Statistics for the LHC

Lecture 4: Bayesian methods and further topics

Academic Training Lectures

CERN, 14–17 June, 2010

indico.cern.ch/conferenceDisplay.py?confId=77830

Glen Cowan
Physics Department
Royal Holloway, University of London
g.cowan@rhul.ac.uk
www.pp.rhul.ac.uk/~cowan

Outline

Lecture 1: Introduction and basic formalism
Probability, statistical tests, parameter estimation.

Lecture 2: Discovery
Quantifying discovery significance and sensitivity
Systematic uncertainties (nuisance parameters)

Lecture 3: Exclusion limits
Frequentist and Bayesian intervals/limits

→ Lecture 4: Further topics
More on Bayesian methods / model selection
The look-elsewhere effect

The Bayesian approach to limits

In Bayesian statistics need to start with 'prior pdf' $\pi(\theta)$, this reflects degree of belief about θ before doing the experiment.

Bayes' theorem tells how our beliefs should be updated in light of the data x:

$$p(\theta|x) = \frac{L(x|\theta)\pi(\theta)}{\int L(x|\theta')\pi(\theta')\,d\theta'} \propto L(x|\theta)\pi(\theta)$$

Integrate posterior pdf $p(\theta\,|\,x)$ to give interval with any desired probability content.

For e.g. $n \sim \text{Poisson}(s+b)$, 95% CL upper limit on s from

$$0.95 = \int_{-\infty}^{s_{\text{up}}} p(s|n)\,ds$$

Bayesian prior for Poisson parameter

Include knowledge that $s \geq 0$ by setting prior $\pi(s) = 0$ for $s<0$.

Could try to reflect 'prior ignorance' with e.g.

$$\pi(s) = \begin{cases} 1 & s \geq 0 \\ 0 & \text{otherwise} \end{cases}$$

Not normalized but this is OK as long as $L(s)$ dies off for large s.

Not invariant under change of parameter — if we had used instead a flat prior for, say, the mass of the Higgs boson, this would imply a non-flat prior for the expected number of Higgs events.

Doesn't really reflect a reasonable degree of belief, but often used as a point of reference;

or viewed as a recipe for producing an interval whose frequentist properties can be studied (coverage will depend on true s).

Bayesian interval with flat prior for s

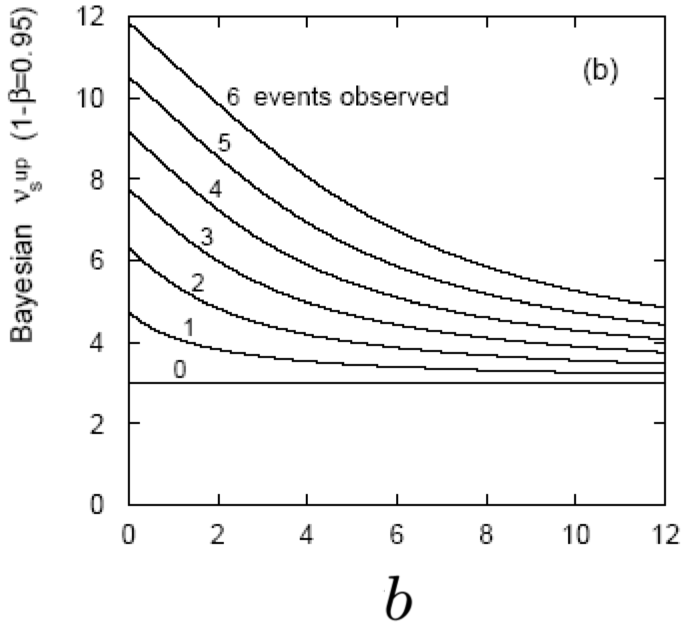
Solve numerically to find limit s_{up}.

For special case $b = 0$, Bayesian upper limit with flat prior numerically same as classical case ('coincidence').

Otherwise Bayesian limit is everywhere greater than classical ('conservative').

Never goes negative.

Doesn't depend on b if $n = 0$.



Priors from formal rules

Because of difficulties in encoding a vague degree of belief in a prior, one often attempts to derive the prior from formal rules, e.g., to satisfy certain invariance principles or to provide maximum information gain for a certain set of measurements.

Often called "objective priors"
Form basis of Objective Bayesian Statistics

The priors do not reflect a degree of belief (but might represent possible extreme cases).

In a Subjective Bayesian analysis, using objective priors can be an important part of the sensitivity analysis.

Priors from formal rules (cont.)

In Objective Bayesian analysis, can use the intervals in a frequentist way, i.e., regard Bayes' theorem as a recipe to produce an interval with certain coverage properties. For a review see:

Robert E. Kass and Larry Wasserman, *The Selection of Prior Distributions by Formal Rules*, J. Am. Stat. Assoc., Vol. 91, No. 435, pp. 1343-1370 (1996).

Formal priors have not been widely used in HEP, but there is recent interest in this direction; see e.g.

L. Demortier, S. Jain and H. Prosper, *Reference priors for high energy physics*, arxiv:1002.1111 (Feb 2010)

Jeffreys' prior

According to *Jeffreys' rule*, take prior according to

$$\pi(\boldsymbol{\theta}) \propto \sqrt{\det(I(\boldsymbol{\theta}))}$$

where

$$I_{ij}(\boldsymbol{\theta}) = -E\left[\frac{\partial^2 \ln L(\boldsymbol{x}|\boldsymbol{\theta})}{\partial\theta_i \partial\theta_j}\right] = -\int \frac{\partial^2 \ln L(\boldsymbol{x}|\boldsymbol{\theta})}{\partial\theta_i \partial\theta_j} L(\boldsymbol{x}|\boldsymbol{\theta})\, d\boldsymbol{x}$$

is the Fisher information matrix.

One can show that this leads to inference that is invariant under a transformation of parameters.

For a Gaussian mean, the Jeffreys' prior is constant; for a Poisson mean μ it is proportional to $1/\sqrt{\mu}$.

Jeffreys' prior for Poisson mean

Suppose $n \sim$ Poisson(μ). To find the Jeffreys' prior for μ,

$$L(n|\mu) = \frac{\mu^n}{n!} e^{-\mu} \qquad \frac{\partial^2 \ln L}{\partial \mu^2} = -\frac{n}{\mu}$$

$$I = -E\left[\frac{\partial^2 \ln L}{\partial \mu^2}\right] = \frac{E[n]}{\mu^2} = \frac{1}{\mu}$$

$$\pi(\mu) \propto \sqrt{I(\mu)} = \frac{1}{\sqrt{\mu}}$$

So e.g. for $\mu = s + b$, this means the prior $\pi(s) \sim 1/\sqrt{(s + b)}$, which depends on b. But this is not designed as a degree of belief about s.

Bayesian limits with uncertainty on *b*

Uncertainty on *b* goes into the prior, e.g.,

$$\pi(s,b) = \pi_s(s)\pi_b(b) \quad \text{(or include correlations as appropriate)}$$

$$\pi_s(s) = \text{const}, \ \sim 1/\sqrt{s+b}\ldots$$

$$\pi_b(b) = \frac{1}{\sqrt{2\pi}\sigma_b} e^{-(b-b_{\text{meas}})^2/2\sigma_b^2} \quad \text{(or whatever)}$$

Put this into Bayes' theorem,

$$p(s,b|n) \propto L(n|s,b)\pi(s,b)$$

Marginalize over *b*, then use $p(s|n)$ to find intervals for *s* with any desired probability content.

Framework for treatment of nuisance parameters well defined; choice of prior can still be problematic, but often less so than finding a "non-informative" prior for a parameter of interest.

Digression: marginalization with MCMC

Bayesian computations involve integrals like

$$p(\theta_0|x) = \int p(\theta_0, \theta_1|x)\, d\theta_1 \ .$$

often high dimensionality and impossible in closed form,
also impossible with 'normal' acceptance-rejection Monte Carlo.

Markov Chain Monte Carlo (MCMC) has revolutionized Bayesian computation.

Google for 'MCMC', 'Metropolis', 'Bayesian computation', ...

MCMC generates correlated sequence of random numbers:

cannot use for many applications, e.g., detector MC;
effective stat. error greater than $\sqrt{n}$.

Basic idea: sample multidimensional $\vec{\theta}$,
look, e.g., only at distribution of parameters of interest.

Comment on priors

Suppose we measure $n \sim \text{Poisson}(s+b)$, goal is to make inference about s.

Suppose b is not known exactly but we have an estimate $\hat{b}$ with uncertainty σ_b.

For Bayesian analysis, first reflex may be to write down a Gaussian prior for b,

$$\pi(b) = \frac{1}{\sqrt{2\pi}\sigma_b} e^{-(b-\hat{b})^2/\sigma_b^2}$$

But a Gaussian could be problematic because e.g.

$b \geq 0$, so need to truncate and renormalize;

tails fall off very quickly, may not reflect true uncertainty.

Gamma prior for b

What is in fact our prior information about b? It may be that we estimated b using a separate measurement (e.g., background control sample) with

$m \sim \text{Poisson}(\tau b)$ (τ = scale factor, here assume known)

Having made the control measurement we can use Bayes' theorem to get the probability for b given m,

$$\pi(b|m) \propto P(m|b)\pi_0(b) \propto \frac{(\tau b)^m}{m!} e^{-\tau b} \pi_0(b)$$

If we take the "original" prior $\pi_0(b)$ to be to be constant for $b \geq 0$, then the posterior $\pi(b|m)$, which becomes the subsequent prior when we measure n and infer s, is a Gamma distribution with:

mean = $(m + 1) / \tau$

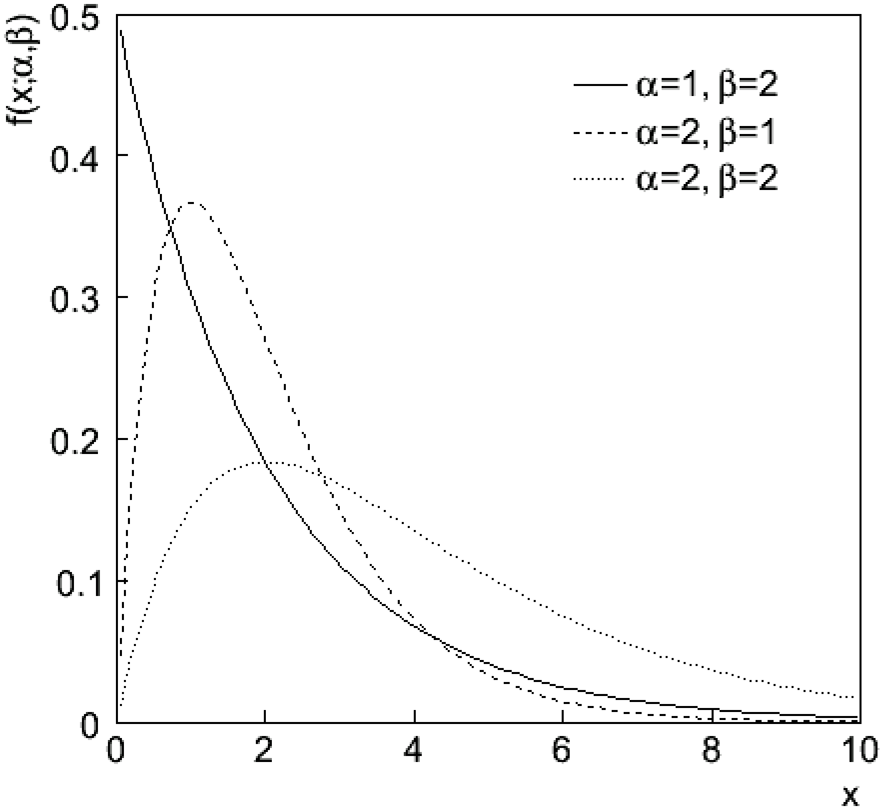
standard dev. = $\sqrt{(m + 1)} / \tau$

Gamma distribution

$$f(x;\alpha,\beta) = \frac{1}{\Gamma(\alpha)\beta^{\alpha}} x^{\alpha-1} e^{-x/\beta}$$

$$E[x] = \alpha\beta$$

$$V[x] = \alpha\beta^2$$



Frequentist approach to same problem

In the frequentist approach we would regard both variables

$n \sim \text{Poisson}(s+b)$
$m \sim \text{Poisson}(\tau b)$

as constituting the data, and thus the full likelihood function is

$$L(s,b) = \frac{(s+b)^n}{n!} e^{-(s+b)} \frac{(\tau b)^m}{m!} e^{-\tau b}$$

Use this to construct test of s with e.g. profile likelihood ratio

$$\lambda(s) = \frac{L(s, \hat{\hat{b}})}{L(\hat{s}, \hat{b})}$$

Note here that the likelihood refers to both n and m, whereas the likelihood used in the Bayesian calculation only modeled n.

Bayesian model selection ('discovery')

The probability of hypothesis H_0 relative to an alternative H_1 is often given by the posterior odds:

no Higgs

$$\frac{P(H_0|x)}{P(H_1|x)} = \frac{P(x|H_0)}{P(x|H_1)} \times \frac{\pi(H_0)}{\pi(H_1)}$$

Higgs

Bayes factor B_{01}

prior odds

The Bayes factor is regarded as measuring the weight of evidence of the data in support of H_0 over H_1.

Interchangeably use $B_{10} = 1/B_{01}$

Assessing Bayes factors

One can use the Bayes factor much like a p-value (or Z value).

There is an "established" scale, analogous to our 5σ rule:

B_{10}	Evidence against H_0
1 to 3	Not worth more than a bare mention
3 to 20	Positive
20 to 150	Strong
> 150	Very strong

Kass and Raftery, *Bayes Factors*, J. Am Stat. Assoc 90 (1995) 773.

Will this be adopted in HEP?

Rewriting the Bayes factor

Suppose we have models H_i, $i = 0, 1, \ldots,$

each with a likelihood $p(x|H_i, \vec{\theta}_i)$

and a prior pdf for its internal parameters $\pi_i(\vec{\theta}_i)$

so that the full prior is $\pi(H_i, \vec{\theta}_i) = p_i \pi_i(\vec{\theta}_i)$

where $p_i = P(H_i)$ is the overall prior probability for H_i.

The Bayes factor comparing H_i and H_j can be written

$$B_{ij} = \frac{P(H_i|\vec{x})}{P(H_i)} \Big/ \frac{P(H_j|\vec{x})}{P(H_j)}$$

Bayes factors independent of $P(H_i)$

For B_{ij} we need the posterior probabilities marginalized over all of the internal parameters of the models:

$$P(H_i|\vec{x}) = \int P(H_i, \vec{\theta}_i|\vec{x})\, d\vec{\theta}_i$$

$$= \frac{\int L(\vec{x}|H_i, \vec{\theta}_i) p_i \pi_i(\vec{\theta}_i)\, d\vec{\theta}_i}{P(x)}$$

Use Bayes theorem

So therefore the Bayes factor is

$$B_{ij} = \frac{\int L(\vec{x}|H_i, \vec{\theta}_i) \pi_i(\vec{\theta}_i)\, d\vec{\theta}_i}{\int L(\vec{x}|H_j, \vec{\theta}_j) \pi_j(\vec{\theta}_j)\, d\vec{\theta}_j}$$

Ratio of marginal likelihoods

The prior probabilities $p_i = P(H_i)$ cancel.

Numerical determination of Bayes factors

Both numerator and denominator of B_{ij} are of the form

$$m = \int L(\vec{x}|\vec{\theta})\pi(\vec{\theta})\, d\vec{\theta} \quad \longleftarrow \quad \text{'marginal likelihood'}$$

These can be very challenging to compute. Methods include:

Harmonic Mean (and improvements)
Importance sampling
Parallel tempering (~thermodynamic integration)
Nested sampling
...

See e.g. Kass and Raftery, *Bayes Factors*, J. Am. Stat. Assoc. 90 (1995) 773-795.

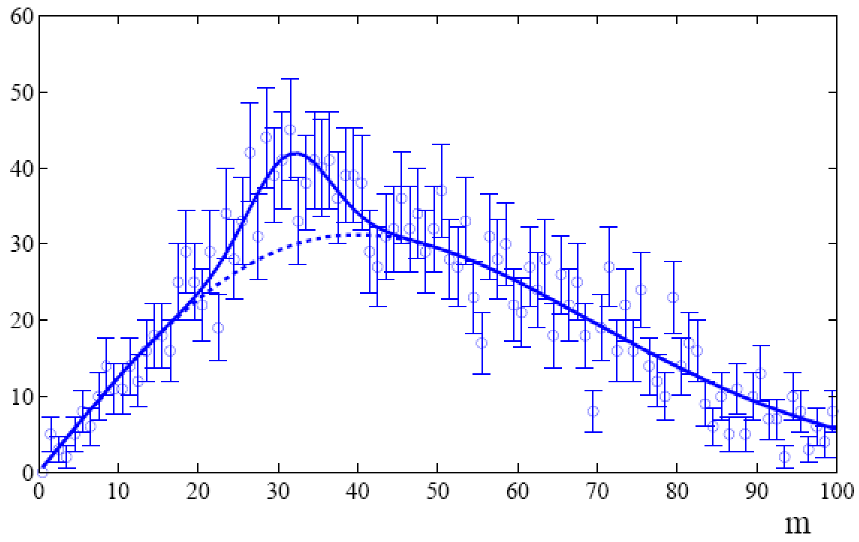
Nested sampling -- see: **`www.inference.phy.cam.ac.uk/bayesys`**

The Look-Elsewhere Effect

Eilam Gross and Ofer Vitells, arXiv:10051891

Suppose a model for a mass distribution allows for a peak at a mass m with amplitude μ.

The data show a bump at a mass m_0.



How consistent is this with the no-bump ($\mu = 0$) hypothesis?

p-value for fixed mass

First, suppose the mass m_0 of the peak was specified a priori.

Test consistency of bump with the no-signal ($\mu = 0$) hypothesis with e.g. likelihood ratio

$$t_{\rm fix} = -2 \ln \frac{L(0, m_0)}{L(\hat{\mu}, m_0)}$$

where "fix" indicates that the mass of the peak is fixed to m_0.

The resulting *p*-value

$$p_{\rm fix} = \int_{t_{\rm fix,obs}}^{\infty} f(t_{\rm fix}|0) \, dt_{\rm fix}$$

gives the probability to find a value of $t_{\rm fix}$ at least as great as observed at the specific mass m_0.

p-value for floating mass

But suppose we did not know where in the distribution to expect a peak.

What we want is the probability to find a peak at least as significant as the one observed anywhere in the distribution.

Include the mass as an adjustable parameter in the fit, test significance of peak using

$$t_{\mathrm{float}} = -2 \ln \frac{L(0)}{L(\hat{\mu}, \hat{m})}$$

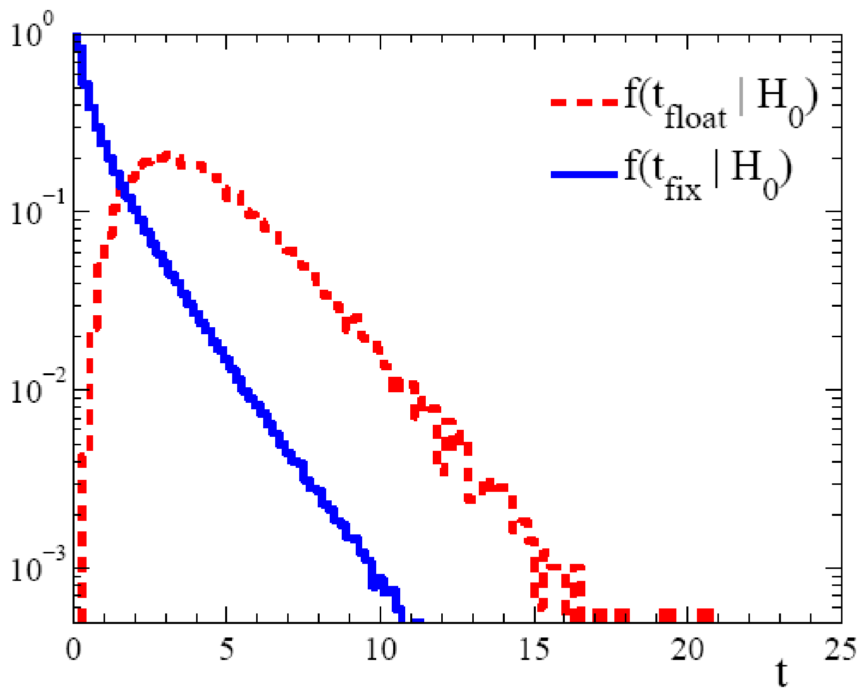
(Note m does not appear in the $\mu = 0$ model.)

$$p_{\mathrm{float}} = \int_{t_{\mathrm{float,obs}}}^{\infty} f(t_{\mathrm{float}}|0)\, dt_{\mathrm{float}}$$

Distributions of t_{fix}, t_{float}

For a sufficiently large data sample, t_{fix} ~chi-square for 1 degree of freedom (Wilks' theorem).

For t_{float} there are two adjustable parameters, μ and m, and naively Wilks theorem says t_{float} ~ chi-square for 2 d.o.f.



In fact Wilks' theorem does not hold in the floating mass case because on of the parameters (m) is not-defined in the $\mu = 0$ model.

So getting t_{float} distribution is more difficult.

Trials factor

We would like to be able to relate the *p*-values for the fixed and floating mass analyses (at least approximately).

Gross and Vitells (arXiv:10051891) argue that the "trials factor" can be approximated by

$$F_{\text{trials}} \equiv \frac{p_{\text{float}}}{p_{\text{fix}}} \approx \langle N \rangle \sqrt{\frac{2}{\pi}} Z_{\text{fix}} \approx \frac{1}{3} \frac{\text{range}}{\text{resolution}} Z_{\text{fix}}$$

where ‹*N*› = average number of local maxima of *L* in fit range and

$$Z_{\text{fix}} = \Phi^{-1}(1 - p_{\text{fix}}) = \sqrt{t_{\text{fix}}}$$

is the significance for the fixed mass case.

So we can either carry out the full floating-mass analysis (e.g. use MC to get *p*-value, or do fixed mass analysis and apply a correction factor.

Wrapping up lecture 4

Bayesian methods for limits

Difficult issues surrounding choice of prior

Marginalize over nuisance parameters (MCMC)

Bayesian model selection

Bayes factors = posterior odds if assume prior odds 1

= ratio of marginalized likelihoods

Can be very difficult to compute.

Look-elsewhere effect

Correct with trials factor or e.g. use floating mass analysis.

Extra slides

MCMC basics: Metropolis-Hastings algorithm

Goal: given an n-dimensional pdf $p(\vec{\theta})$,

generate a sequence of points $\vec{\theta}_1, \vec{\theta}_2, \vec{\theta}_3, \ldots$

1) Start at some point $\vec{\theta}_0$

2) Generate $\vec{\theta} \sim q(\vec{\theta}; \vec{\theta}_0)$

Proposal density $q(\vec{\theta}; \vec{\theta}_0)$ e.g. Gaussian centred about $\vec{\theta}_0$

3) Form Hastings test ratio $\alpha = \min\left[1, \dfrac{p(\vec{\theta})q(\vec{\theta}_0; \vec{\theta})}{p(\vec{\theta}_0)q(\vec{\theta}; \vec{\theta}_0)}\right]$

4) Generate $u \sim \mathrm{Uniform}[0, 1]$

5) If $u \leq \alpha$, $\vec{\theta}_1 = \vec{\theta}$, $\leftarrow$ move to proposed point

else $\vec{\theta}_1 = \vec{\theta}_0$ $\leftarrow$ old point repeated

6) Iterate

Metropolis-Hastings (continued)

This rule produces a *correlated* sequence of points (note how each new point depends on the previous one).

For our purposes this correlation is not fatal, but statistical errors larger than naive $\sqrt{n}$.

The proposal density can be (almost) anything, but choose so as to minimize autocorrelation. Often take proposal density symmetric: $q(\vec{\theta}; \vec{\theta}_0) = q(\vec{\theta}_0; \vec{\theta})$

Test ratio is (*Metropolis*-Hastings): $\alpha = \min \left[1, \frac{p(\vec{\theta})}{p(\vec{\theta}_0)} \right]$

I.e. if the proposed step is to a point of higher $p(\vec{\theta})$, take it; if not, only take the step with probability $p(\vec{\theta})/p(\vec{\theta}_0)$.
If proposed step rejected, hop in place.

Metropolis-Hastings caveats

Actually one can only prove that the sequence of points follows the desired pdf in the limit where it runs forever.

There may be a "burn-in" period where the sequence does not initially follow $p(\vec{\theta})$.

Unfortunately there are few useful theorems to tell us when the sequence has converged.

Look at trace plots, autocorrelation.

Check result with different proposal density.

If you think it's converged, try starting from a different point and see if the result is similar.