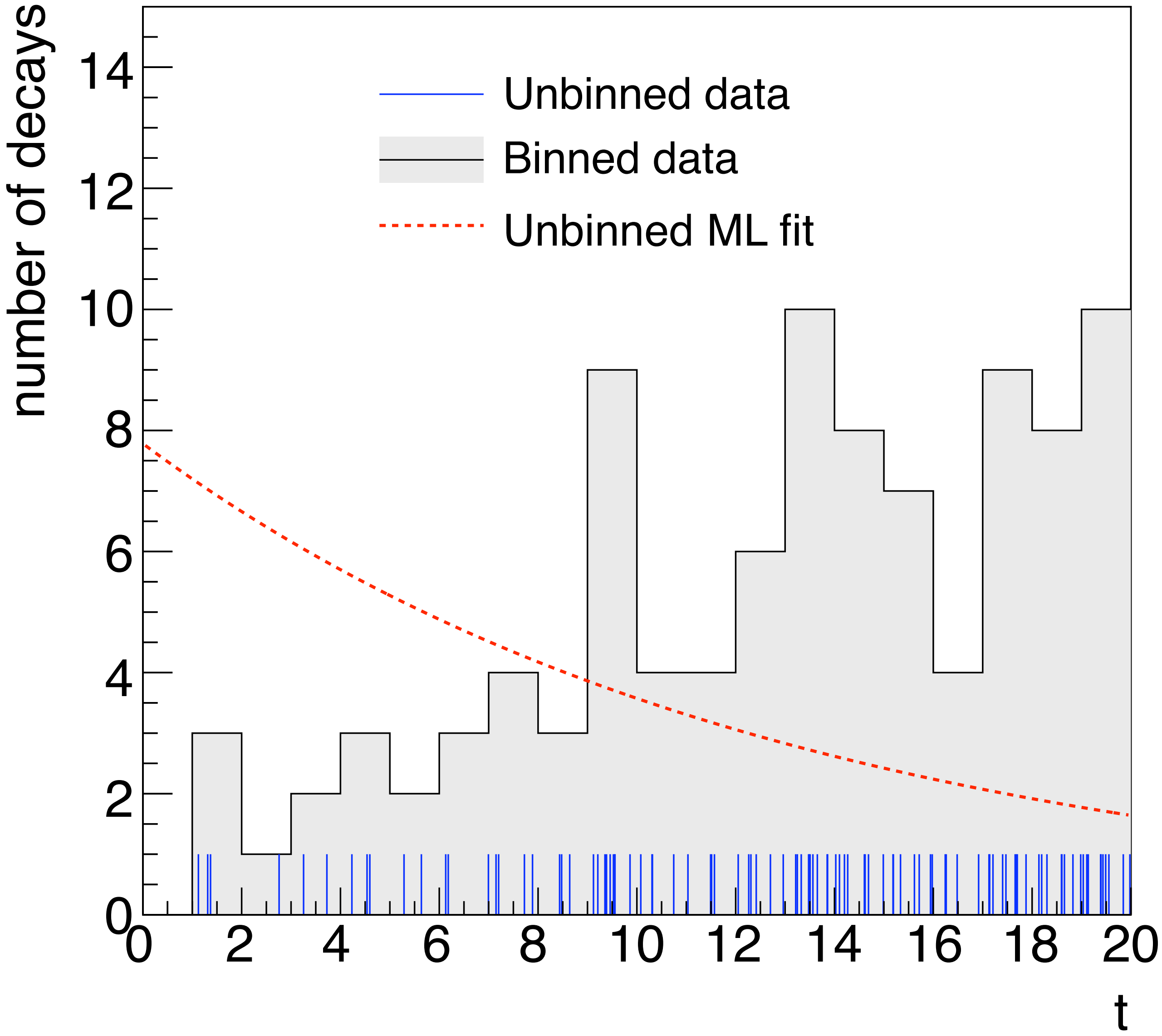
$$P(\vec{t}|\tau) = \prod_{i=1}^{N} \frac{1}{\tau} e^{-t_i/\tau}$$

Binned Poisson distribution

$$P(\vec{t}|\tau) = \prod_{j=1}^{M} \frac{e^{-\nu_j} \nu_j^{n_j}}{n_j!}$$

$$\nu_j = \text{expected events in bin j}$$
$$n_j = \text{observed events in bin j}$$

pitfalls



Assumed model is exponential. Data actually from linearly increasing function.

pitfalls

We take the best fit probability as our test statistic.   For the unbinned fit

$$\tau^* = \frac{1}{N}\sum_{i=1}^{N} t_i$$

$$p = \int_{\sum t_i' > \xi} \mathrm{d}t_1' \int \mathrm{d}t_2' \ldots (\tau^*)^{-N}\, e^{-\sum t_i'/\tau^*} = 1 - P(N,N)$$

Regularized incomplete gamma function

$$P\left(s,x\right) = \frac{\gamma\left(s,x\right)}{\Gamma\left(s\right)} = \frac{\int_0^x t^{s-1} e^{-t}\mathrm{d}t}{\int_0^\infty t^{s-1} e^{-t}\mathrm{d}t}$$

Doesn't depend on the data ! In fact, for large *N*, $p \approx 0.5$

pitfalls

The p-value from the maximum likelihood is about 0.5 !

The p-value from the binned fit is 0

What happened ? The maximum likelihood quantity does not know anything about the distribution of the events, and the result only depends on

$$\tau^* = \frac{1}{N} \sum_{i=1}^{N} t_i$$

and the p-value only depends on N !

Lesson: make sure your test statistic is sensitive to what you want to test ! The fitting program may give you a high p-value and it could well be that the fit function looks nothing like the data.

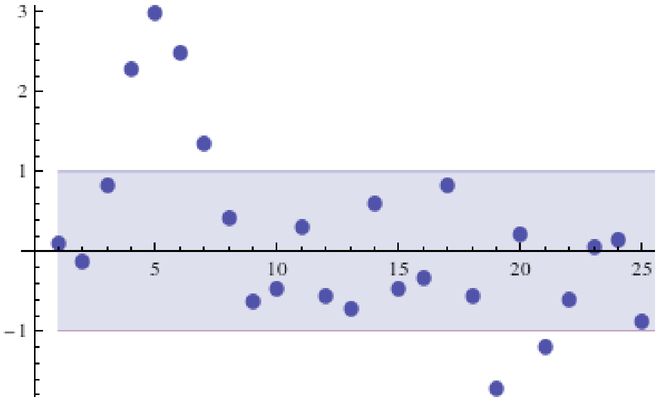
χ^2

- Most statistics disrespect order of data, information wasted

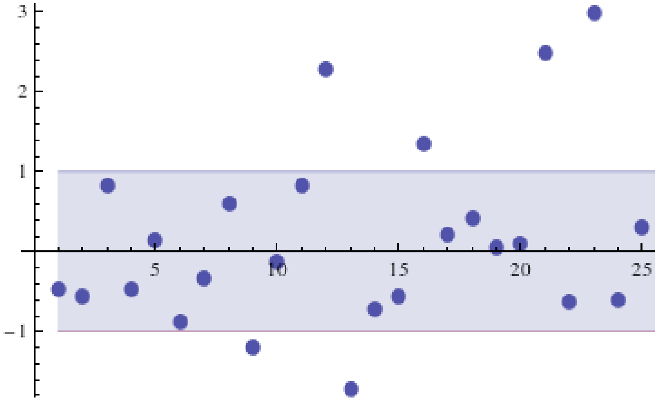
- Human brain good for simple problems

Example:

- Series of N=25 datapoints
- Each Gaussian with mean = 0 and variance = 1



$$\chi^2 = 32.1 \Rightarrow p = 0.16$$



$\Rightarrow$ Can we combine information about **order** and **magnitude of deviation**?

F. Beaujean, A. Caldwell, Jour. Stat. Plan. & Infer. 141 (2011) 3437.

Bayesians and Frequentists

Frequentists make statements of the kind:

‘Assuming the model is correct, this result will occur in XX% of the experiments’

The model is **assumed true**, and estimators for the true parameters in the model are produced from the data.

In the ‘classical’ approach, this is then converted to ‘assuming the model, the bounds [a,b] will contain the true value in XX% of experiments performed’ (confidence levels). Does not imply that the true value is in the range [a,b] with probability XX !

The decision on whether to then believe the model/parameters is left to the individual (subjective). *The inductive part of the reasoning is left out of the analysis.*

Bayesians and Frequentists

Bayesians make statements of the kind:

‘the degree-of-belief in model A is XX (between 0,1)’

Given the new data, the degree-of-belief is updated using the frequencies of possible outcomes in the context of the models (full set)

Credible regions are then defined: with XX% credibility, the parameter is in the interval [a,b]. **Note – very different from a CL.**

The inductive part of the reasoning is built in to the analysis, and the connection between prior beliefs and posterior beliefs is made clear.

Subjective, but the subjective element is made explicit.

Bayesians and Frequentists

In both approaches, work with models and frequencies of outcomes within the model.

Many elements are the same: modeling; picking the most sensitive variables to test the theory, …

There is no right and wrong approach, but you have to understand what you get out of each type of analysis. E.g., don’t confuse confidence levels with probabilities, p-values with support for a model, …

BAT → Software package for solving data analysis problems

Code structured on Bayes' formula for parameter estimation

$$\boxed{P(\vec{\lambda}, M|\vec{D}) = \frac{P(\vec{D}|\vec{\lambda}, M)P(\vec{\lambda}, M)}{P(\vec{D})}}$$

- **The idea behind BAT**
- Merge common parts of every Bayesian analysis into a software package
- Provide flexible environment to phrase arbitrary problems
- Provide a set of well tested/tuned numerical algorithms and tools
- C++ based framework (flexible, modular)
- Interfaces to ROOT, Cuba, Minuit, user defined, ..
- can be downloaded from: http://www.mppmu.mpg.de/bat

Parameter Estimation

The posterior pdf gives the full probability distribution for all parameters, including all correlations – no approximations. If interested in subset of parameters, then marginalize. E.g., for one parameter:

$$P(\lambda_i|\vec{D},M) = \int P(\vec{\lambda}|\vec{D},M)d\vec{\lambda}_{\mathrm{J}\neq i}$$

Can calculate what you need from the posterior pdf. E.g.,

Mode $\overset{\lambda_i}{\max}\{P(\lambda_i|D,M)\}$

+ probability intervals, …

Mean of λ_i $<\lambda_i>=\int P(\lambda_i|\vec{D},M)\lambda_i d\lambda_i$

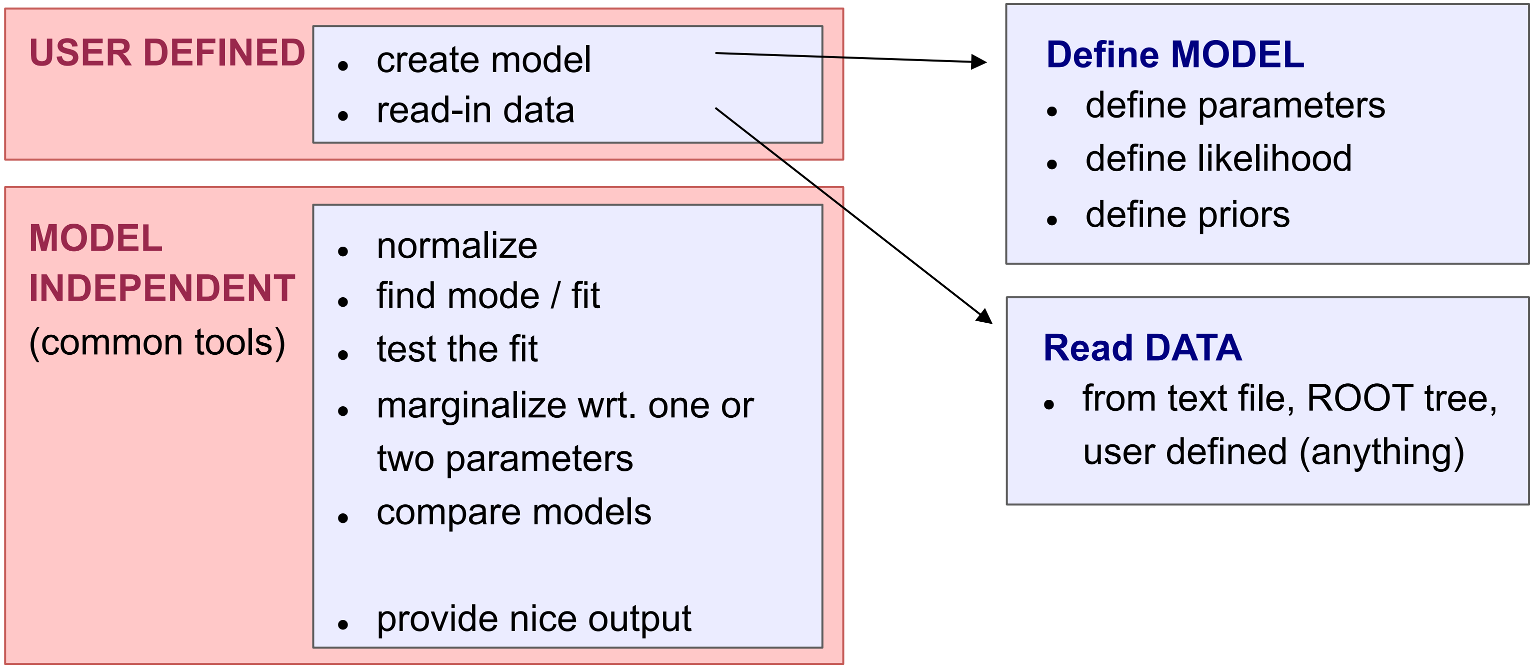
Median $\int_{\lambda_{min}}^{\lambda_{med}} P(\lambda_i|\vec{D},M)d\lambda_i = 0.5$

Can also perform uncertainty propagation w/o approximations

The idea

Separate the common parts from the rest

- case specific: the model and the data
- common tools: all the rest



USER DEFINED

- create model
- read-in data

MODEL INDEPENDENT (common tools)

- normalize
- find mode / fit
- test the fit
- marginalize wrt. one or two parameters
- compare models
- provide nice output

Define MODEL

- define parameters
- define likelihood
- define priors

Read DATA

- from text file, ROOT tree, user defined (anything)

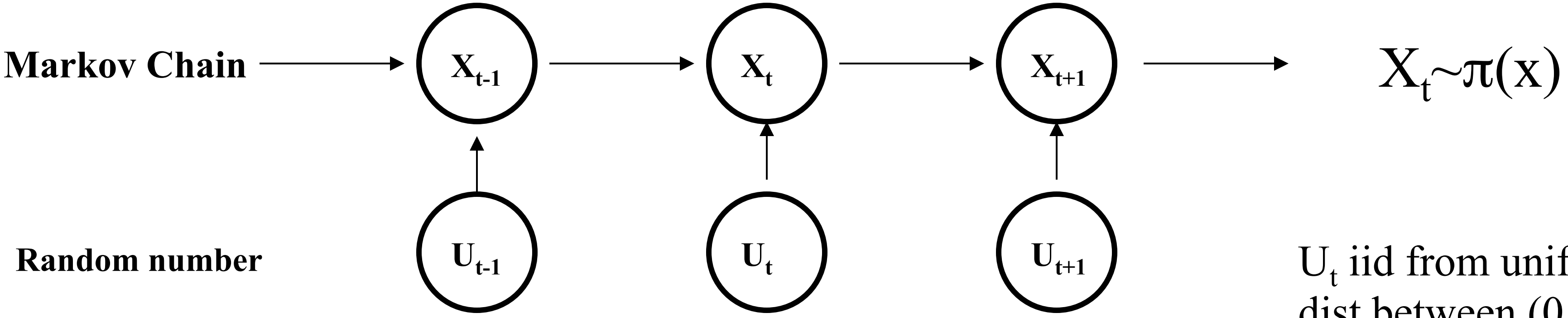
Markov Chain Monte Carlo (MCMC)

- generally it is very difficult to obtain the full posterior PDF
  - number of parameters can be large
  - different input data will result in a different posterior
- also the visualization of the PDF in more than 3 dimensions is rather impractical and hard to understand
- usually one looks at marginalized posterior wrt. one, two or three parameters
  - a projection of the posterior onto one (two, three) parameter
  - integrating all the other parameters out
  - still numerically difficult

- the Markov Chain Monte Carlo revolutionized the area of Bayesian analysis

Markov Chain Monte Carlo

Goal of MCMC is to find a chain with $(\pi_i)_{i=0}^{\infty}$=pdf of interest. Sampling according to the Markov Chain will then correspond to sampling from the desired pdf.



U_t iid from uniform dist between (0,1)

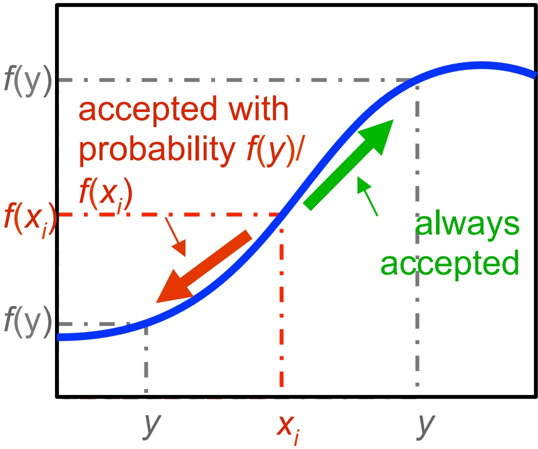
Markov Chain Monte Carlo is any method producing an ergodic Markov chain X_t whose stationary distribution in the distribution of interest.

The original algorithm is due to Metropolis. Later generalized by Hastings.

Metropolis algorithm

- In BAT implemented Metropolis algorithm
- Map positive function ***f*(*x*)** by random walk towards higher probabilities
- Algorithm:

  - Start at some randomly chosen x_i
  - Randomly generate y around x_i
  - If $f(y) \geq f(x_i)$, set $x_{i+1} = y$
  - If $f(y) < f(x_i)$, set $x_{i+1} = y$ with probability $f(y)/f(x_i)$
  - If y not accepted, stay where you are, i.e., set $x_{i+1} = x_i$
  - Generate new y , repeat



- For each step fill the histogram with x_{i+1}
- For infinite number of steps the distribution in the histogram converges to ***f(x)***

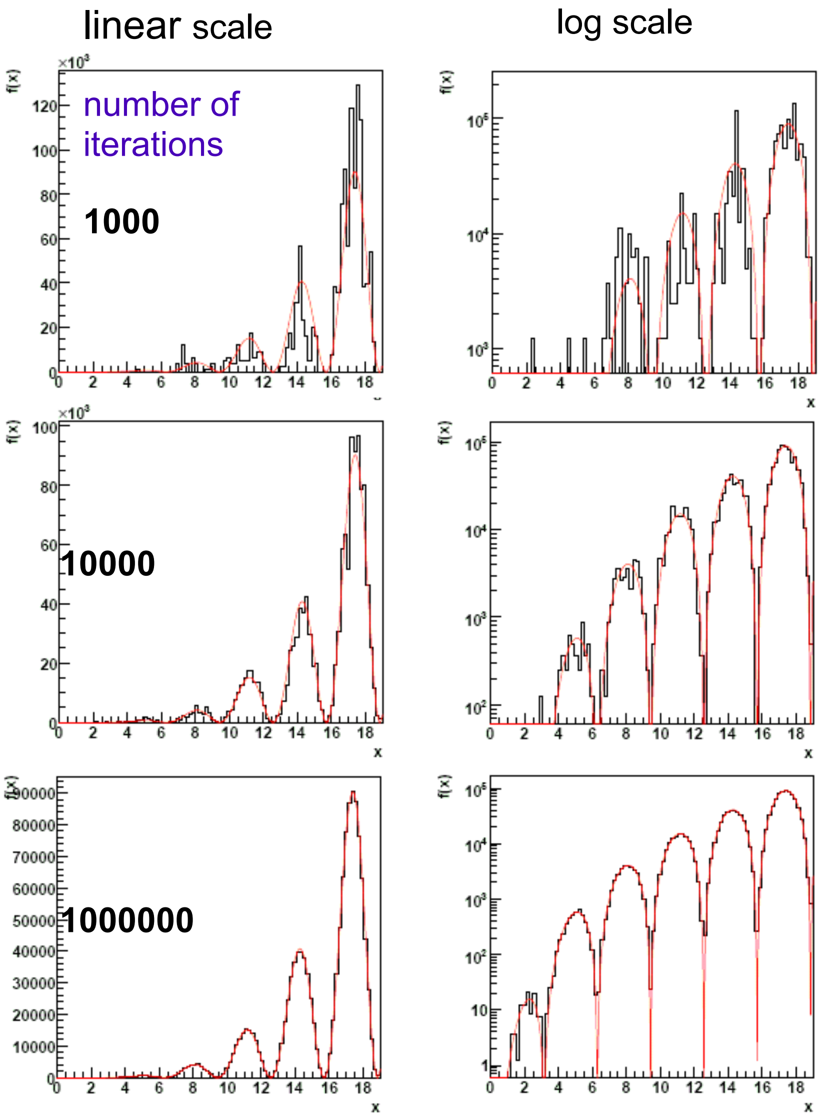
Exercise: try out the Metropolis algorithm to generate a Gaussian distribution from flat rn [0,1]

MCMC: an example

- mapping an arbitrary function:

$$\text{e.g.} \quad f(x) = x^4 \sin^2 x$$

- distribution sampled by MCMC in this case quickly converges towards the underlying distribution
- **mapping of complicated shapes with multiple minima and maxima**

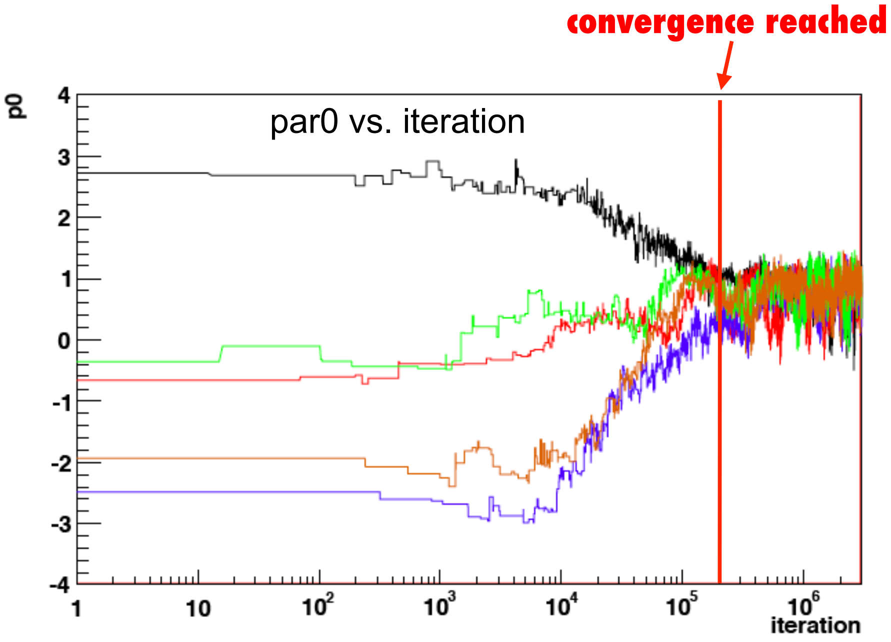


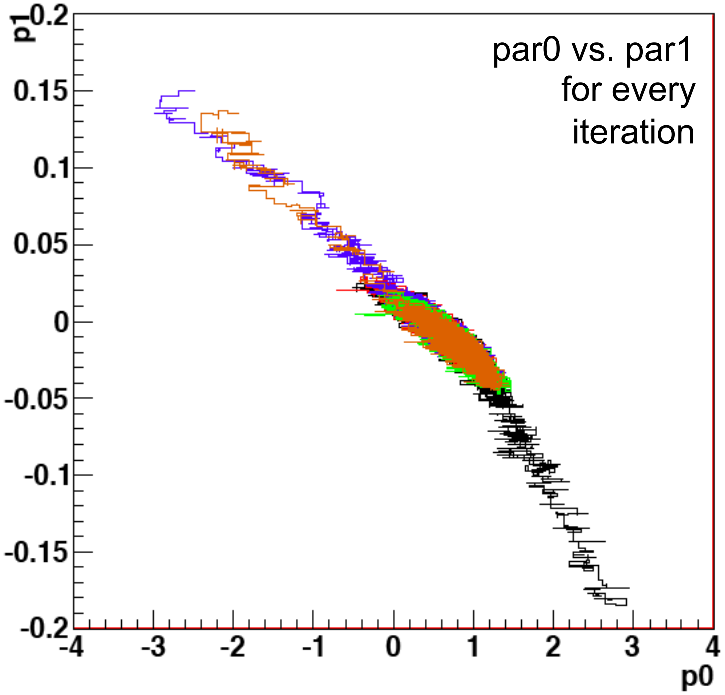
Note:

- MCMC has to become stationary to sample from underlying distribution
- in general the convergence is a non-trivial problem

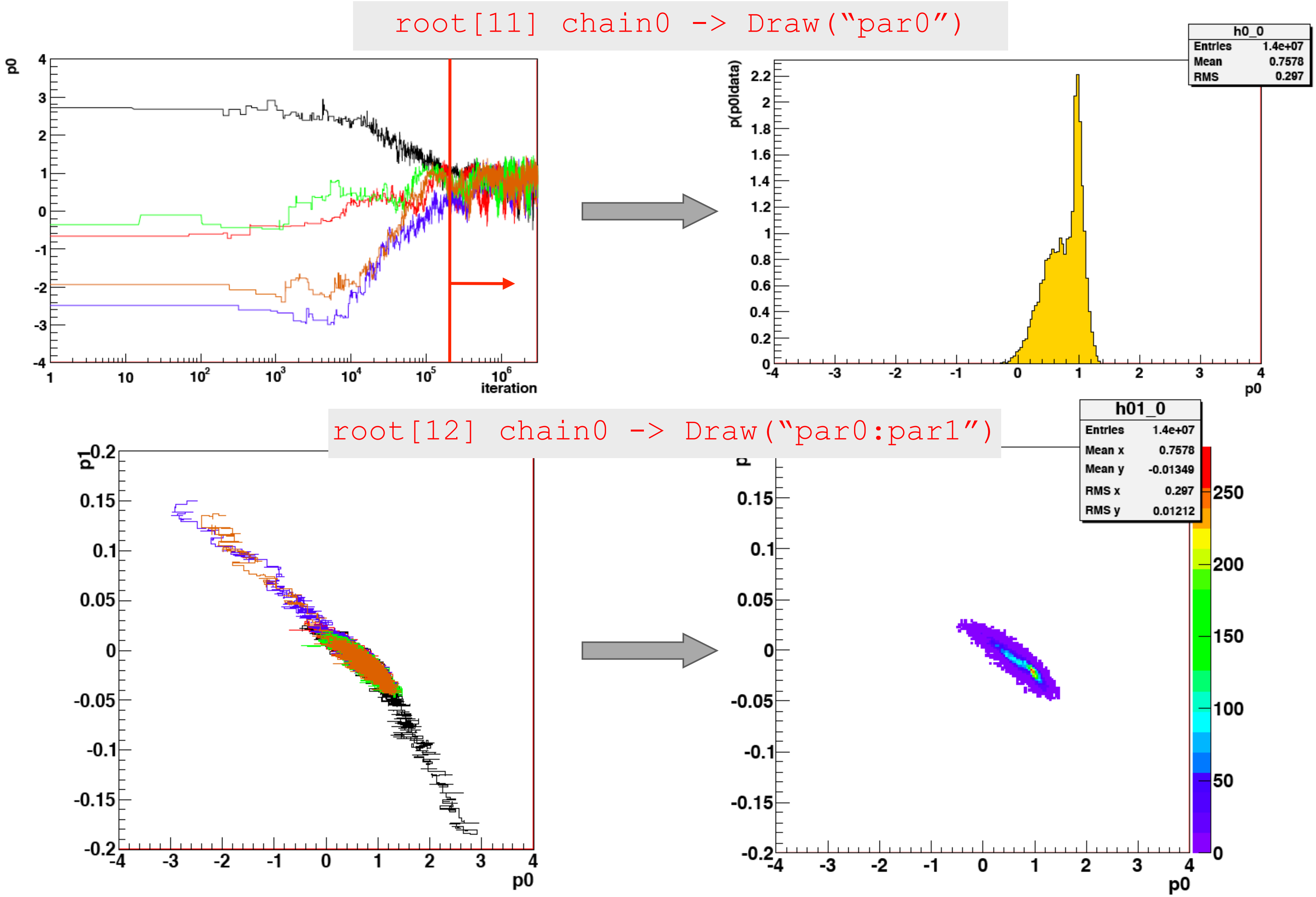
Analysis of Markov Chain

- the full chain(s) can be stored for further analysis and parameter tuning as ROOT TTree(s)
  - allows direct usage of standard ROOT tools for analysis
- Markov Chain contains the complete information about the posterior (except for the normalization)





Obtaining marginalized distributions from TTree



```
root[11] chain0 -> Draw("par0")
```

```
root[12] chain0 -> Draw("par0:par1")
```

Using the Markov Chain

Once you have the chain, it is simple to calculate quantities of interest.

Chain is $\{\lambda_1, \lambda_2, \dots, \lambda_n\}_i \quad i = 1, N$

E.g., pdf for one parameter: just plot $\{\lambda_j\}_i$ joint $\{\lambda_j, \lambda_k\}_i$

Expectation value of a function $E[f(\vec{\lambda})] = \dfrac{1}{N}\displaystyle\sum_{i=1}^{N} f(\lambda_{1i}, \dots, \lambda_{ni})$

Probability distribution of your function: just plot $\{f(\lambda_1, \dots, \lambda_n)\}_i$