Lecture 4

Interval estimation — introduction

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

Desirable properties of such an interval may include:

communicate objectively the result of the experiment;
have a given probability of containing the true parameter;
provide information needed to draw conclusions about the parameter possibly incorporating stated prior beliefs.

Often use +/– the estimated standard deviation of the estimator.
In some cases, however, this is not adequate:

estimate near a physical boundary,
e.g., an observed event rate consistent with zero.

We will look briefly at Frequentist and Bayesian intervals.

Frequentist confidence intervals

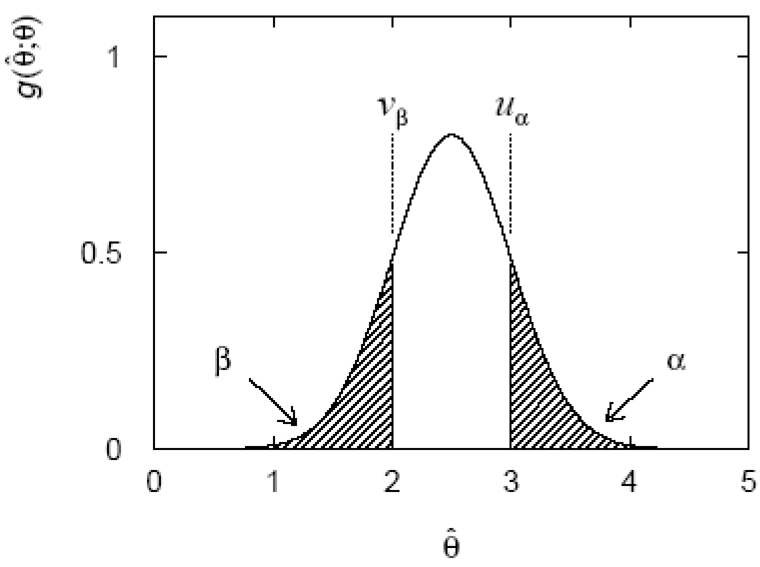
Consider an estimator $\hat{\theta}$ for a parameter θ and an estimate $\hat{\theta}_{\text{obs}}$.

We also need for all possible θ its sampling distribution $g(\hat{\theta};\theta)$.

Specify upper and lower tail probabilities, e.g., $\alpha = 0.05$, $\beta = 0.05$, then find functions $u_\alpha(\theta)$ and $v_\beta(\theta)$ such that:

$$\begin{aligned}\alpha &= P(\hat{\theta} \geq u_\alpha(\theta)) \\ &= \int_{u_\alpha(\theta)}^{\infty} g(\hat{\theta};\theta)\,d\hat{\theta}\end{aligned}$$

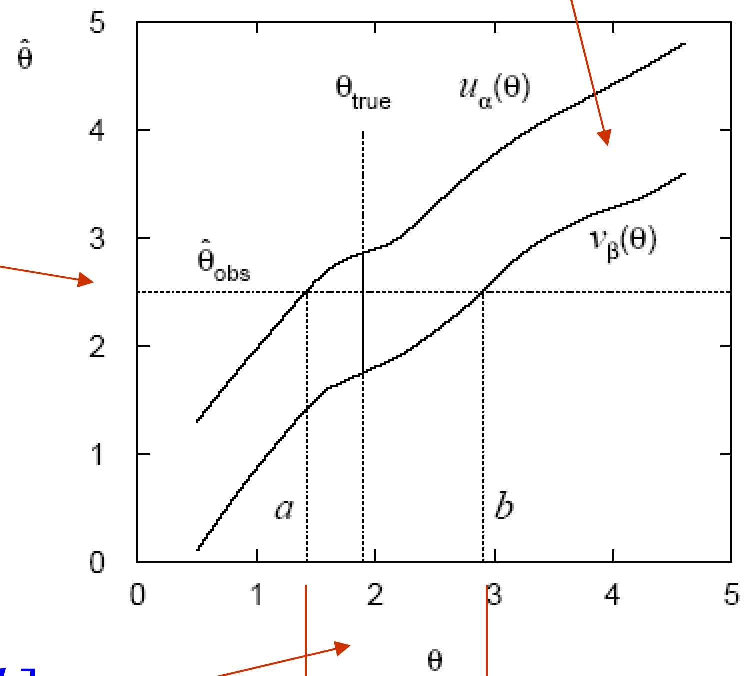
$$\begin{aligned}\beta &= P(\hat{\theta} \leq v_\beta(\theta)) \\ &= \int_{-\infty}^{v_\beta(\theta)} g(\hat{\theta};\theta)\,d\hat{\theta}\end{aligned}$$



Confidence interval from the confidence belt

The region between $u_\alpha(\theta)$ and $v_\beta(\theta)$ is called the confidence belt.

Find points where observed estimate intersects the confidence belt.



This gives the confidence interval $[a, b]$

Confidence level $= 1 - \alpha - \beta =$ probability for the interval to cover true value of the parameter (holds for any possible true θ).

Confidence intervals by inverting a test

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

Specify values of the data that are 'disfavoured' by θ (critical region) such that P(data in critical region) $\leq \gamma$ for a prespecified γ, e.g., 0.05 or 0.1.

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 would not be rejected in a test of size γ (confidence level is $1 - \gamma$).

The interval will cover the true value of θ with probability $\geq 1 - \gamma$.

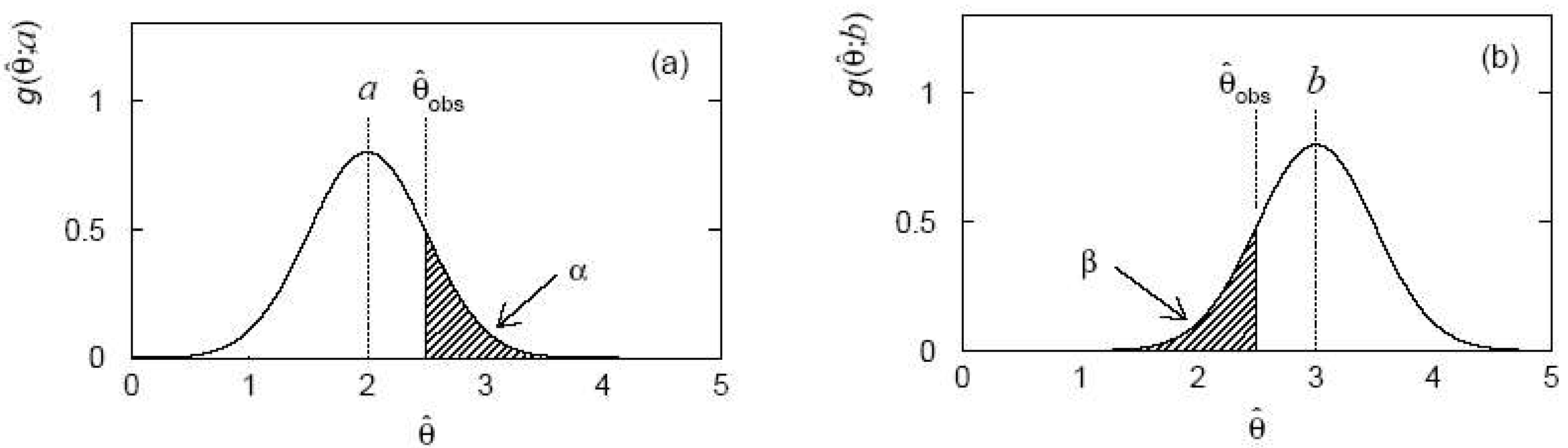
Equivalent to confidence belt construction; confidence belt is acceptance region of a test.

Confidence intervals in practice

The recipe to find the interval [a, b] boils down to solving

$$\alpha = \int_{u_\alpha(\theta)}^{\infty} g(\hat{\theta};\theta)\,d\hat{\theta} = \int_{\hat{\theta}_{\rm obs}}^{\infty} g(\hat{\theta};a)\,d\hat{\theta}\,,$$

$$\beta = \int_{-\infty}^{v_\beta(\theta)} g(\hat{\theta};\theta)\,d\hat{\theta} = \int_{-\infty}^{\hat{\theta}_{\rm obs}} g(\hat{\theta};b)\,d\hat{\theta}\,.$$



→ a is hypothetical value of θ such that $P(\hat{\theta} > \hat{\theta}_{\rm obs}) = \alpha\,.$

→ b is hypothetical value of θ such that $P(\hat{\theta} < \hat{\theta}_{\rm obs}) = \beta\,.$

Meaning of a confidence interval

N.B. the interval is random, the true θ is an unknown constant.

Often report interval $[a, b]$ as $\hat{\theta}^{+d}_{-c}$, i.e. $c = \hat{\theta} - a$, $d = b - \hat{\theta}$.

So what does $\hat{\theta} = 80.25^{+0.31}_{-0.25}$ mean? It does not mean:

$P(80.00 < \theta < 80.56) = 1 - \alpha - \beta$, but rather:

repeat the experiment many times with same sample size,

construct interval according to same prescription each time,

in $1 - \alpha - \beta$ of experiments, interval will cover θ.

Central vs. one-sided confidence intervals

Sometimes only specify α or β, $\rightarrow$ one-sided interval (limit)

Often take $\alpha = \beta = \dfrac{\gamma}{2}$ $\rightarrow$ coverage probability $= 1 - \gamma$

$\rightarrow$ central confidence interval

N.B. 'central' confidence interval does not mean the interval is symmetric about $\hat{\theta}$, but only that $\alpha = \beta$.

The HEP error 'convention': 68.3% central confidence interval.

Intervals from the likelihood function

In the large sample limit it can be shown for ML estimators:

$\hat{\vec{\theta}} \sim N(\vec{\theta}, V)$ (n-dimensional Gaussian, covariance V)

$$L(\vec{\theta}) = L_{\max} \exp\left[-\frac{1}{2} Q(\hat{\vec{\theta}}, \vec{\theta})\right], \quad Q(\hat{\vec{\theta}}, \vec{\theta}) = (\hat{\vec{\theta}} - \vec{\theta})^T V^{-1} (\hat{\vec{\theta}} - \vec{\theta})$$

$Q(\hat{\vec{\theta}}, \vec{\theta}) = Q_\gamma$ defines a hyper-ellipsoidal confidence region,

$$P(\text{ellipsoid covers true } \vec{\theta}) = P(Q(\hat{\vec{\theta}}, \vec{\theta}) \leq Q_\gamma)$$

If $\hat{\vec{\theta}} \sim N(\vec{\theta}, V)$ then $Q(\hat{\vec{\theta}}, \vec{\theta}) \sim \text{Chi-square}(n)$

$$\text{coverage probability} \equiv 1 - \gamma = \int_0^{Q_\gamma} f_{\chi^2}(z; n)\, dz = F_{\chi^2}(Q_\gamma; n)$$

Approximate confidence regions from $L(\theta)$

So the recipe to find the confidence region with CL = $1-\gamma$ is:

$$\ln L(\vec{\theta}) = \ln L_{\max} - \frac{Q_\gamma}{2} \quad \text{or} \quad \chi^2(\vec{\theta}) = \chi^2_{\min} + Q_\gamma$$

where $\quad Q_\gamma = F^{-1}_{\chi^2}(1-\gamma; n)$

Q_γ	$1-\gamma$				
	$n=1$	$n=2$	$n=3$	$n=4$	$n=5$
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

$1-\gamma$	Q_γ				
	$n=1$	$n=2$	$n=3$	$n=4$	$n=5$
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

For finite samples, these are approximate confidence regions.

Coverage probability not guaranteed to be equal to $1-\gamma$;

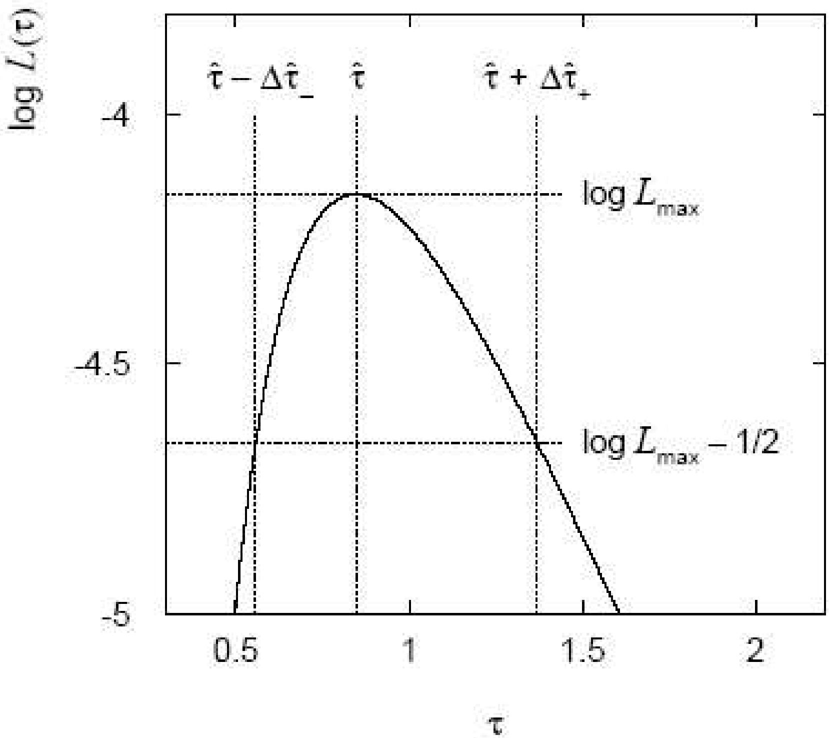
no simple theorem to say by how far off it will be (use MC).

Remember here the interval is random, not the parameter.

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

For n=1 parameter, CL = 0.683, $Q_\gamma = 1$.

Our exponential example, now with $n = 5$ observations:



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

Setting limits on Poisson parameter

Consider again the case of finding $n = n_s + n_b$ events where

n_b events from known processes (background)

n_s events from a new process (signal)

are Poisson r.v.s with means s, b, and thus $n = n_s + n_b$ is also Poisson with mean $= s + b$. Assume b is known.

Suppose we are searching for evidence of the signal process, but the number of events found is roughly equal to the expected number of background events, e.g., $b = 4.6$ and we observe $n_{obs} = 5$ events.

The evidence for the presence of signal events is not statistically significant,

$\rightarrow$ set upper limit on the parameter s.

Upper limit for Poisson parameter

Find the hypothetical value of s such that there is a given small probability, say, $\gamma = 0.05$, to find as few events as we did or less:

$$\gamma = P(n \leq n_{\mathrm{obs}}; s, b) = \sum_{n=0}^{n_{\mathrm{obs}}} \frac{(s+b)^n}{n!} e^{-(s+b)}$$

Solve numerically for $s = s_{\mathrm{up}}$, this gives an upper limit on s at a confidence level of $1-\gamma$.

Example: suppose $b = 0$ and we find $n_{\mathrm{obs}} = 0$. For $1-\gamma = 0.95$,

$$\gamma = P(n = 0; s, b = 0) = e^{-s} \quad \rightarrow \quad s_{\mathrm{up}} = -\ln\gamma \approx 3.00$$

Calculating Poisson parameter limits

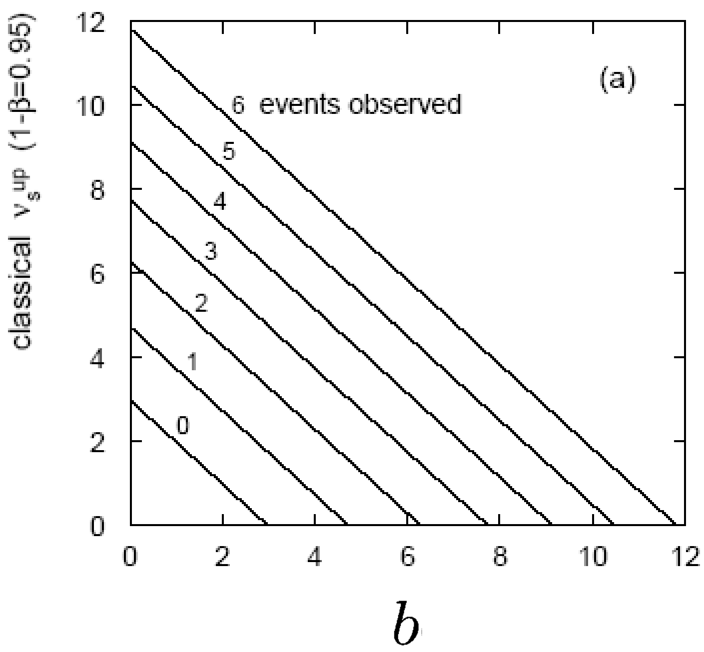
To solve for s_{lo}, s_{up}, can exploit relation to χ^2 distribution:

$$s_{\rm lo} = \frac{1}{2} F^{-1}_{\chi^2}(\alpha; 2n) - b$$

Quantile of χ^2 distribution

$$s_{\rm up} = \frac{1}{2} F^{-1}_{\chi^2}(1-\beta; 2(n+1)) - b$$

For low fluctuation of n this can give negative result for s_{up}; i.e. confidence interval is empty.



Limits near a physical boundary

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

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

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

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 limit of parameter is close to a physical boundary, cf. m_ν estimated using $E^2 - p^2$.

Expected limit for $s = 0$

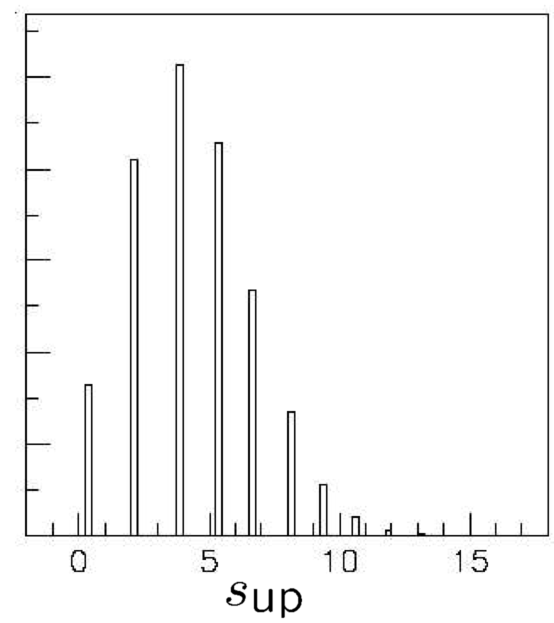
Physicist: I should have used CL = 0.95 — then $s_{up} = 0.496$

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

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 ($s = 0$) hypothesis (sensitivity).

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



The Bayesian approach

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. Poisson parameter 95% CL upper limit from

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

Bayesian prior for Poisson parameter

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

Often 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*

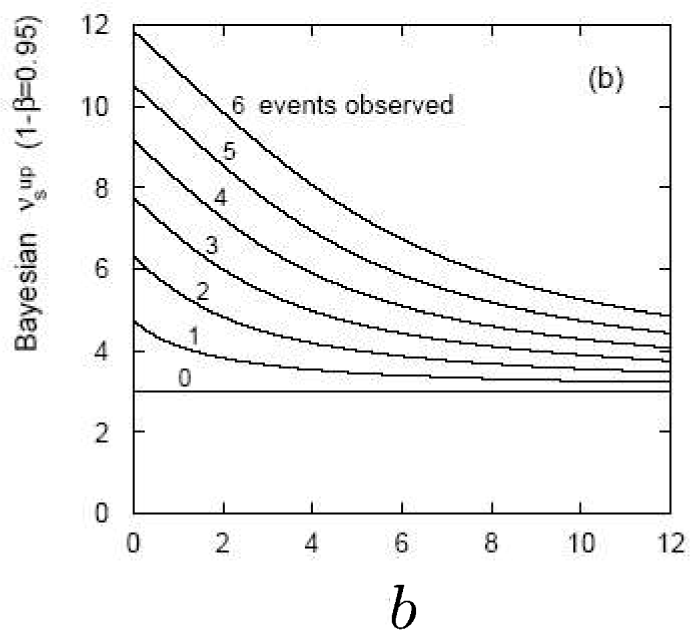
Solve numerically to find limit s_{up}.

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 $n = 0$.



Likelihood ratio limits (Feldman-Cousins)

Define likelihood ratio for hypothesized parameter value *s*:

$$l(s) = \frac{L(n|s,b)}{L(n|\hat{s},b)} \quad \text{where} \quad \hat{s} = \begin{cases} n-b & n \geq b, \\ 0 & \text{otherwise} \end{cases}$$

Here $\hat{s}$ is the ML estimator, note $0 \leq l(s) \leq 1$.

Critical region defined by low values of likelihood ratio.

Resulting intervals can be one- or two-sided (depending on *n*).

(Re)discovered for HEP by Feldman and Cousins,
Phys. Rev. D 57 (1998) 3873.

More on intervals from LR test (Feldman-Cousins)

Caveat with coverage: suppose we find $n >> b$.
Usually one then quotes a measurement: $\hat{s} = n - b\,, \quad \hat{\sigma}_{\hat{s}} = \sqrt{n}$

If, however, n isn't large enough to claim discovery, one sets a limit on s.

FC pointed out that if this decision is made based on n, then the actual coverage probability of the interval can be less than the stated confidence level ('flip-flopping').

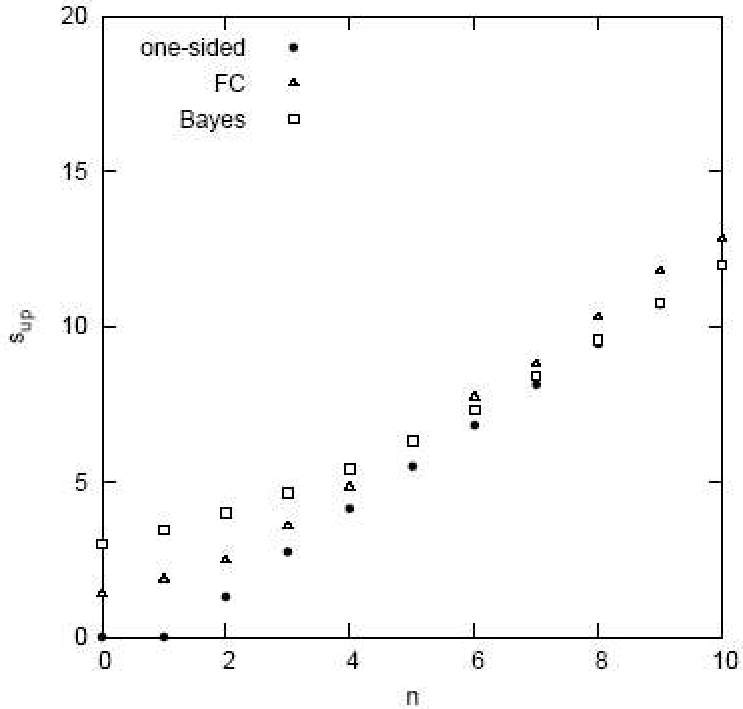
FC intervals remove this, providing a smooth transition from 1- to 2-sided intervals, depending on n.

But, suppose FC gives e.g. $0.1 < s < 5$ at 90% CL, p-value of s=0 still substantial. Part of upper-limit 'wasted'?

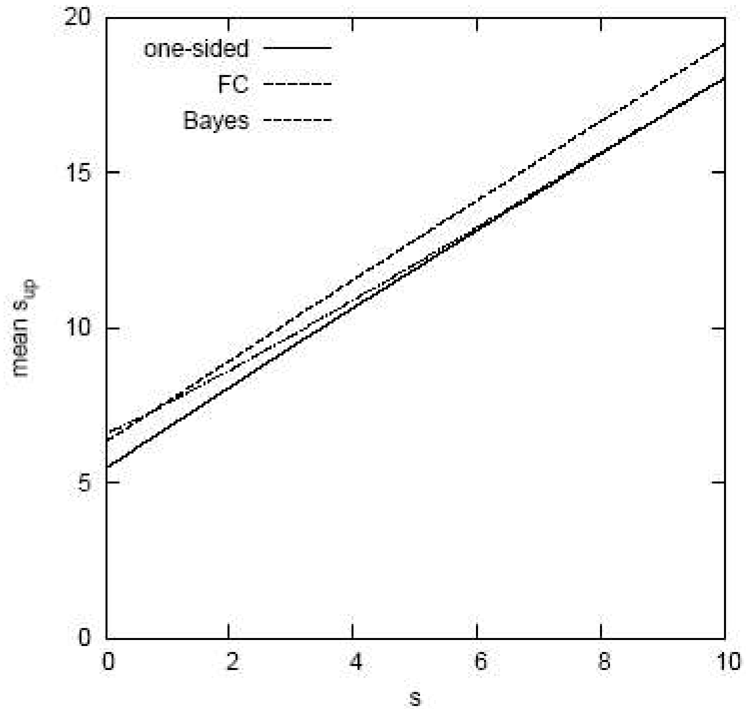
Properties of upper limits

Example: take $b = 5.0$, $1 - \gamma = 0.95$

Upper limit s_{up} vs. n

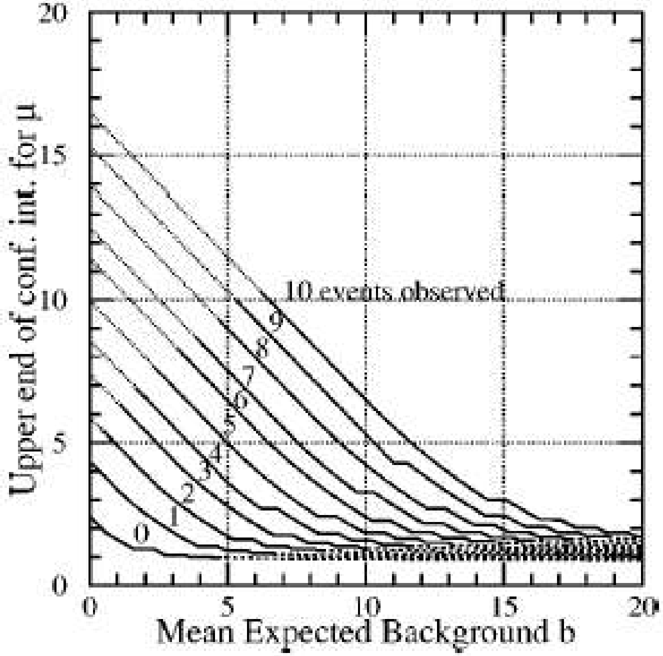


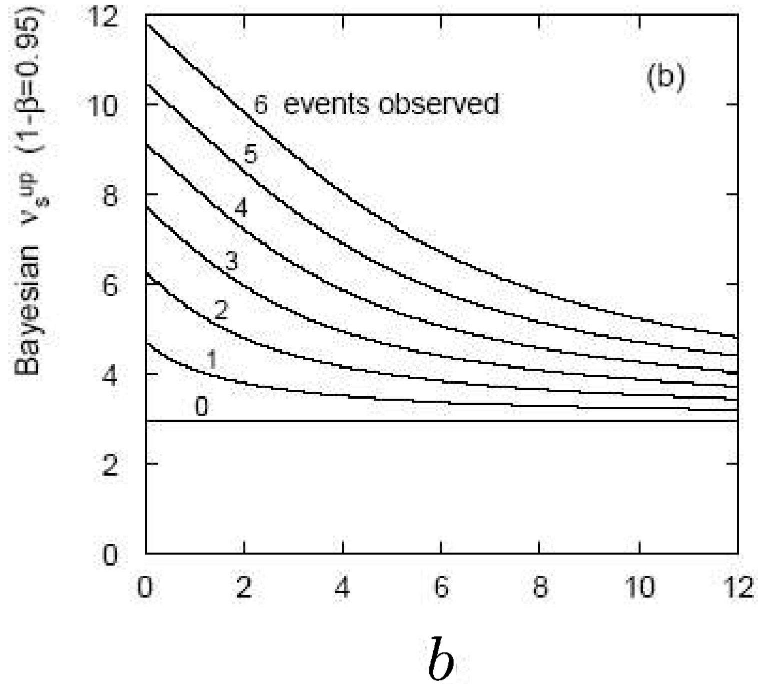
Mean upper limit vs. s



Upper limit versus b

Feldman & Cousins, PRD 57 (1998) 3873





If $n = 0$ observed, should upper limit depend on b?

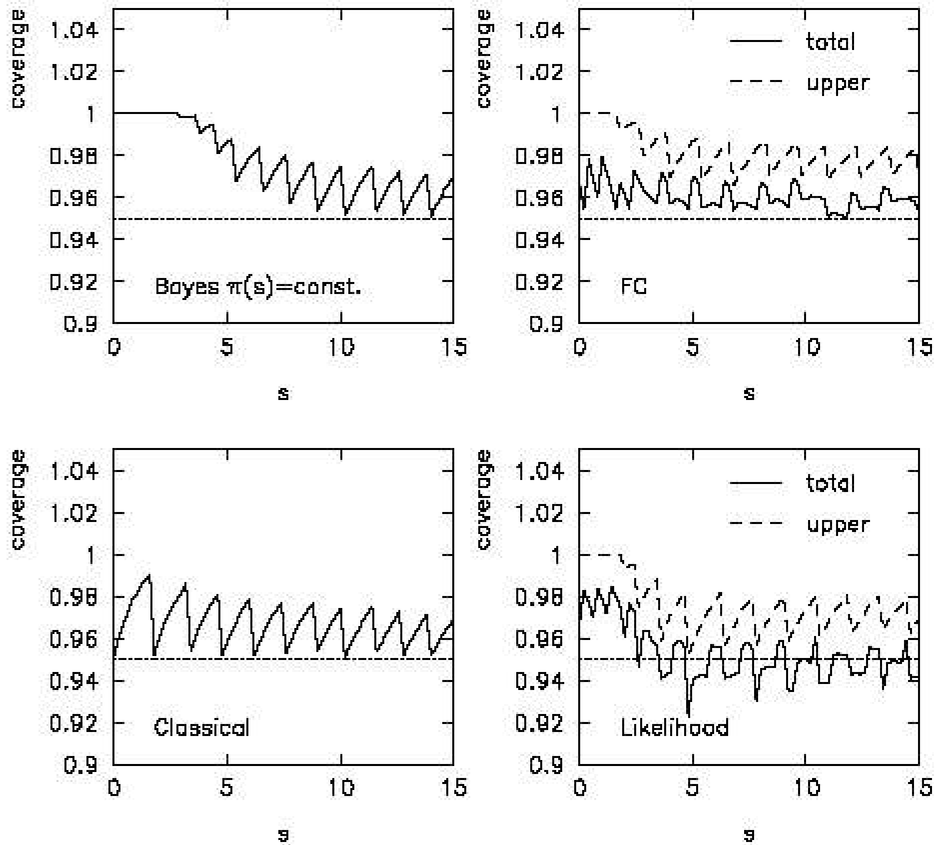
Classical: yes

Bayesian: no

FC: yes

Coverage probability of intervals

Because of discreteness of Poisson data, probability for interval to include true value in general > confidence level ('over-coverage')



Wrapping up lecture 4

In large sample limit and away from physical boundaries, +/– 1 standard deviation is all you need for 68% CL.

Frequentist confidence intervals

Complicated! Random interval that contains true parameter with fixed probability.

Can be obtained by inversion of a test; freedom left as to choice of test.

Log-likelihood can be used to determine approximate confidence intervals (or regions)

Bayesian intervals

Conceptually easy — just integrate posterior pdf.

Requires choice of prior.

Lecture 4 — extra slides

Interval from Gaussian distributed estimator

Suppose we have $g(\hat{\theta};\theta) = \frac{1}{\sqrt{2\pi\sigma_{\hat{\theta}}^2}} \exp\left(\frac{-(\hat{\theta}-\theta)^2}{2\sigma_{\hat{\theta}}^2}\right)$.

To find confidence interval for θ, solve

$$\alpha = 1 - G(\hat{\theta}_{\rm obs}; a, \sigma_{\hat{\theta}}) = 1 - \Phi\left(\frac{\hat{\theta}_{\rm obs} - a}{\sigma_{\hat{\theta}}}\right),$$

$$\beta = G(\hat{\theta}_{\rm obs}; b, \sigma_{\hat{\theta}}) = \Phi\left(\frac{\hat{\theta}_{\rm obs} - b}{\sigma_{\hat{\theta}}}\right),$$

for a, b, where G is cumulative distribution for $\hat{\theta}$ and

$\Phi(x) = \int_{-\infty}^{x} \frac{1}{\sqrt{2\pi}} e^{-x'^2/2}\, dx'$ is cumulative of standard Gaussian.

Interval for Gaussian estimator (2)

$$\rightarrow \quad a = \hat{\theta}_{\mathrm{obs}} - \sigma_{\hat{\theta}} \Phi^{-1}(1-\alpha),$$

$$b = \hat{\theta}_{\mathrm{obs}} + \sigma_{\hat{\theta}} \Phi^{-1}(1-\beta).$$

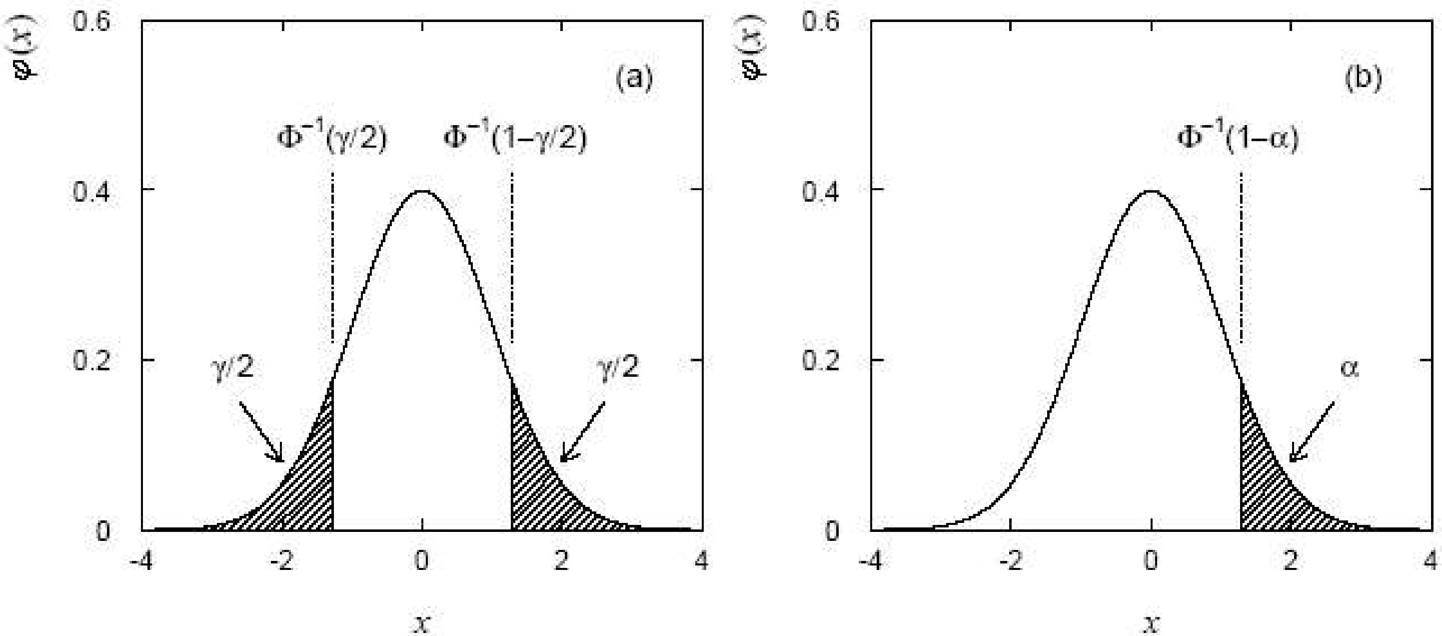
$\Phi^{-1} =$ quantile of standard Gaussian

(inverse of cumulative distribution, CERNLIB routine **GAUSIN**).

$\rightarrow$ $\Phi^{-1}(1-\alpha)$, $\Phi^{-1}(1-\beta)$ give how many standard deviations a, b are from $\hat{\theta}$.

Quantiles of the standard Gaussian

To find the confidence interval for a parameter with a Gaussian, estimator we need the following quantiles:



Quantiles of the standard Gaussian (2)

Usually take a round number for the quantile …

central		one-sided	
$\Phi^{-1}(1-\gamma/2)$	$1-\gamma$	$\Phi^{-1}(1-\alpha)$	$1-\alpha$
1	0.6827	1	0.8413
2	0.9544	2	0.9772
3	0.9973	3	0.9987

Sometimes take a round number for the coverage probability …

central		one-sided	
$1-\gamma$	$\Phi^{-1}(1-\gamma/2)$	$1-\alpha$	$\Phi^{-1}(1-\alpha)$
0.90	1.645	0.90	1.282
0.95	1.960	0.95	1.645
0.99	2.576	0.99	2.326