Parameter Estimation
Lecture 2

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Outline

Lecture 1: Introduction, Maximum Likelihood

→ Lecture 2: Least squares, Bayesian approach, confidence intervals

For some slides/links with exercises and code you can see:

https://www.pp.rhul.ac.uk/~cowan/stat/exercises/cowan_stat_exercises.pdf

https://www.pp.rhul.ac.uk/~cowan/stat/exercises/cowan_stat_exercises_full.pdf

Most material here is taken from the University of London course:

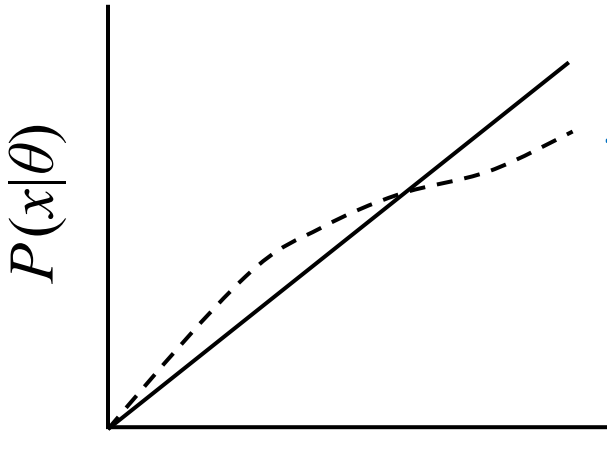
https://www.pp.rhul.ac.uk/~cowan/stat_course.html

Parameter Estimation 2-1

- Nuisance parameters, systematic uncertainties
- From Maximum Likelihood to Least Squares
- Bayesian parameter estimation
- Marginalization of posterior pdf
- Markov Chain Monte Carlo

Systematic uncertainties and nuisance parameters

In general, our model of the data is not perfect:



model: $P(x|\theta) = \theta x$

truth: $P(x|\theta) = \theta x + \alpha x^2 + \beta x^3 + \cdots$

Can improve model by including additional adjustable parameters.

$$P(x|\theta) \to P(x|\theta, \nu)$$

Nuisance parameter ↔ systematic uncertainty. Some point in the parameter space of the enlarged model should be "true".

Presence of nuisance parameter decreases sensitivity of analysis to the parameter of interest (e.g., increases variance of estimate).

Example: fitting a straight line

Data: (x_i, y_i, σ_i) , $i = 1, \ldots, n$.

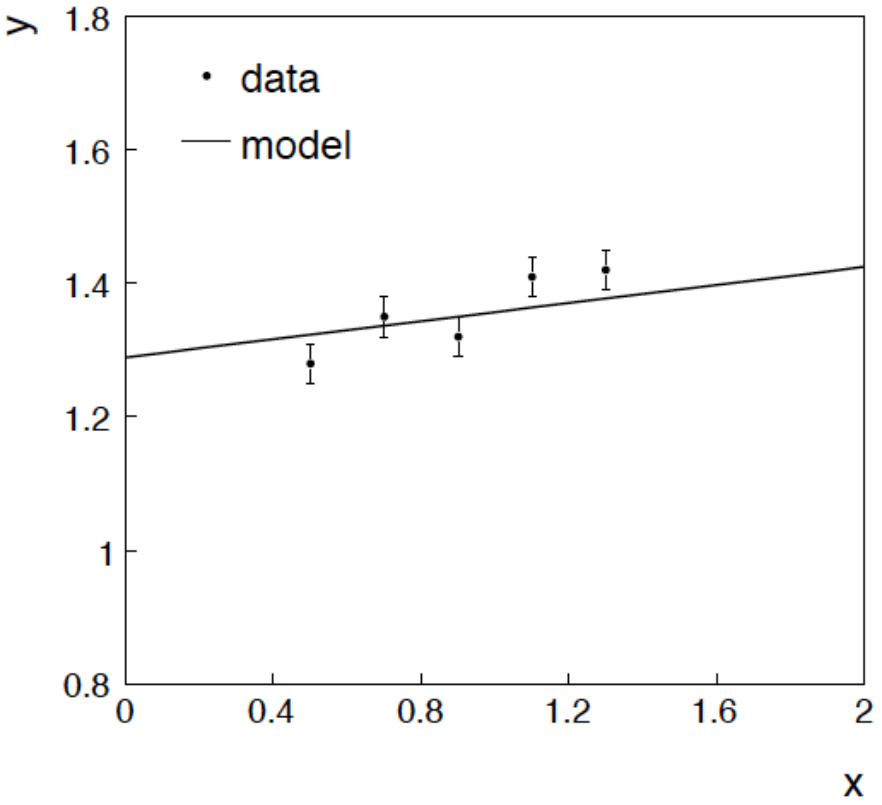
Model: y_i independent and all follow $y_i \sim \text{Gauss}(\mu(x_i), \sigma_i)$

$$\mu(x; \theta_0, \theta_1) = \theta_0 + \theta_1 x \ ,$$

assume x_i and σ_i known.

Goal: estimate θ_0

Here suppose we don't care about θ_1 (example of a "nuisance parameter")



Maximum likelihood fit with Gaussian data

In this example, the y_i are assumed independent, so the likelihood function is a product of Gaussians:

$$L(\theta_0, \theta_1) = \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi}\sigma_i} \exp\left[-\frac{1}{2}\frac{(y_i - \mu(x_i; \theta_0, \theta_1))^2}{\sigma_i^2}\right] ,$$

Maximizing the likelihood is here equivalent to minimizing

$$\chi^2(\theta_0, \theta_1) = -2 \ln L(\theta_0, \theta_1) + \text{const} = \sum_{i=1}^{n} \frac{(y_i - \mu(x_i; \theta_0, \theta_1))^2}{\sigma_i^2} .$$

i.e., for Gaussian data, ML same as Method of Least Squares (LS)

θ_1 known a priori

$$L(\theta_0) = \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi}\sigma_i} \exp\left[-\frac{1}{2}\frac{(y_i - \mu(x_i;\theta_0,\theta_1))^2}{\sigma_i^2}\right] .$$

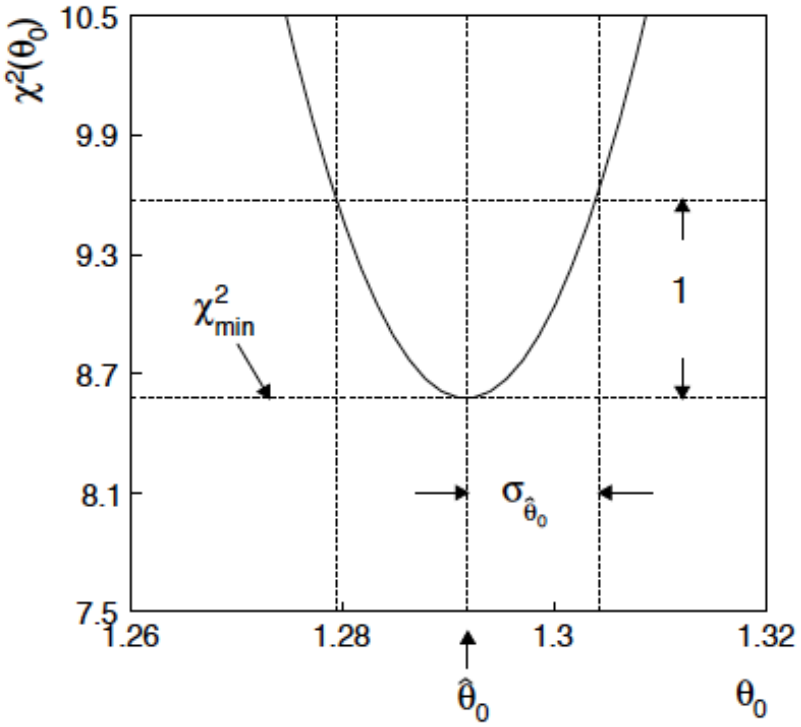
$$\chi^2(\theta_0) = -2\ln L(\theta_0) + \text{const} = \sum_{i=1}^{n} \frac{(y_i - \mu(x_i;\theta_0,\theta_1))^2}{\sigma_i^2} .$$

For Gaussian y_i, ML same as LS

Minimize $\chi^2 \rightarrow$ estimator $\hat{\theta}_0$.

Come up one unit from χ^2_{min}

to find $\sigma_{\hat{\theta}_0}$.



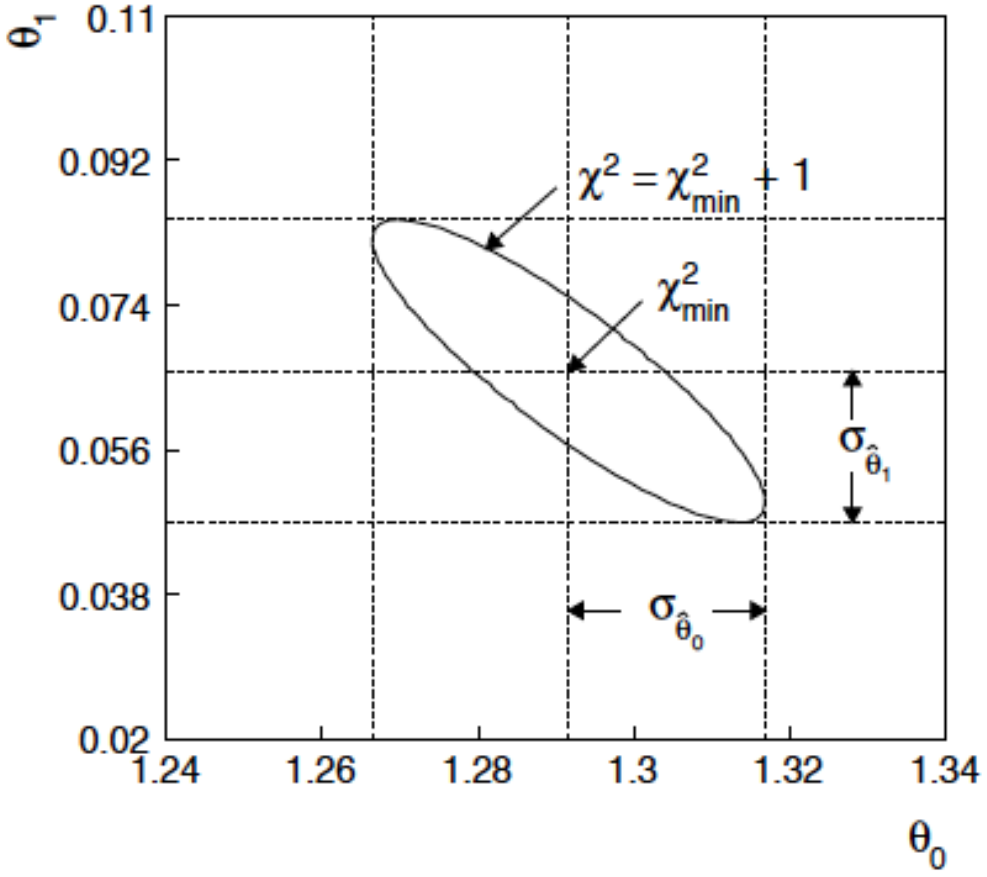
ML (or LS) fit of θ_0 and θ_1

$$\chi^2(\theta_0, \theta_1) = -2 \ln L(\theta_0, \theta_1) + \text{const} = \sum_{i=1}^{n} \frac{(y_i - \mu(x_i; \theta_0, \theta_1))^2}{\sigma_i^2} \, .$$

Standard deviations from tangent lines to contour

$$\chi^2 = \chi^2_{\text{min}} + 1 \, .$$

Correlation between $\hat{\theta}_0, \hat{\theta}_1$ causes errors to increase.

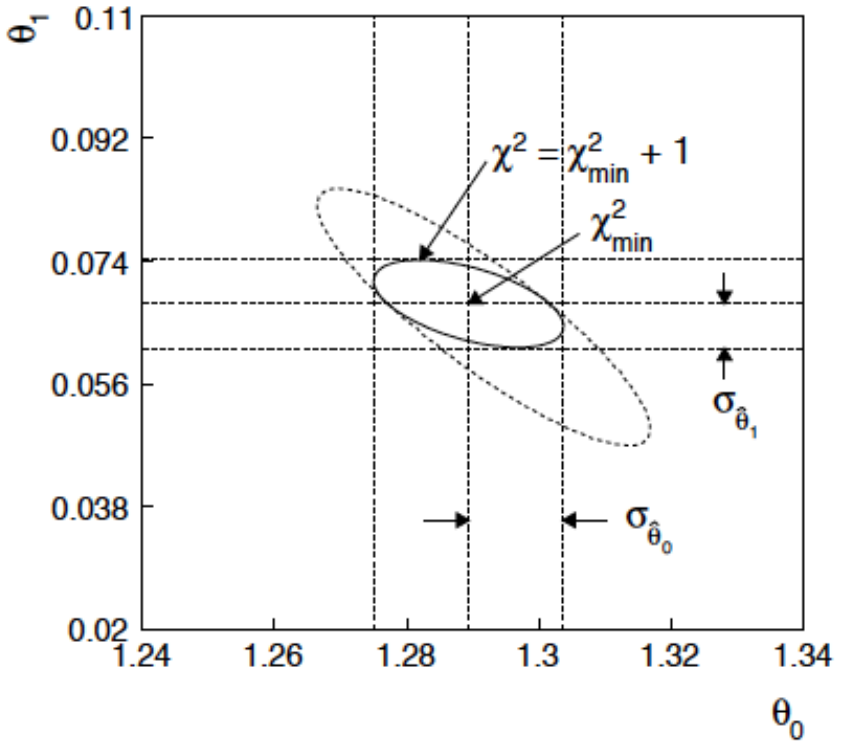


If we have a measurement $t_1 \sim \text{Gauss}\,(\theta_1, \sigma_{t1})$

$$L(\theta_0, \theta_1) = \frac{1}{\sqrt{2\pi}\sigma_t} e^{-(t_1-\theta_1)^2/2\sigma_{t_1}^2} \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi}\sigma_i} \exp\left[-\frac{1}{2}\frac{(y_i - \mu(x_i;\theta_0,\theta_1))^2}{\sigma_i^2}\right]$$

$$\chi^2(\theta_0, \theta_1) = \sum_{i=1}^{n} \frac{(y_i - \mu(x_i;\theta_0,\theta_1))^2}{\sigma_i^2} + \frac{(t_1 - \theta_1)^2}{\sigma_{t_1}^2}$$

The information on θ_1 improves accuracy of $\hat{\theta}_0$.



Reminder of Bayesian approach

In Bayesian statistics we can associate a probability with a hypothesis, e.g., a parameter value θ.

Interpret probability of θ as 'degree of belief' (subjective).

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

Our experiment has data x, $\rightarrow$ likelihood $P(x|\theta)$.

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

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

Posterior pdf $p(\theta|x)$ contains all our knowledge about θ.

Bayesian approach: $y_i \sim \text{Gauss}(\mu(x_i;\theta_0,\theta_1), \sigma_i)$

We need to associate prior probabilities with θ_0 and θ_1, e.g.,

$$\pi(\theta_0, \theta_1) = \pi_0(\theta_0)\pi_1(\theta_1)$$

← suppose knowledge of θ_0 has no influence on knowledge of θ_1

$$\pi_0(\theta_0) = \text{const.}$$

← 'non-informative', in any case much broader than $L(\theta_0)$

$$\pi_1(\theta_1) = p(\theta_1|t_1) \propto p(t_1|\theta_1)\pi_{\text{Ur}}(\theta_1) = \frac{1}{\sqrt{2\pi}\sigma_t} e^{-(t_1-\theta_1)^2/2\sigma_t^2} \times \text{const.}$$

prior after t_1, before $\boldsymbol{y}$

Ur = "primordial" prior

Likelihood for control measurement t_1

Bayesian example: $y_i \sim \text{Gauss}(\mu(x_i;\theta_0,\theta_1), \sigma_i)$

Putting the ingredients into Bayes' theorem gives:

$$p(\theta_0,\theta_1|\vec{y}) \propto \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi}\sigma_i} e^{-(y_i-\mu(x_i;\theta_0,\theta_1))^2/2\sigma_i^2} \; \pi_0 \; \frac{1}{\sqrt{2\pi}\sigma_{t_1}} e^{-(\theta_1-t_1)^2/2\sigma_{t_1}^2}$$

posterior $\propto$ likelihood $\times$ prior

Note here the likelihood only reflects the measurements $\boldsymbol{y}$.

The information from the control measurement t_1 has been put into the prior for θ_1.

We would get the same result using the likelihood $P(\boldsymbol{y},t|\theta_0,\theta_1)$ and the constant "Ur-prior" for θ_1.

Marginalizing the posterior pdf

We then integrate (marginalize) $p(\theta_0, \theta_1 | \boldsymbol{y})$ to find $p(\theta_0 | \boldsymbol{y})$:

$$p(\theta_0|\mathbf{y}) = \int p(\theta_0, \theta_1|\mathbf{y})\, d\theta_1$$

In this example we can do the integral (rare). We find

$$p(\theta_0|\mathbf{y}) = \frac{1}{\sqrt{2\pi}\sigma_{\theta_0}} e^{-(\theta_0 - \hat{\theta}_0)^2/2\sigma_{\theta_0}^2}$$

$$\hat{\theta}_0 = \text{same as MLE}$$

$$\sigma_{\theta_0} = \sigma_{\hat{\theta}_0} \qquad \text{(same as for MLE)}$$

For this example, numbers come out same as in frequentist approach, but interpretation different.

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.

MCMC (e.g., Metropolis-Hastings algorithm) generates correlated sequence of random numbers:

cannot use for many applications, e.g., detector MC;
effective stat. error greater than if all values independent .

Basic idea: sample multidimensional θ but look only at distribution of parameters of interest.

MCMC basics: Metropolis-Hastings algorithm

Goal: given an n-dimensional pdf $p(\boldsymbol{\theta})$, generate a sequence of points $\boldsymbol{\theta}_1, \boldsymbol{\theta}_2, \boldsymbol{\theta}_3, \ldots$

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

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

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

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 $u \sim \text{Uniform}[0, 1]$

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

else $\vec{\theta}_1 = \vec{\theta}_0$ ← 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).

Still works if $p(\boldsymbol{\theta})$ is known only as a proportionality, which is usually what we have from Bayes' theorem: $p(\boldsymbol{\theta}|\boldsymbol{x}) \propto p(\boldsymbol{x}|\boldsymbol{\theta})\pi(\boldsymbol{\theta})$.

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

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

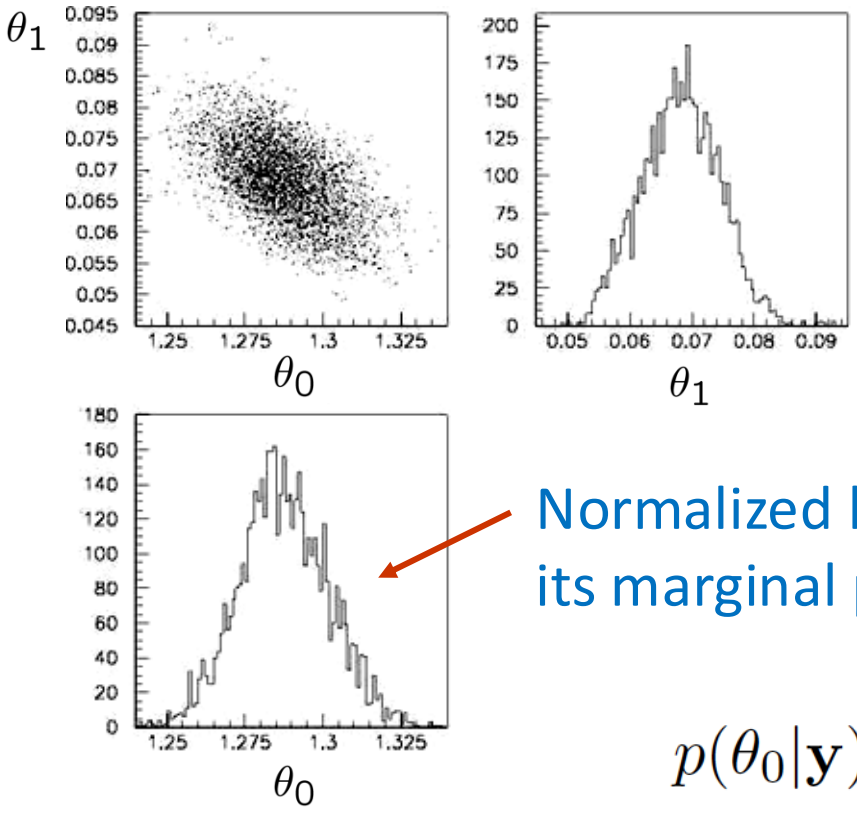
I.e. if the proposed step is to a point of higher $p(\boldsymbol{\theta})$, take it;

if not, only take the step with probability $p(\boldsymbol{\theta})/p(\boldsymbol{\theta}_0)$.

If proposed step rejected, repeat the current point.

Example: posterior pdf from MCMC

Sample the posterior pdf from previous example with MCMC:



Normalized histogram of θ_0 gives its marginal posterior pdf:

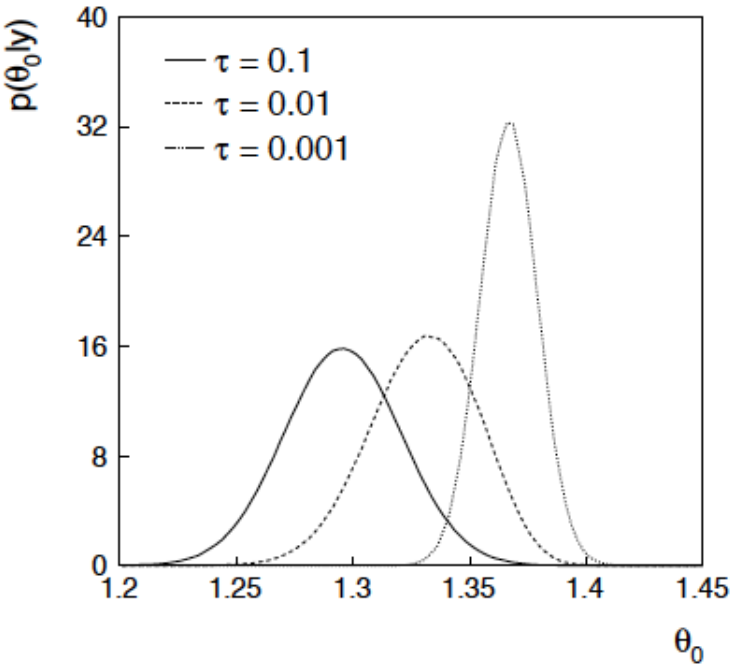
$$p(\theta_0|\mathbf{y}) = \int p(\theta_0, \theta_1|\mathbf{y})\, d\theta_1$$

Bayesian method with alternative priors

Suppose we don't have a previous measurement of θ_1 but rather, an "expert" says it should be positive and not too much greater than 0.1 or so, i.e., something like

$$\pi_1(\theta_1) = \frac{1}{\tau} e^{-\theta_1/\tau} , \quad \theta_1 \geq 0 , \quad \tau = 0.1 .$$

From this we obtain (numerically) the posterior pdf for θ_0:



This summarizes all knowledge about θ_0.

Look also at result from variety of priors.

Confidence Intervals

- Interval estimation
- Confidence interval from inverting a test
- Example: limits on mean of Gaussian
- Confidence intervals from the likelihood function
- Confidence intervals in problems with nuisance parameters
- The CL_s method

Confidence intervals by inverting a test

In addition to a 'point estimate' of a parameter we should report an interval reflecting its statistical uncertainty.

Confidence intervals for a parameter θ can be found by defining a test of the hypothesized value θ (do this for all θ):

Specify region of data 'disfavoured' by θ (critical region w_θ),

i.e., more favoured by some relevant alternative value of θ,

$P(\text{data in critical region}|\theta) \leq \alpha$ for prespecified α, e.g., 0.05.

If data observed in the critical region, reject the value θ.

Now invert the test to define a confidence interval as:

set of θ values that are not rejected in a test of size α (confidence level CL is $1-\alpha$).

Confidence interval from p-values

Equivalently, define a p-value for all hypothesized values of θ.

p_θ = P(data having incompatibility with θ ≥ observed | θ)

Critical region of size α = data values for which p-value ≤ α.

Then the confidence region at confidence level CL = $1-\alpha$ is

the set of θ values for which $p_\theta > \alpha$.

E.g. an upper limit on θ is the greatest value for which $p_\theta > \alpha$.

In practice find by setting $p_\theta = \alpha$ and solve for θ.

Same idea for multidimensional parameter space $\boldsymbol{\theta} = (\theta_1, \ldots \theta_M)$, result is confidence "region" with boundary determined by $p_{\boldsymbol{\theta}} = \alpha$.

Coverage probability of confidence interval

If the true value of θ is rejected, then it's not in the confidence interval. The probability for this is by construction (equality for continuous data):

$$P(\text{reject } \theta | \theta) \leq \alpha = \text{type-I error rate}$$

Therefore, the probability for the interval to contain or "cover" θ is

$$P(\text{conf. interval "covers" } \theta | \theta) \geq 1 - \alpha$$

This assumes that the set of θ values considered includes the true value, i.e., it assumes the composite hypothesis $P(\boldsymbol{x}|H,\theta)$.

The Poisson counting experiment

Suppose we do a counting experiment and observe n events.

Events could be from *signal* process or from *background* – we only count the total number.

Poisson model:

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

s = mean (i.e., expected) # of signal events

b = mean # of background events

Goal is to make inference about s, e.g.,

test $s = 0$ (rejecting $H_0 \approx$ "discovery of signal process")

test all non-zero s (values not rejected = confidence interval)

In both cases need to ask what is relevant alternative hypothesis.

Frequentist upper limit on Poisson parameter

Consider again the case of observing $n \sim \text{Poisson}(s + b)$.

Suppose $b = 4.5$, $n_{\text{obs}} = 5$. Find upper limit on s at 95% CL.

Relevant alternative is $s = 0$ (critical region at low n)

p-value of hypothesized s is $P(n \leq n_{\text{obs}}; s, b)$

Upper limit s_{up} at $\text{CL} = 1 - \alpha$ found from

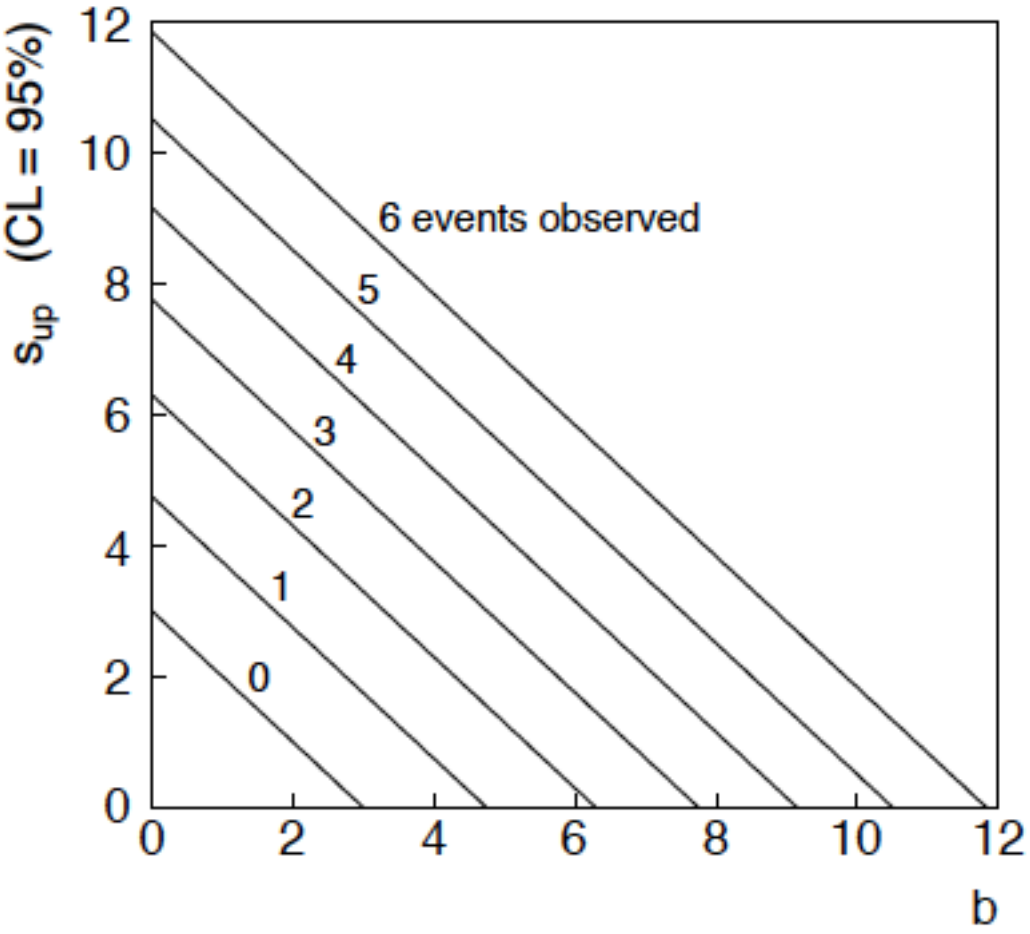
$$\alpha = P(n \leq n_{\text{obs}}; s_{\text{up}}, b) = \sum_{n=0}^{n_{\text{obs}}} \frac{(s_{\text{up}} + b)^n}{n!} e^{-(s_{\text{up}}+b)}$$

$$s_{\text{up}} = \frac{1}{2} F^{-1}_{\chi^2}(1 - \alpha; 2(n_{\text{obs}} + 1)) - b$$

$$= \frac{1}{2} F^{-1}_{\chi^2}(0.95; 2(5 + 1)) - 4.5 = 6.0$$

$n \sim$ Poisson(s+b): frequentist upper limit on s

For low fluctuation of n, formula can give negative result for $s_{\rm up}$; i.e. confidence interval is empty; all values of $s \geq 0$ have $p_s \leq \alpha$.



Limits near a boundary of the parameter space

Suppose e.g. $b = 2.5$ and we observe $n = 0$.

If we choose CL $= 0.9$, we find from the formula for s_{up}

$$s_{\text{up}} = -0.197 \quad (\text{CL} = 0.90)$$

Physicist:

We already knew $s \geq 0$ before we started; can't use negative upper limit to report result of expensive experiment!

Statistician:

The interval is designed to cover the true value only 90% of the time — this was clearly not one of those times.

Not uncommon dilemma when testing parameter values for which one has very little experimental sensitivity, e.g., very small s.

Expected limit for $s = 0$

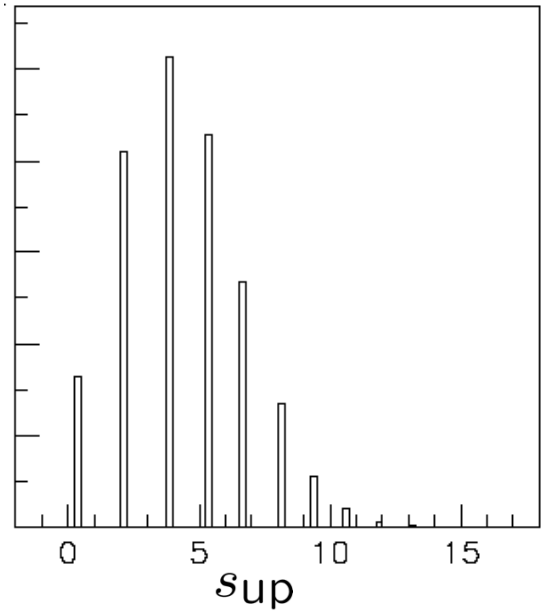
Physicist: I should have used CL = 0.95 — then $s_{\rm up} = 0.496$

Even better: for CL = 0.917923 we get $s_{\rm up} = 10^{-4}$!

Reality check: with $b = 2.5$, typical Poisson fluctuation in n is at least $\sqrt{2.5} = 1.6$. How can the limit be so low?

Look at the mean limit for the no-signal hypothesis ($s = 0$) (sensitivity).

Distribution of 95% CL limits with $b = 2.5$, $s = 0$.
Mean upper limit = 4.44



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:

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

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

For e.g. $n \sim$ 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; can be OK provided $p(n|s)$ dies off quickly for large s.

Not invariant under change of parameter — if we had used instead a flat prior for a nonlinear function of s, then this would imply a non-flat prior for s.

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 (e.g., coverage probability, which will depend on true s).

Bayesian upper limit with flat prior for s

Put Poisson likelihood and flat prior into Bayes' theorem:

$$p(s|n) \propto p(n|s)\pi(s) = \frac{(s+b)^n}{n!} e^{-(s+b)} \times 1\,, \quad s \geq 0$$

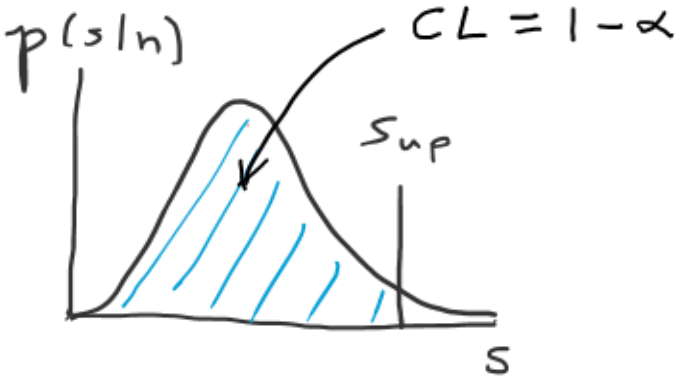
Normalize to unit area:

$$p(s|n) = \frac{(s+b)^n e^{-(s+b)}}{\Gamma(b, n+1)}$$

upper incomplete gamma function

Upper limit $s_{\rm up}$ determined by

$$1 - \alpha = \int_0^{s_{\rm up}} p(s|n)\, ds$$



Bayesian interval with flat prior for s

Solve to find limit s_{up}:

$$s_{\text{up}} = \frac{1}{2} F_{\chi^2}^{-1}[p, 2(n+1)] - b$$

where

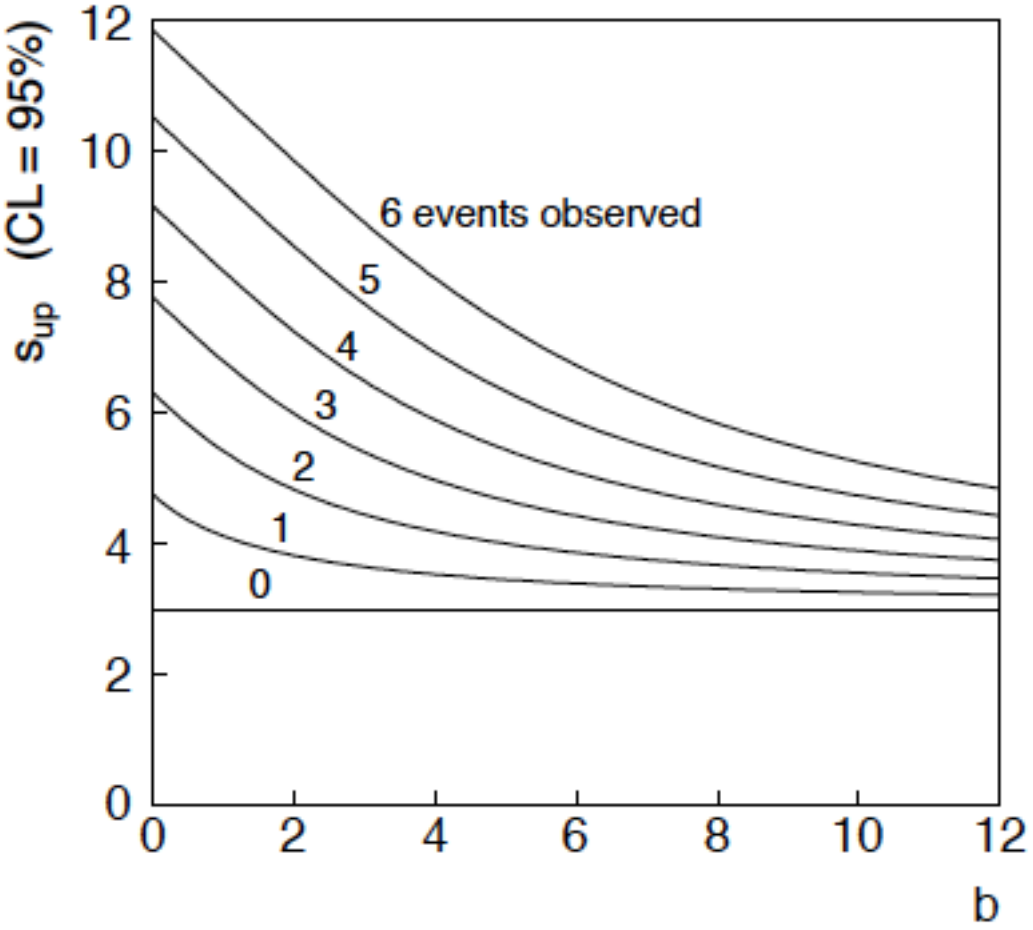
$$p = 1 - \alpha \left(1 - F_{\chi^2}[2b, 2(n+1)]\right)$$

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

Bayesian interval with flat prior for *s*

For $b > 0$ Bayesian limit is everywhere greater than the (one sided) frequentist upper limit.

Never goes negative. Doesn't depend on b if $n = 0$.



Approximate confidence intervals/regions from the likelihood function

Suppose we test parameter value(s) $\boldsymbol{\theta} = (\theta_1, \ldots, \theta_N)$ using the ratio

$$\lambda(\boldsymbol{\theta}) = \frac{L(\boldsymbol{\theta})}{L(\hat{\boldsymbol{\theta}})} \qquad 0 \leq \lambda(\boldsymbol{\theta}) \leq 1$$

Lower $\lambda(\boldsymbol{\theta})$ means worse agreement between data and hypothesized $\boldsymbol{\theta}$. Equivalently, usually define

$$t_{\boldsymbol{\theta}} = -2 \ln \lambda(\boldsymbol{\theta})$$

so higher $t_{\boldsymbol{\theta}}$ means worse agreement between $\boldsymbol{\theta}$ and the data.

p-value of $\boldsymbol{\theta}$ therefore

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

need pdf

Confidence region from Wilks' theorem

Wilks' theorem says (in large-sample limit and provided certain conditions hold...)

$$f(t_{\boldsymbol{\theta}}|\boldsymbol{\theta}) \sim \chi^2_N$$

chi-square dist. with # d.o.f. = # of components in $\boldsymbol{\theta} = (\theta_1, \ldots, \theta_N)$.

Assuming this holds, the p-value is

$$p_{\boldsymbol{\theta}} = 1 - F_{\chi^2_N}(t_{\boldsymbol{\theta}}|\boldsymbol{\theta}) \quad \leftarrow \text{set equal to } \alpha$$

To find boundary of confidence region set $p_{\boldsymbol{\theta}} = \alpha$ and solve for $t_{\boldsymbol{\theta}}$:

$$t_{\boldsymbol{\theta}} = F^{-1}_{\chi^2_N}(1-\alpha)$$

Recall also

$$t_\theta = -2\ln\frac{L(\theta)}{L(\hat{\theta})}$$

Confidence region from Wilks' theorem (cont.)

i.e., boundary of confidence region in $\boldsymbol{\theta}$ space is where

$$\ln L(\boldsymbol{\theta}) = \ln L(\hat{\boldsymbol{\theta}}) - \tfrac{1}{2} F^{-1}_{\chi^2_N}(1-\alpha)$$

For example, for $1-\alpha = 68.3\%$ and $n = 1$ parameter,

$$F^{-1}_{\chi^2_1}(0.683) = 1$$

and so the 68.3% confidence level interval is determined by

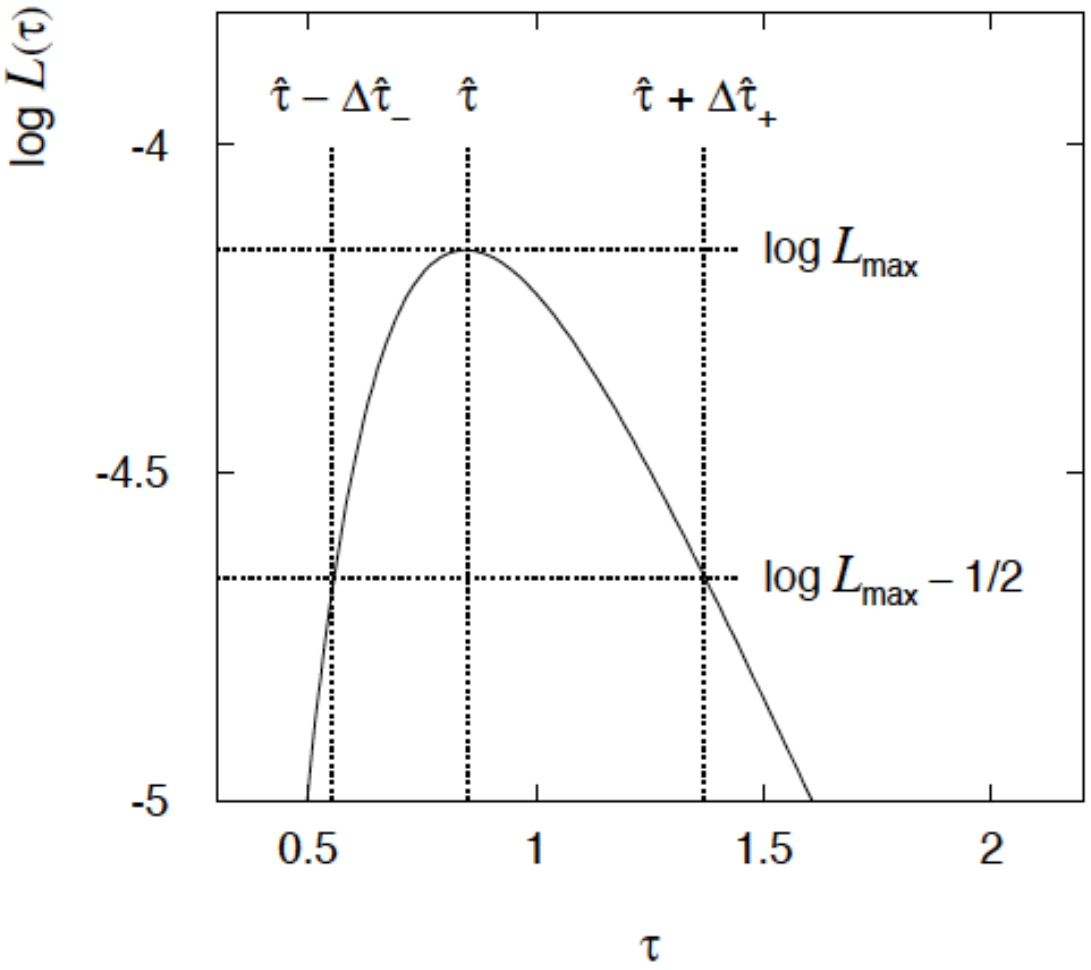
$$\ln L(\theta) = \ln L(\hat{\theta}) - \frac{1}{2}$$

Same as recipe for finding the estimator's standard deviation, i.e.,

$[\hat{\theta} - \sigma_{\hat{\theta}}, \hat{\theta} + \sigma_{\hat{\theta}}]$ is a 68.3% CL confidence interval.

Example of interval from $\ln L(\theta)$

For $N = 1$ parameter, CL = 0.683, $Q_\alpha = 1$.



Our exponential example, now with only $n = 5$ events.

Can report ML estimate with approx. confidence interval from $\ln L_{\max} - 1/2$ as "asymmetric error bar":

$$\hat{\tau} = 0.85^{+0.52}_{-0.30}$$

Multiparameter case

For increasing number of parameters, CL $= 1 - \alpha$ decreases for confidence region determined by a given

$$Q_\alpha = F^{-1}_{\chi^2_n}(1-\alpha)$$

Q_α	$1-\alpha$				
	$n=1$	$n=2$	$n=3$	$n=4$	$n=5$
1.0	0.683	0.393	0.199	0.090	0.037
2.0	0.843	0.632	0.428	0.264	0.151
4.0	0.954	0.865	0.739	0.594	0.451
9.0	0.997	0.989	0.971	0.939	0.891

← # of par.

Multiparameter case (cont.)

Equivalently, Q_α increases with n for a given CL $= 1 - \alpha$.

$1-\alpha$	$\hat{Q}_\alpha$				
	$n=1$	$n=2$	$n=3$	$n=4$	$n=5$
0.683	1.00	2.30	3.53	4.72	5.89
0.90	2.71	4.61	6.25	7.78	9.24
0.95	3.84	5.99	7.82	9.49	11.1
0.99	6.63	9.21	11.3	13.3	15.1

← # of par.

Profile Likelihood

Suppose we have a likelihood $L(\boldsymbol{\mu},\boldsymbol{\theta}) = P(\boldsymbol{x}|\boldsymbol{\mu},\boldsymbol{\theta})$ with N parameters of interest $\boldsymbol{\mu} = (\mu_1,..., \mu_N)$ and M nuisance parameters $\boldsymbol{\theta} = (\theta_1,..., \theta_M)$. The "profiled" (or "constrained") values of $\boldsymbol{\theta}$ are:

$$\hat{\hat{\boldsymbol{\theta}}}(\boldsymbol{\mu}) = \underset{\boldsymbol{\theta}}{\operatorname{argmax}}\, L(\boldsymbol{\mu}, \boldsymbol{\theta})$$

and the profile likelihood is: $L_{\mathrm{p}}(\boldsymbol{\mu}) = L(\boldsymbol{\mu}, \hat{\hat{\boldsymbol{\theta}}})$

The profile likelihood depends only on the parameters of interest; the nuisance parameters are replaced by their profiled values.

The profile likelihood can be used to obtain confidence intervals/regions for the parameters of interest in the same way as one would for all of the parameters from the full likelihood.

Profile Likelihood Ratio – Wilks theorem

Goal is to test/reject regions of $\boldsymbol{\mu}$ space (param. of interest).

Rejecting a point $\boldsymbol{\mu}$ should mean $p_{\boldsymbol{\mu}} \leq \alpha$ for all possible values of the nuisance parameters $\boldsymbol{\theta}$.

Test $\boldsymbol{\mu}$ using the "profile likelihood ratio": $\lambda(\boldsymbol{\mu}) = \dfrac{L(\boldsymbol{\mu}, \hat{\hat{\boldsymbol{\theta}}})}{L(\hat{\boldsymbol{\mu}}, \hat{\boldsymbol{\theta}})}$

Let $t_{\boldsymbol{\mu}} = -2\ln\lambda(\boldsymbol{\mu})$. Wilks' theorem says in large-sample limit:

$$t_{\boldsymbol{\mu}} \sim \text{chi-square}(N)$$

where the number of degrees of freedom is the number of parameters of interest (components of $\boldsymbol{\mu}$). So p-value for $\boldsymbol{\mu}$ is

$$p_{\boldsymbol{\mu}} = \int_{t_{\mu,\text{obs}}}^{\infty} f(t_{\boldsymbol{\mu}}|\boldsymbol{\mu}, \boldsymbol{\theta})\, dt_{\boldsymbol{\mu}} = 1 - F_{\chi^2_N}(t_{\boldsymbol{\mu},\text{obs}})$$

Profile Likelihood Ratio – Wilks theorem (2)

If we have a large enough data sample to justify use of the asymptotic chi-square pdf, then if $\boldsymbol{\mu}$ is rejected, it is rejected for any values of the nuisance parameters.

The recipe to get confidence regions/intervals for the parameters of interest at CL = 1 – α is thus the same as before, simply use the profile likelihood:

$$\ln L_{\rm p}(\boldsymbol{\mu}) = \ln L_{\rm max} - \frac{1}{2} F^{-1}_{\chi^2_N}(1-\alpha)$$

where the number of degrees of freedom N for the chi-square quantile is equal to the number of parameters of interest.

If the large-sample limit is not justified, then use e.g. Monte Carlo to get distribution of $t_{\boldsymbol{\mu}}$.

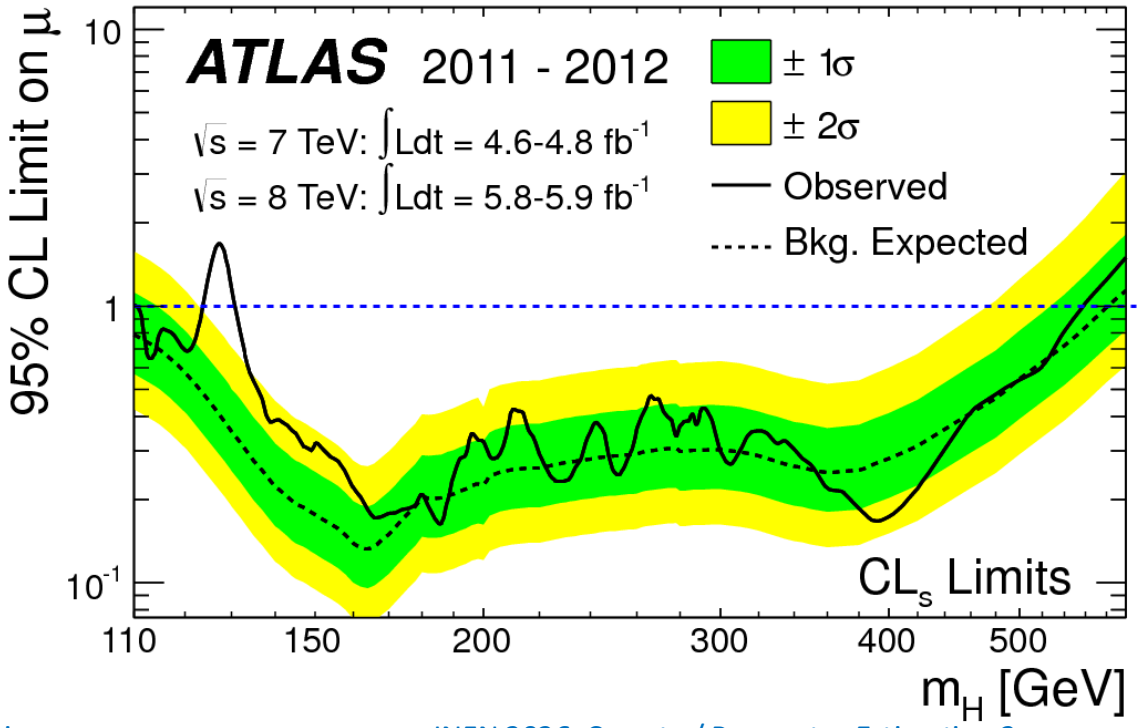
How to read the green and yellow limit plots

For every value of m_{H}, find the upper limit on μ.

Also for each m_{H}, determine the distribution of upper limits μ_{up} one would obtain under the hypothesis of $\mu = 0$.

The dashed curve is the median μ_{up}, and the green (yellow) bands give the $\pm\, 1\sigma\, (2\sigma)$ regions of this distribution.

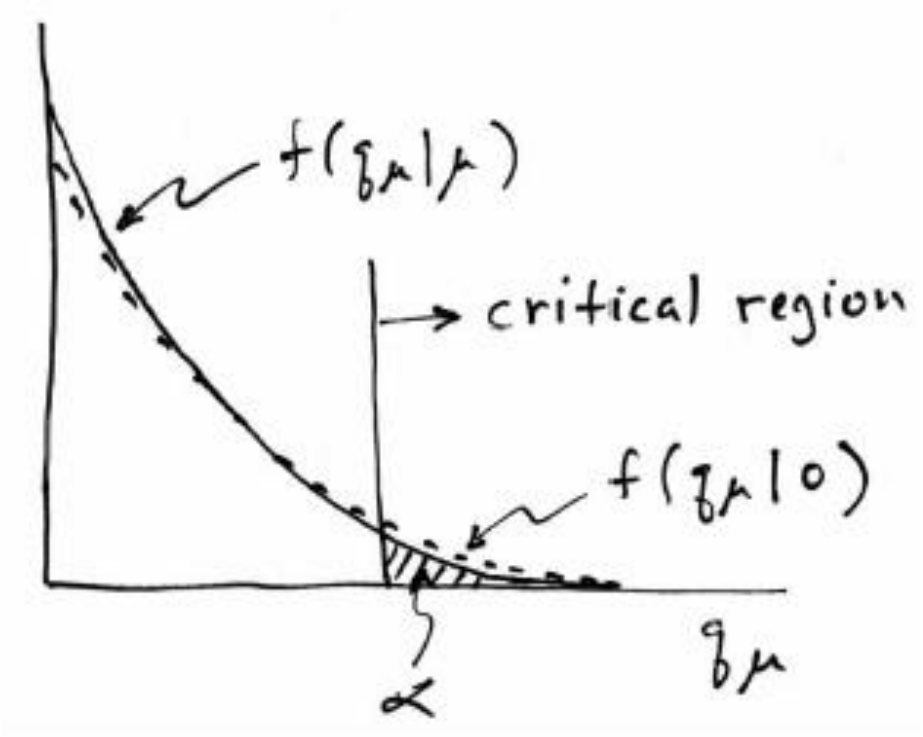
ATLAS, Phys. Lett. B 716 (2012) 1-29



Low sensitivity to μ

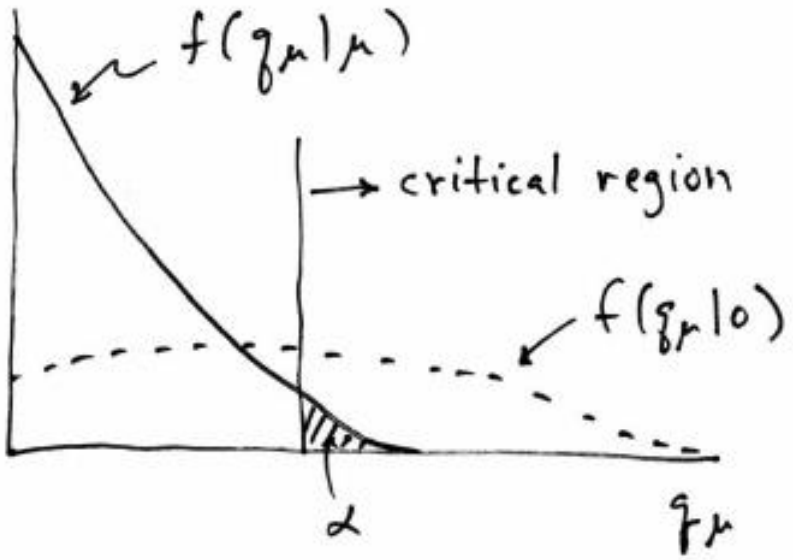
It can be that the effect of a given hypothesized μ is very small relative to the background-only ($\mu = 0$) prediction.

This means that the distributions $f(q_\mu|\mu)$ and $f(q_\mu|0)$ will be almost the same:



Having sufficient sensitivity

In contrast, having sensitivity to μ means that the distributions $f(q_\mu|\mu)$ and $f(q_\mu|0)$ are more separated:

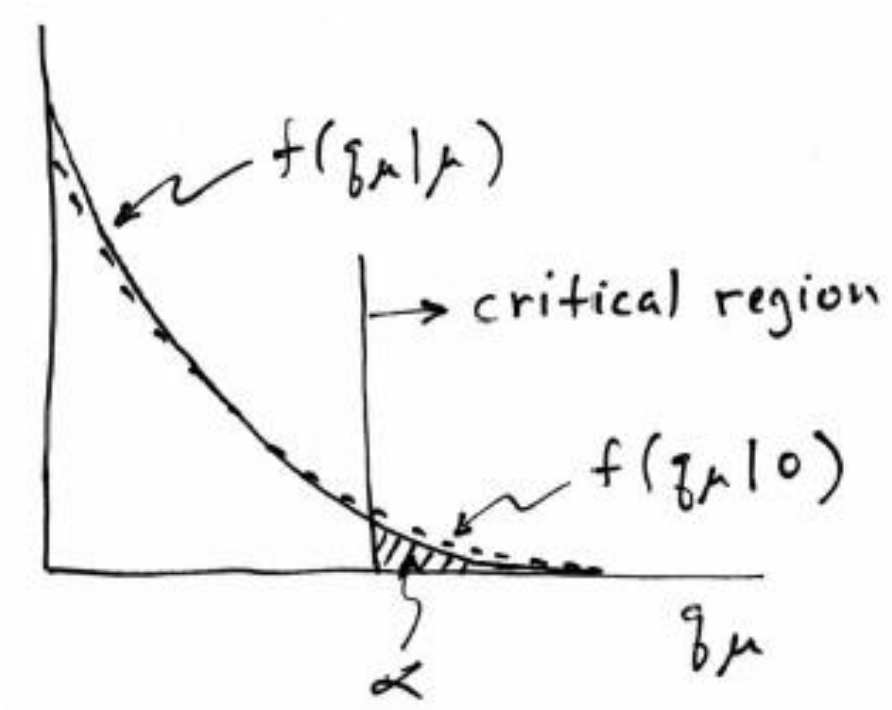


That is, the power (probability to reject μ if $\mu = 0$) is substantially higher than α. Use this power as a measure of the sensitivity.

Spurious exclusion

Consider again the case of low sensitivity. By construction the probability to reject μ if μ is true is α (e.g., 5%).

And the probability to reject μ if $\mu = 0$ (the power) is only slightly greater than α.



This means that with probability of around $\alpha = 5\%$ (slightly higher), one excludes hypotheses to which one has essentially no sensitivity (e.g., $m_{\mathrm{H}} = 1000$ TeV).

"Spurious exclusion"

Ways of addressing spurious exclusion

The problem of excluding parameter values to which one has no sensitivity known for a long time; see e.g.,

Virgil L. Highland, *Estimation of Upper Limits from Experimental Data*, July 1986, Revised February 1987, Temple University Report C00-3539-38.

In the 1990s this was re-examined for the LEP Higgs search by Alex Read and others

T. Junk, Nucl. Instrum. Methods Phys. Res., Sec. A **434**, 435 (1999); A.L. Read, J. Phys. G **28**, 2693 (2002).

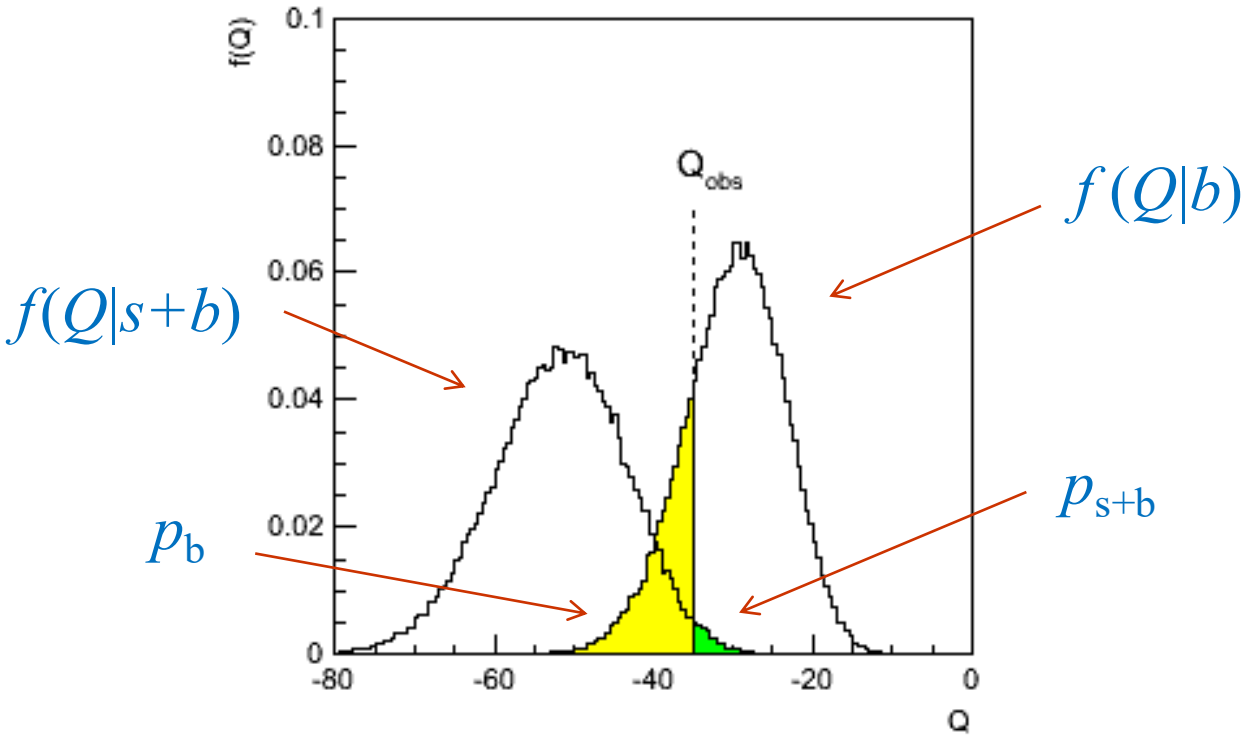
and led to the "CL_s" procedure for upper limits.

Unified (Feldman-Cousins) intervals also effectively reduce spurious exclusion by the particular choice of critical region.

Gary J. Feldman and Robert D. Cousins, Phys. Rev. D **57**, 3873 (1998)

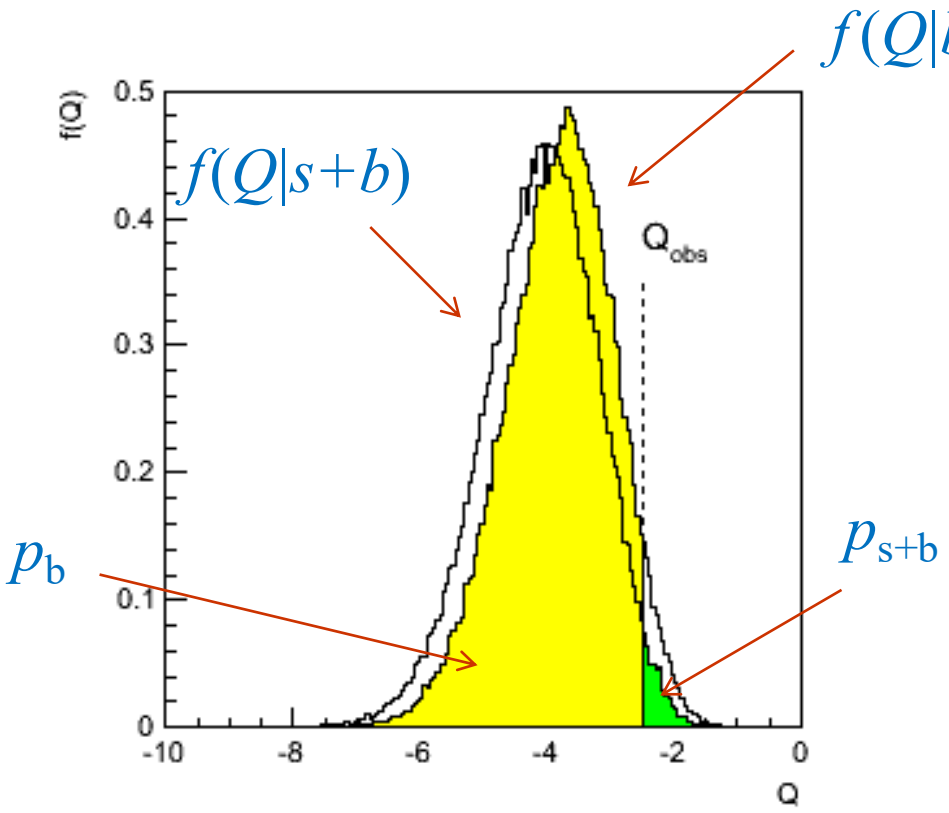
The CL_s procedure

In the usual formulation of CL_s, one tests both the $\mu = 0$ (b) and $\mu > 0$ $(\mu s+b)$ hypotheses with the same statistic $Q = -2\ln L_{s+b}/L_b$:



The CL_s procedure (2)

As before, "low sensitivity" means the distributions of Q under b and $s+b$ are very close:



The CL_s procedure (3)

The CL_s solution (A. Read et al.) is to base the test not on the usual p-value (CL_{s+b}), but rather to divide this by CL_b (~one minus the p-value of the b-only hypothesis), i.e.,

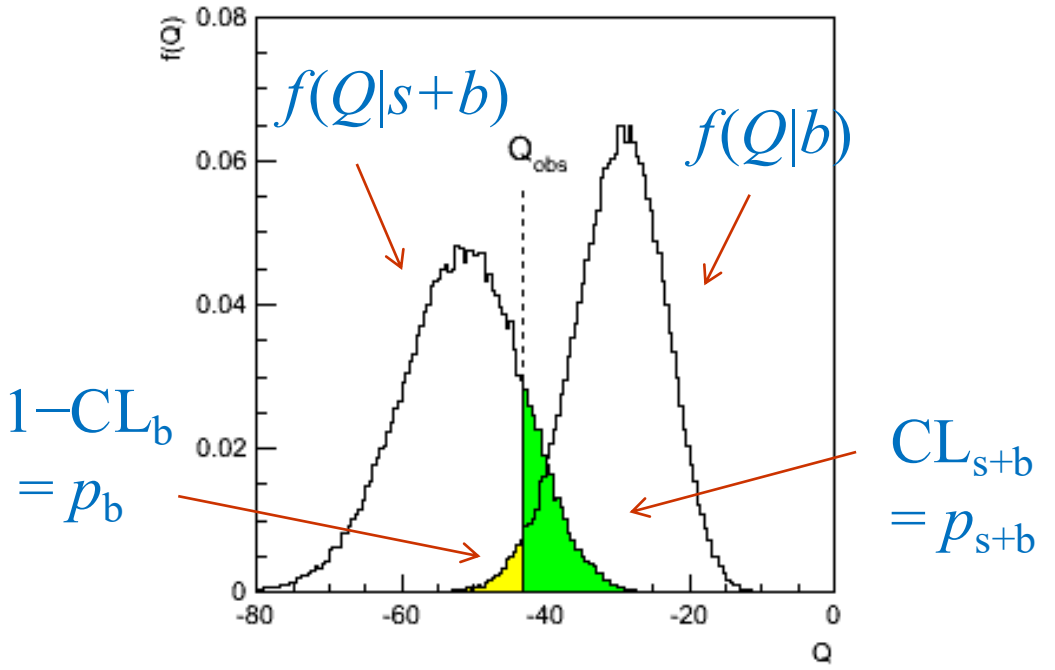
Define:

$$CL_s = \frac{CL_{s+b}}{CL_b}$$

$$= \frac{p_{s+b}}{1 - p_b}$$

Reject $s+b$ hypothesis if:

$$CL_s \leq \alpha$$



Increases "effective" p-value when the two distributions become close (prevents exclusion if sensitivity is low).

Finally...

Estimation of parameters is usually the "easy" part of statistics:

Frequentist: maximize the likelihood.

Bayesian: find posterior pdf and summarize (e.g. mode).

Standard tools for quantifying precision of estimates:
Variance of estimators, confidence intervals,...

But there are many potential stumbling blocks:

bias versus variance trade-off (how many parameters to fit?);

goodness of fit (usually only for LS or binned data);

choice of prior for Bayesian approach;

unexpected behaviour in LS averages with correlations,

confidence intervals can be empty, $\rightarrow$ CL_s, F-C,...

Extra Slides

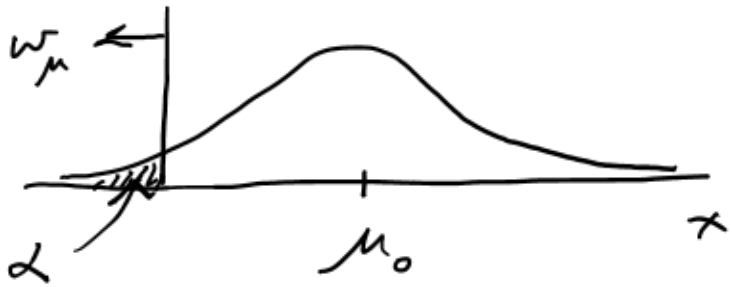
Example: upper limit on mean of Gaussian

When we test the parameter, we should take the critical region to maximize the power with respect to the relevant alternative(s).

Example: $x \sim \text{Gauss}(\mu, \sigma)$ (take σ known)

Test $H_0 : \mu = \mu_0$ versus the alternative $H_1 : \mu < \mu_0$

$\rightarrow$ Put w_μ at region of x-space characteristic of low μ (i.e. at low x)

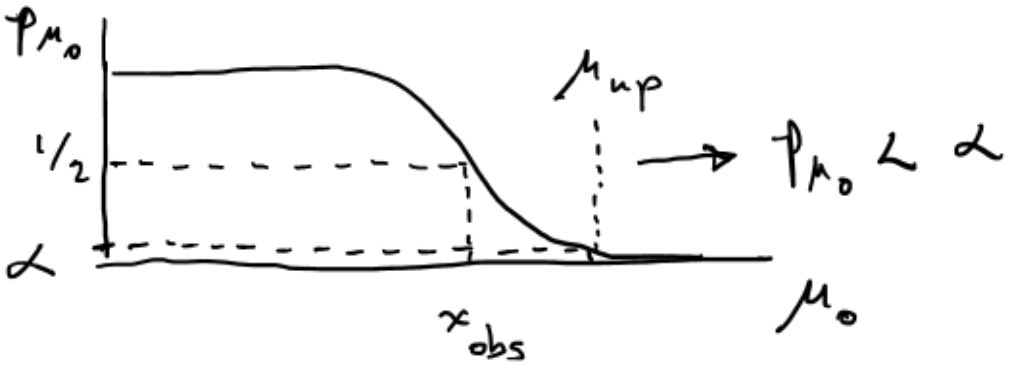


Equivalently, take the p-value to be

$$p_{\mu_0} = P(x \leq x_{\text{obs}}|\mu_0) = \int_{-\infty}^{x_{\text{obs}}} \frac{1}{\sqrt{2\pi}\sigma} e^{-(x-\mu_0)^2/2\sigma^2}\, dx = \Phi\left(\frac{x_{\text{obs}} - \mu_0}{\sigma}\right)$$

Upper limit on Gaussian mean (2)

To find confidence interval, repeat for all μ_0, i.e., set $p_{\mu 0} = \alpha$ and solve for μ_0 to find the interval's boundary



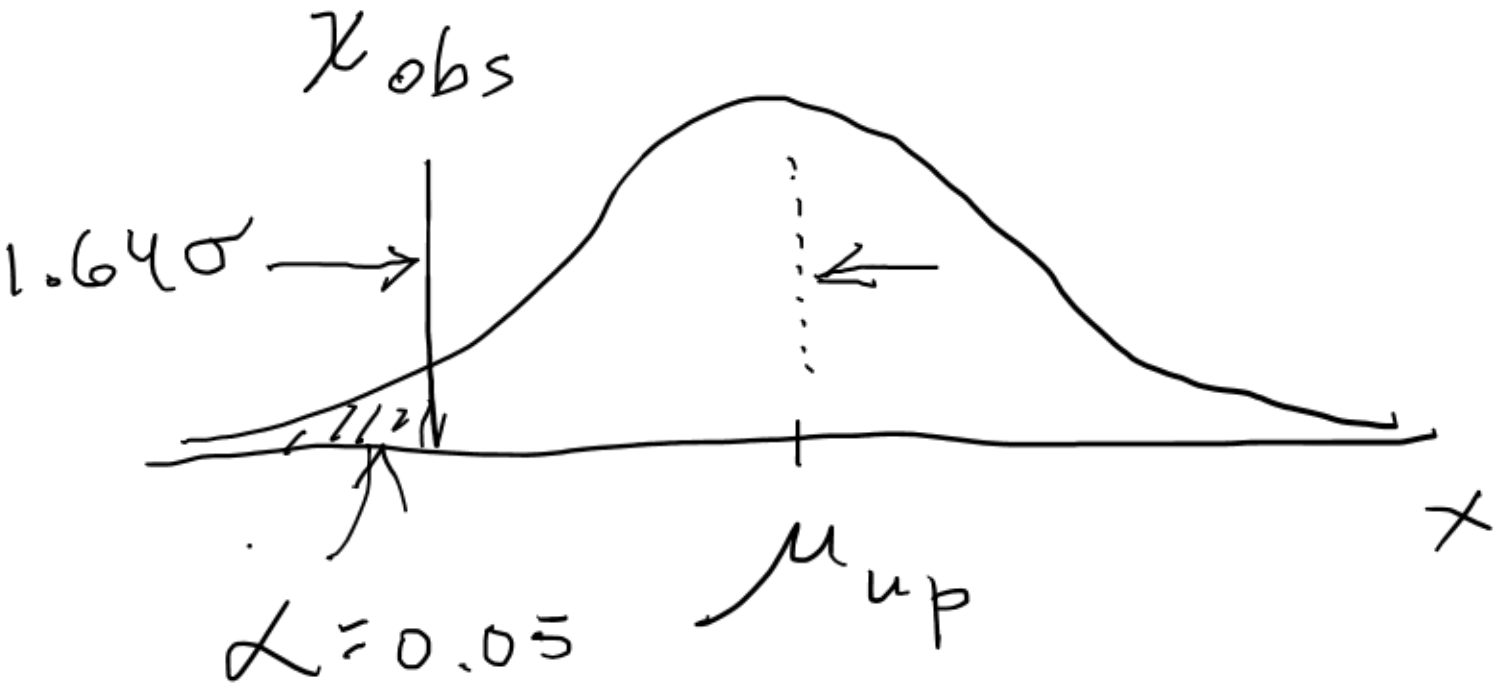
$$\mu_0 \to \mu_{\rm up} = x_{\rm obs} - \sigma\Phi^{-1}(\alpha) = x_{\rm obs} + \sigma\Phi^{-1}(1-\alpha)$$

This is an upper limit on μ, i.e., higher μ have even lower p-value and are in even worse agreement with the data.

Usually use $\Phi^{-1}(\alpha) = -\Phi^{-1}(1-\alpha)$ so as to express the upper limit as $x_{\rm obs}$ plus a positive quantity. E.g. for α = 0.05, $\Phi^{-1}(1-0.05)$ = 1.64.

Upper limit on Gaussian mean (3)

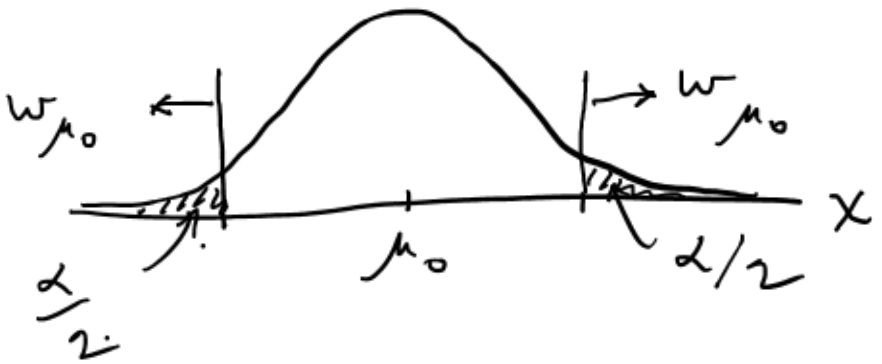
μ_{up} = the hypothetical value of μ such that there is only a probability α to find $x \leq x_{\text{obs}}$.



1- vs. 2-sided intervals

Now test: $H_0 : \mu = \mu_0$ versus the alternative $H_1 : \mu \neq \mu_0$

I.e. we consider the alternative to μ_0 to include higher and lower values, so take critical region on both sides:



Result is a "central" confidence interval $[\mu_{\rm lo}, \mu_{\rm up}]$:

$$\mu_{\rm lo} = x_{\rm obs} - \sigma\Phi^{-1}\left(1 - \frac{\alpha}{2}\right)$$

$$\mu_{\rm up} = x_{\rm obs} + \sigma\Phi^{-1}\left(1 - \frac{\alpha}{2}\right)$$

E.g. for $\alpha = 0.05$

$$\Phi^{-1}\left(1 - \frac{\alpha}{2}\right) = 1.96 \approx 2$$

Note upper edge of two-sided interval is higher (i.e. not as tight of a limit) than obtained from the one-sided test.

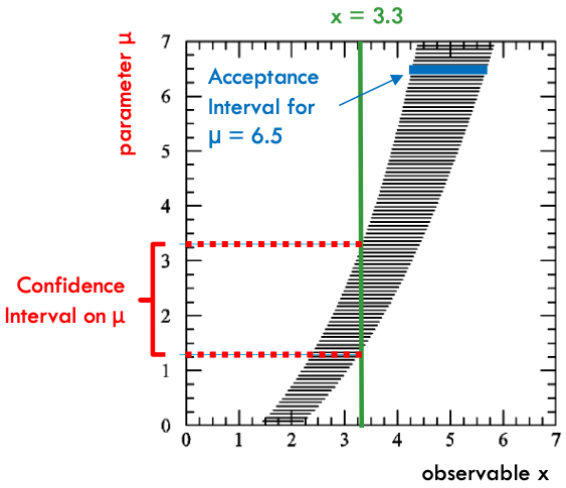
Confidence belt of Neyman construction is a graphical representation of the acceptance region (complement of critical region) of the test of the parameter.

André David

inspired by W. Verkerke and N. Smith

FREQUENTIST UNCERTAINTIES IN HEPP

Single measurement interval inversion



Neyman construction of the confidence belt

Acceptance intervals defined by

$$P(x_{low} < x < x_{high}; \mu) = \int_{x_{low}}^{x_{high}} p(x;\mu)\, dx \geq 1 - \alpha$$

where $\mathbf{1 - \alpha}$ is the **confidence level**.

Procedure in a nutshell:

1. For a given μ generate distribution of x, p(x; μ).
2. Use p(x; μ) to determine x_{low} and x_{high} and make horizontal line.
   - NB: acceptance interval depends on 1-α choice and can be one-sided (for limits).
3. Repeat for many values of μ to construct the belt.
4. For a given x = 3.3 look up the confidence interval for μ from the belt.

(Detailed step-by-step in backup.)

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