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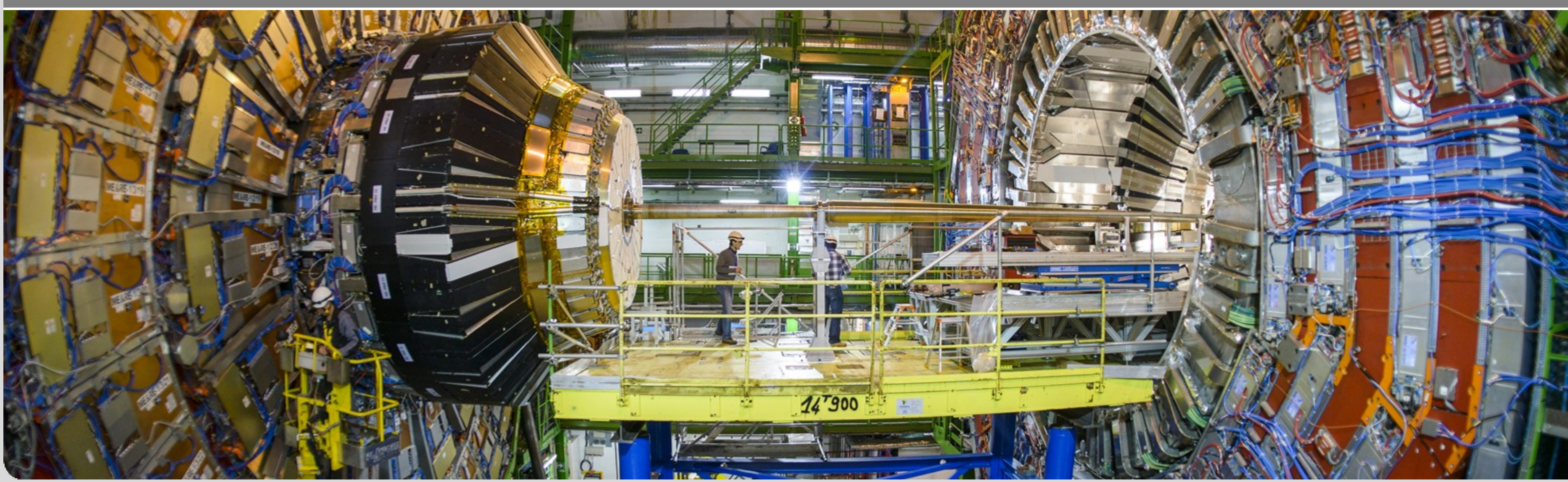
Tutorial Lecture on Limit Setting in High Energy Physics

Roger Wolf (based on material by Stefan Schmitt)

07. March 2017

INSTITUTE OF EXPERIMENTAL PARTICLE PHYSICS (IEKP) – PHYSICS FACULTY



Probability

Think of throwing a coin three times in a row:

- $\Omega = \{(\mathrm{Head}, \mathrm{Head}, \mathrm{Head}), (\mathrm{Tail}, \mathrm{Head}, \mathrm{Head}), \ldots\} \rightarrow$ (all possible outcomes) **sample space**.
- Each subset $A \subset \Omega$ is called **event**.
- The set of all possible events (σ-algebra) $\mathfrak{S}(\Omega)$.
- **Probability**:

  $\mathcal{P} : \mathfrak{S}(\Omega) \rightarrow \mathbb{R} \quad ; \quad A \rightarrow \mathcal{P}(A),$

  - Non-negative: $\mathcal{P}(A) \geq 0 \quad \forall A$
  - Linear : $\mathcal{P}(A \cup B) = \mathcal{P}(A) + \mathcal{P}(B) \quad \forall A \cap B = \emptyset$
  - Normalized : $\mathcal{P}(\mathfrak{S}(\Omega)) = 1$

Probability (conditional)

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Probability of event A given event $B(\neq \emptyset)$:

- $\mathcal{P}_B(A) = \mathcal{P}(A|B) = \frac{\mathcal{P}(A\cap B)}{\mathcal{P}(B)}$ $\rightarrow$ (**conditional probability**).

Bayes theorem:

- $\mathcal{P}_A(B) \cdot \mathcal{P}(A) = \mathcal{P}_B(A) \cdot \mathcal{P}(B)$ $\rightarrow$ (**Bayes theorem**).

(Statistically) independent events:

- $\mathcal{P}(A \cap B) = \mathcal{P}(A) \cdot \mathcal{P}(B)$ $\rightarrow$ (**statistical independent**).

  $\mathcal{P}_A(B) = \mathcal{P}(B)$

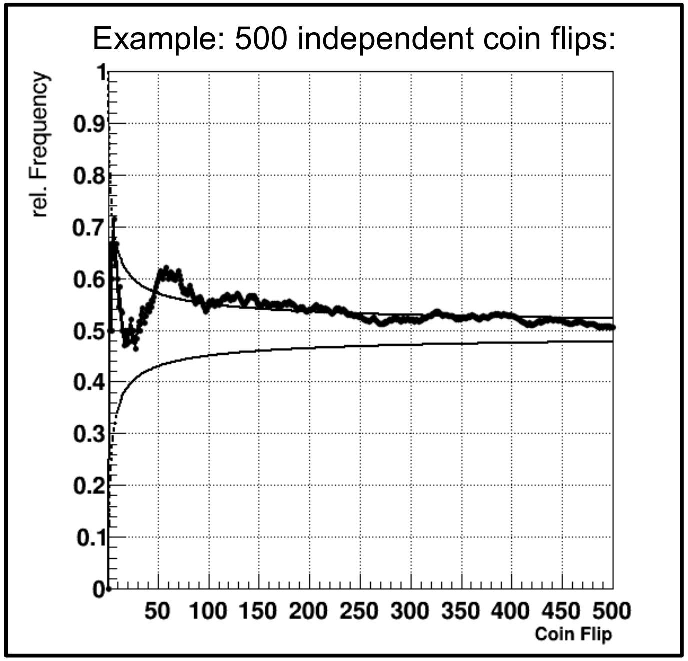
  $\mathcal{P}_B(A) = \mathcal{P}(A)$

- Particle physics is a unique field where statistical independence of event is perfectly fulfilled for an incredibly large sample space.

Interpretation paradigms

- Mathematical results need to be interpreted:

- **Frequentist**:



Relative frequency converges to probability.

- **Bayesian**:

  Quantification of my degree of belief that event A turns out to be true.

+ Makes sense also for "experiments", which can not be repeated.

- Requires reasonable implementation of probability distribution (usually coincides with Frequentist interpretation, where overlaps, but not always).

Bayesian statistics and prior knowledge

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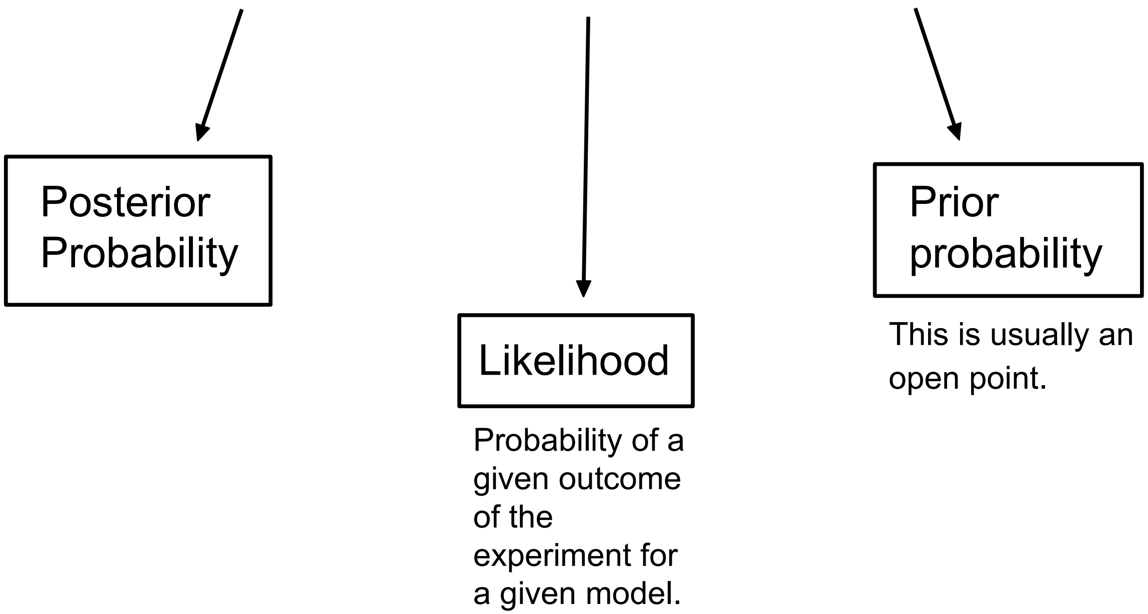
- In Bayesian statistics: “my degree of belief” that event A turns out to be true depends on my prejudice (→ prior knowledge):

$$\mathcal{P}_{\mathrm{Data}}(\mathrm{Model}) \propto \mathcal{P}_{\mathrm{Model}}(\mathrm{Data}) \cdot \mathcal{P}(\mathrm{Model}) \qquad \rightarrow \textbf{(Bayes theorem)}.$$



- Mapped to our use case: does the measurement support my physics model?

Exercise-1: Prior @ work

Assume there is a decease which 0.1% of the population have (→ this is your prior). Assume there is a test that diagnoses this decease with a probability of 98%, while it gives false positive results with a probability of 3% .

a) Your test is positive. Calculate the probability that you are ill.

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a) Your test is positive. Calculate the probability that you are ill.

$$\mathcal{P}_+(\text{ill}) = \frac{\mathcal{P}_{\text{ill}}(+)\cdot\mathcal{P}(\text{ill})}{\mathcal{P}_{\text{ill}}(+)\cdot\mathcal{P}(\text{ill})+\mathcal{P}_{\text{not ill}}(+)\cdot\mathcal{P}(\text{not ill})}$$

$$= \frac{0.98\cdot 0.001}{0.98\cdot 0.001+0.03\cdot 0.999} = 0.032$$

b) How does the result change if you redo the test and it is positive again?

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$$= \frac{0.98\cdot 0.032}{0.98\cdot 0.032+0.03\cdot 0.968} = 0.519$$

Probability density functions

- In general we assume the underlying statistics model to follow a given probability density function.

- Most prominent examples:

Poisson:

$$\mathcal{P}(k, \mu) = \frac{\mu^k}{k!} e^{-\mu}$$

e.g. for counting experiments (like for cross sections).

Gaussian:

$$\varphi(x, \mu, \sigma) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-(x-\mu)^2/2\sigma^2}$$

e.g. for parameter estimates (like for mass measurements) .

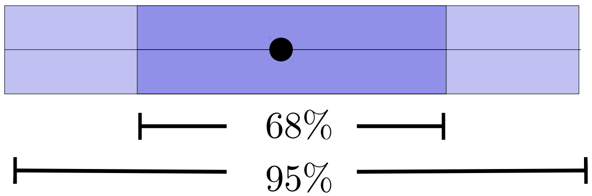
- Probability density distributions are themselves functions of parameters.

- If it is the target of the measurement we often call it parameter of interest (POI), otherwise we often call it nuisance parameter (often indicated by θ).

Confidence intervals

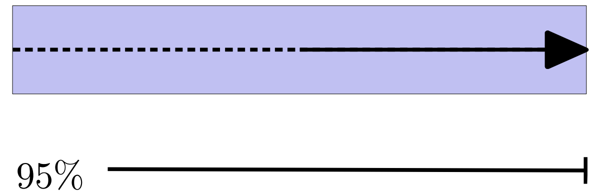
- Confidence intervals allow statements about parameters in models.

Double sided (measurement):



$$m = \mu \pm \sigma_{0.68} \text{ @ } 68\%\ CL$$

Single sided (limit):



$$BR \leq \mu_{0.95} \text{ @ } 95\%\ CL$$

- Interpretation depending on paradigm:

Frequentist:

Probability to make given observation for a given truth. Esp. no probability for “truth to be true”

Bayesian:

Probability of truth to lie in given interval.

- We will concentrate on single sided confidence intervals (→ used for upper limits).

Upper limit

- With the upper limit on a model POI μ, for a given observation x_{obs} (or N_{obs}) we search for the largest value of μ for which the probability to make an observation of $x \leq x_{obs}$ (or $N \leq N_{obs}$) is less than a value α.
- We call this value of μ the upper limit on μ at the confidence level (CL) $1 - \alpha$. During the next slides we will indicate this quantity by $\mu_{1-\alpha}$.
- We particle physics we usually use $\alpha = 0.05$ (→ 95% CL limit).

Meaning:

For $\mu = \mu_{0.95}$ in 95% of all outcomes of the same experiment x (or N) would have been larger then x_{obs} (or N_{obs}) . For $\mu > \mu_{0.95}$ this fraction would be even larger. The observation restricts μ to be not larger than $\mu_{0.95}$ at 95% CL.

Question:

Is $\mu_{0.90} < \mu_{0.95}$ or $\mu_{0.90} > \mu_{0.95}$?

Confidence interval construction (Frequentist)

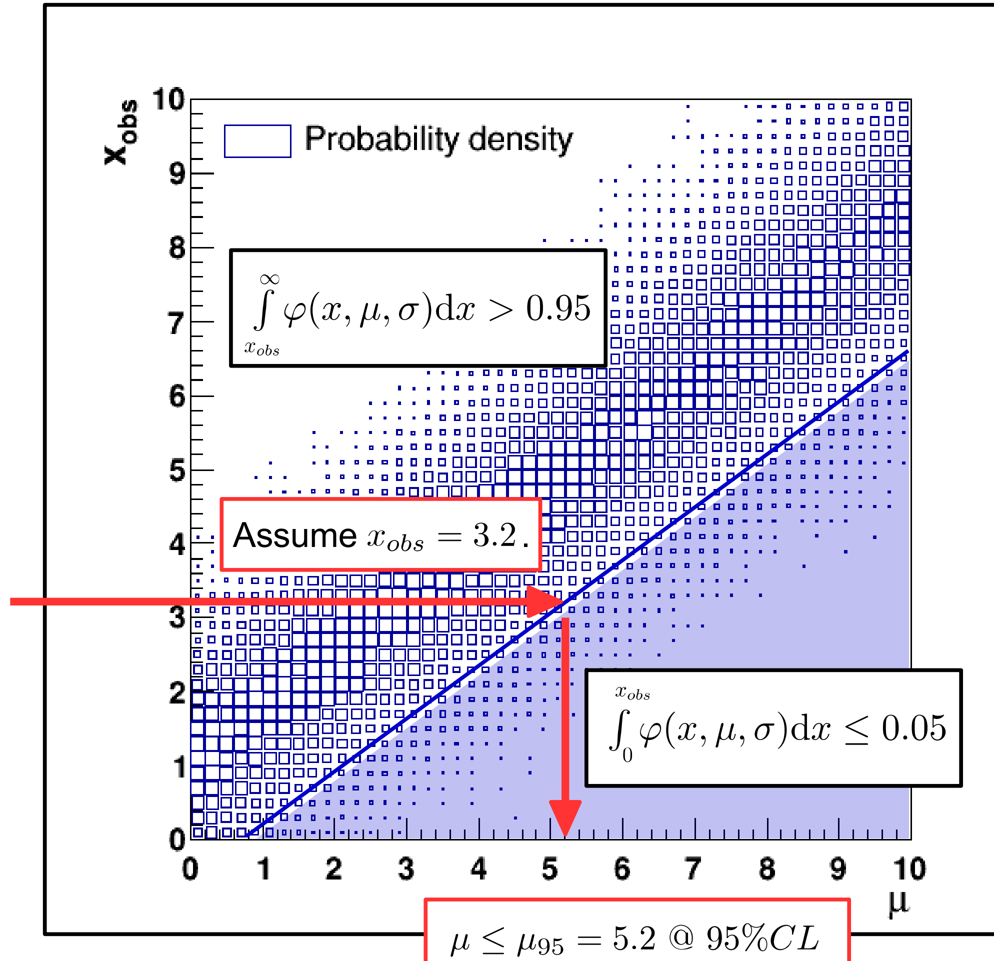
- Here shown for 95% CL upper limit on a parameter μ of a Gaussian distributed random variable x_{obs} :

- **Neyman construction**:

- For each value of μ find single sided confidence interval for given α (e.g. $\alpha = 0.05$).

- Interconnect interval edges.

- For a given observation find the largest value for μ where x_{obs} is still contained in the interval.



Confidence interval construction (Frequentist)

- Here shown for 95% CL upper limit on a parameter μ of a Poisson distributed random variable N_{obs}:

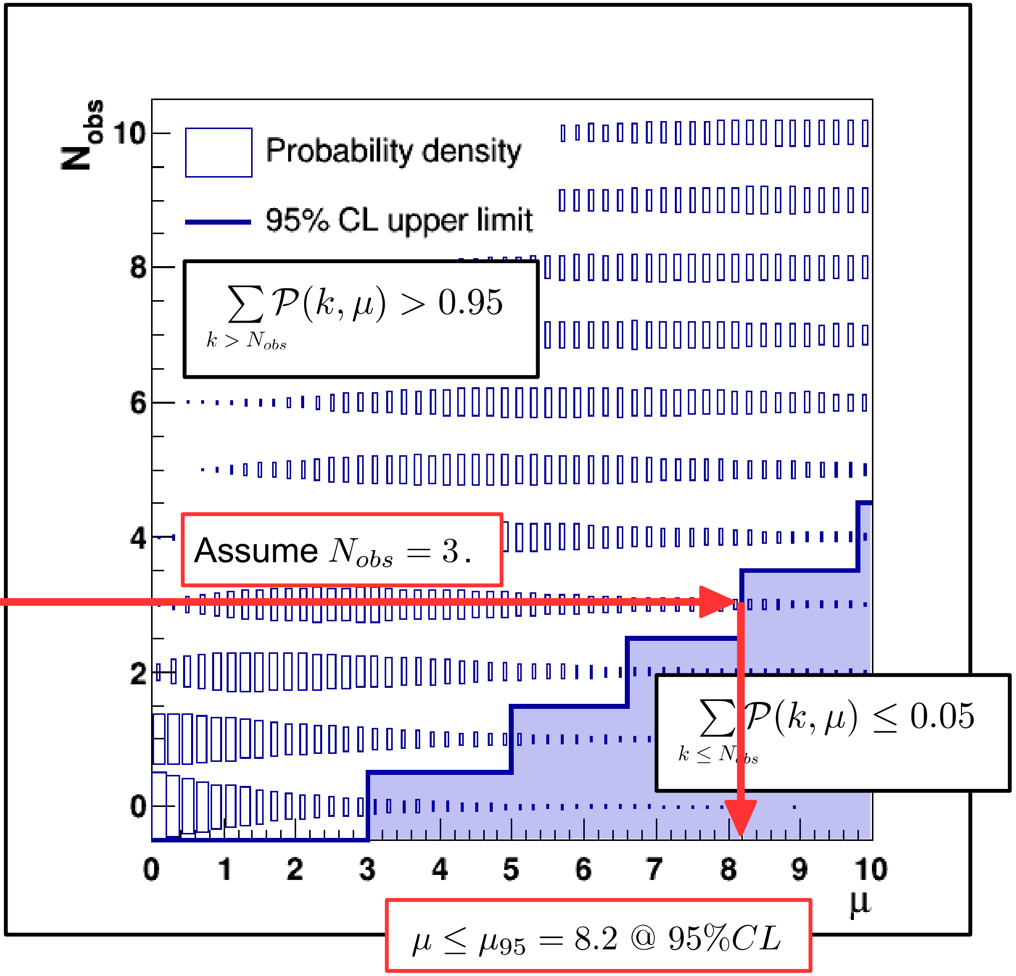
- **Neyman construction**:

- For each value of μ find single sided confidence interval for given α (e.g. $\alpha = 0.05$).

- Interconnect interval edges.

- For a given observation find the largest value for μ where x_{obs} is still contained in the interval.

- Note steps due to discrete nature of Poisson distribution.



Coverage

- For a given limit procedure you can calculate for each value of μ the exact probability to exclude the theory:

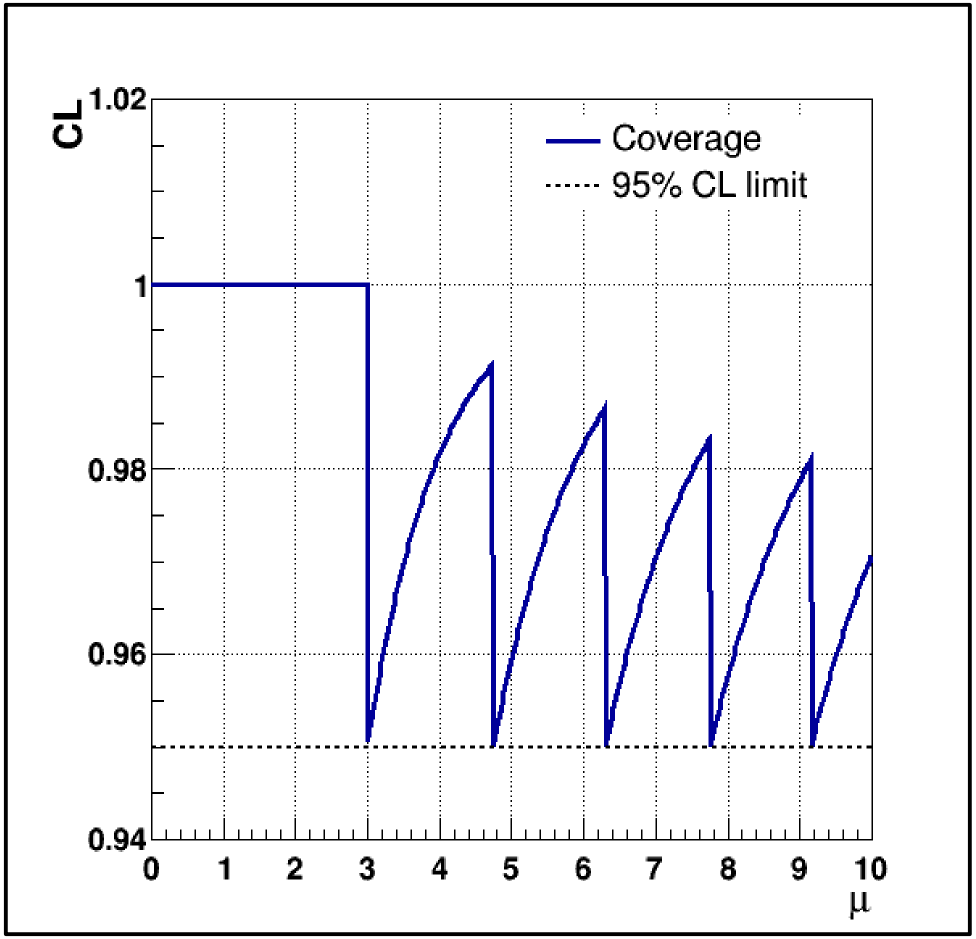
- **Coverage**:

- For our Poisson example:

$$P_{excl}(\mu) = \sum_{N \geq N_{obs}} P_\mu(N) \cdot \theta(\mu \leq \mu_{0.95})$$

$$P_{excl}(\mu) \begin{cases} > 0.95 & \text{over coverage} \\ = 0.95 & \text{exact coverage} \\ < 0.95 & \text{under coverage} \end{cases}$$

- Over coverage ($\rightarrow$ exclusion statement more conservative).



Exercise-2: Frequentist limit

Assume you have an observation of 1 event, were you expect 0 due to already known processes. You want to quote a 95% CL upper limit on the true value μ of the expected events for a Poisson distributed signal model.

a) Calculate the exclusion probability (i.e. the probability to observe more than 2 events) for the values of μ given in the table on the right:

μ	P_{excl}
2	
3	
4	
5	

$N_{obs} = 1$

NB: in root you can use the function given below for your calculation. Vary μ for fixed $N = N_{obs}$ until $\alpha < 0.05$.

$$\alpha \quad = \texttt{TMath::Prob}(2\,\mu, 2(N+1)) = \sum_{N \leq N_{obs}} \frac{e^{-\mu}\mu^N}{N!}$$

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μ	P_{excl}
2	0.59
3	0.80
4	0.91
5	0.96

$N_{obs} = 1$

b) Calculate the 95% CL limit on μ for the values of N_{obs} given in the table on the right:

N_{obs}	$\mu_{0.95}$
0	
1	
2	
4	

NB: in root you can use the function given below for your calculation. Vary μ for fixed $N = N_{obs}$ until $\alpha < 0.05$.

$$\alpha = \texttt{TMath::Prob}(2\,\mu, 2(N+1)) = \sum_{N \leq N_{obs}} \frac{e^{-\mu}\mu^N}{N!}$$

$$\mu_{1-\alpha} = \texttt{TMath::ChisquareQuantile}(1-\alpha, 2(N+1))/2$$

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$N_{obs} = 1$

N_{obs}	$\mu_{0.95}$
0	3.00
1	4.74
2	6.30
4	9.15

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Confidence interval construction (Bayesian)

- Here shown for 95% CL upper limit on a parameter μ of an arbitrarily distributed random variable x_{obs} :

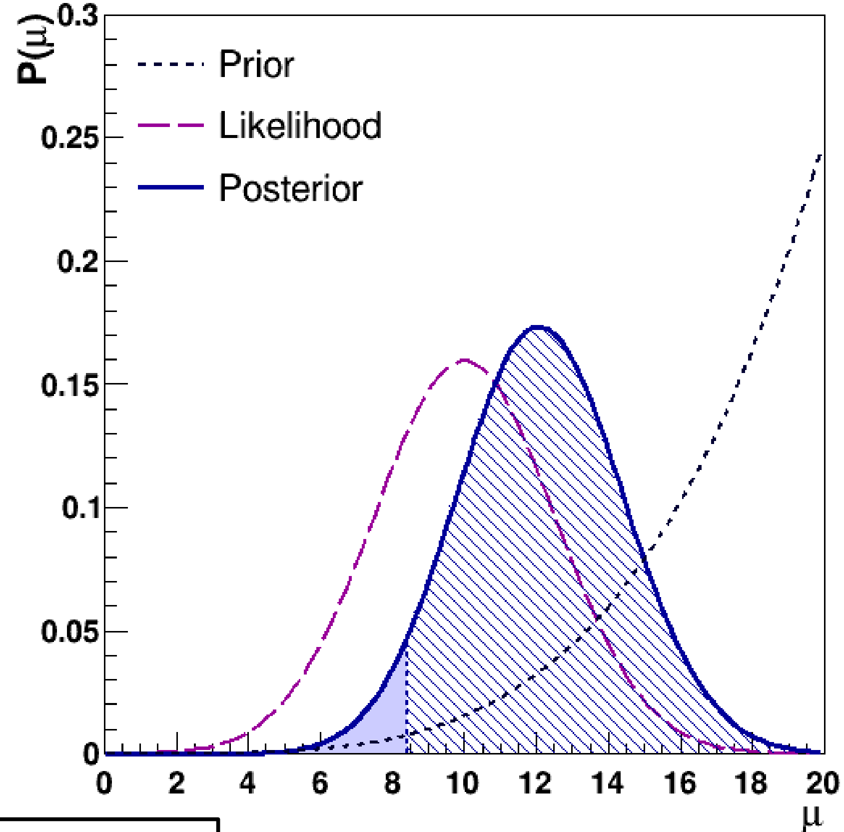
- **Bayesian limit:**

- Assign prior $\mathcal{P}(\text{Model})$ to model to be true and likelihood $\mathcal{P}_{\text{Model}}(x_{obs})$.

- Calculate posterior $\mathcal{P}_{x_{obs}}(\text{Model})$ for known prior, likelihood & x_{obs} .

- Determine $\mu_{0.95}$ such that:

$$\underbrace{\frac{\int_0^{\mu_{0.95}} \mathcal{P}_{x_{obs}}(\text{Model}) \cdot \mathcal{P}(\text{Model}) \mathrm{d}\mu}{\int_0^{\infty} \mathcal{P}_{x_{obs}}(\text{Model}) \cdot \mathcal{P}(\text{Model}) \mathrm{d}\mu}}_{\equiv \alpha(\mu, N)} \leq 0.05$$



Requires numerical integration of posterior.

Exercise-3: Bayesian limit

Assume you have an observation of 1 event, were you expect 0 due to already known processes. You want to quote a 95% CL upper limit on the true value μ of the expected events for a Poisson distributed signal model.

a) Calculate the 95% CL limit on μ for $N_{obs} = 1$ and a flat prior.

NB: the macro below calculates α for you by numerical integration of the posterior. Vary μ for fixed $N = N_{obs}$ until $\alpha < 0.05$.

GetPosterior.C(μ, N)$= \alpha(\mu, N)$

Exercise-3: Bayesian limit

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b) Do the same calculation for the prior $\mathcal{P}(\mathrm{Model}) \propto \mu$.

N_{obs}	μ_{95}
1	3.00
2	4.74
3	6.30
5	9.15

$\mathcal{P}(\mathrm{Model}) = \mathrm{const}$

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`GetPosterior.C`(μ, N)$= \alpha(\mu, N)$

For exercise b) modify the function `GetBayesPosterior(mu)` in the macro.

Exercise-3: Bayesian limit

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a) Calculate the 95% CL limit on μ for $N_{obs} = 2$ and a flat prior.

b) Do the same calculation for the prior $\mathcal{P}(\text{Model}) \propto \mu$.

N_{obs}	μ_{95}
1	3.00
2	4.74
3	6.30
5	9.15

$\mathcal{P}(\text{Model}) = \text{const}$

N_{obs}	μ_{95}
1	4.75
2	6.27
3	7.76
5	10.51

$\mathcal{P}(\text{Model}) \propto \mu$

NB: the macro below calculates α for you by numerical integration of the posterior. Vary μ for fixed $N = N_{obs}$ until $\alpha < 0.05$.

`GetPosterior.C`$(\mu, N) = \alpha(\mu, N)$

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Summary (lecture part-I)

- Short recap of basics about probabilities.
- Confidence intervals and limits.
- Frequentist limit construction.
- Bayesian limit construction.

Excluding signal on top of a known background

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- Usually expected number of events is a sum of (perfectly known) number of background events plus potential signal events:

$$\mu = s + b$$

s: expected signal

b: expected background

- Determine limit on μ. To obtain limit on s use $s = \mu - b$. Assume b to be perfectly known for the time being.

Exclusion sensitivity

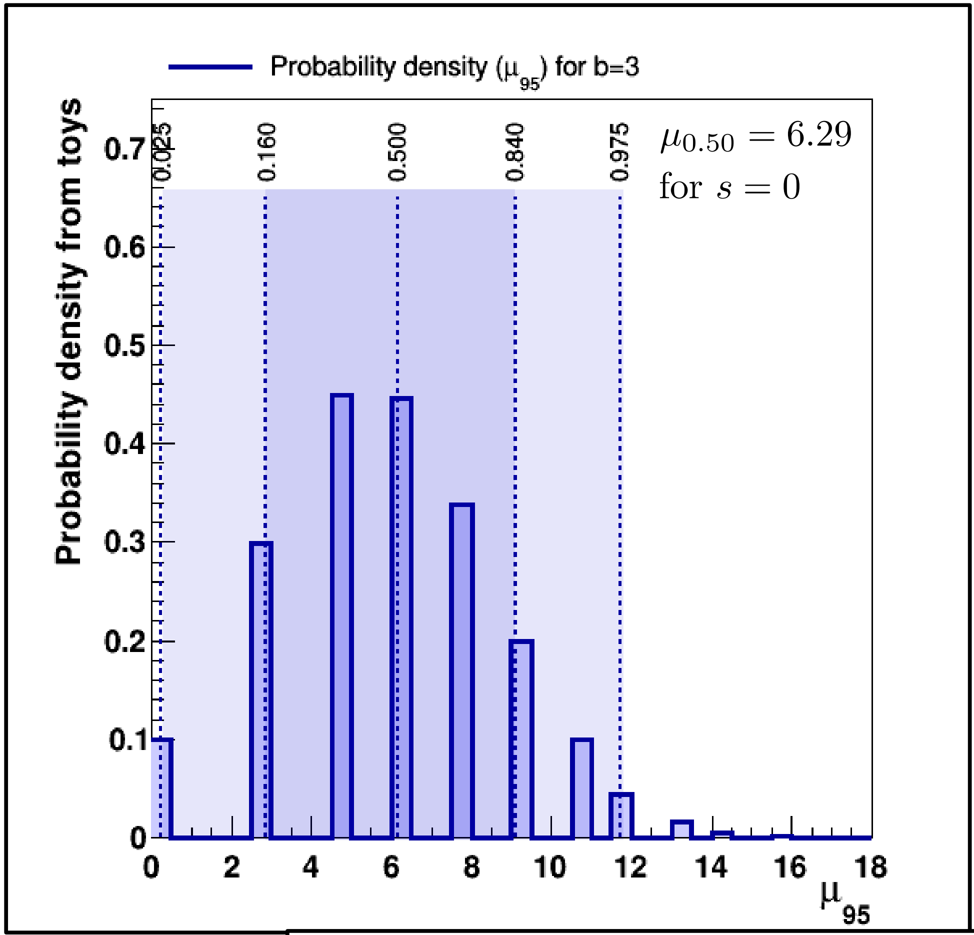
- With $b > 0$ it makes sense to talk about the sensitivity of an experiment to exclude a certain model.

- Assume additional number of events due to s (in signal region) to be small:

  b large $\rightarrow$ low sensitivity.
  b small $\rightarrow$ high sensitivity.

- Calculate limit for toy experiments for $s = 0$ ($b \neq 0$, here Poisson distributed).

- Usually quote expected exclusion limit in terms of quantiles of the resulting probability distribution for $\mu_{0.95}$.



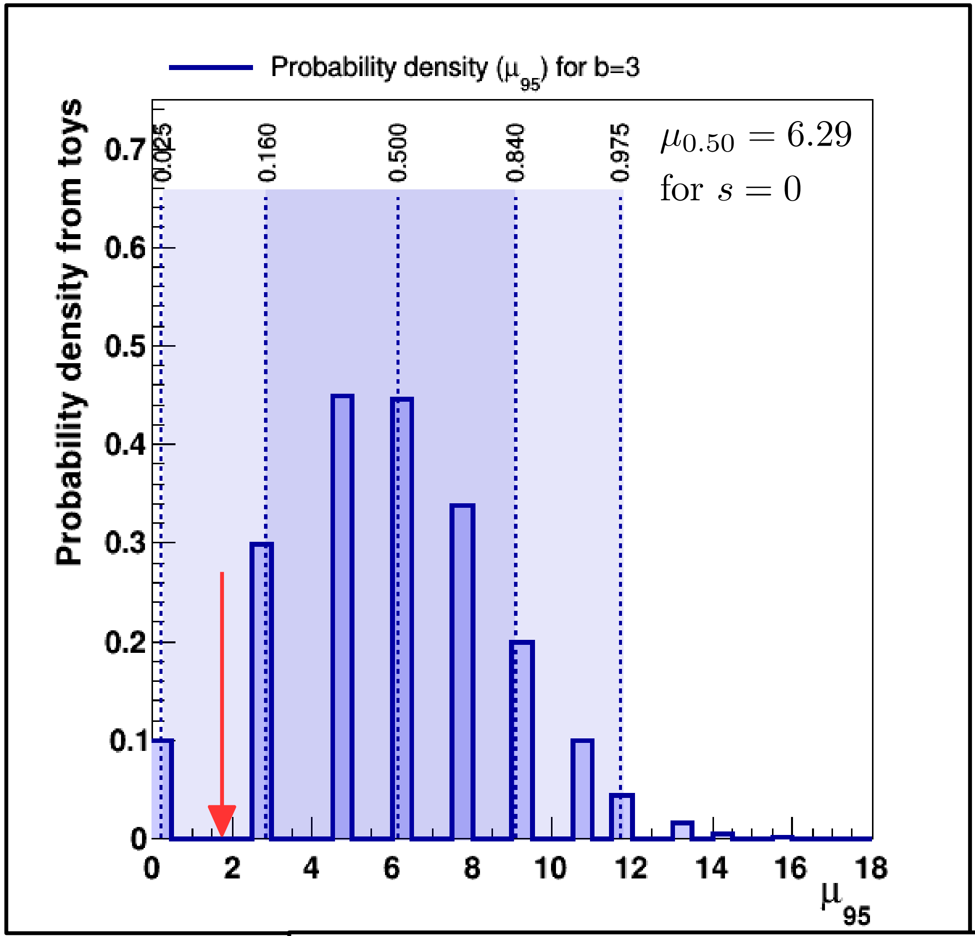
Example: 95% CL upper limit on $\mu = b$ in absence of signal for $b = 3$ and using Frequentist limit setting.

Limits near boundaries

- **Problem**: Frequentist limit can fall far below actual exclusion sensitivity and even lead to unphysical results (e.g. in case of "under fluctuations" of b.)

b	$\mu_{0.95} - b$	$\mu_{0.50}^{exp}(s=0)$
0	4.74	0
2	2.74	$4.75\pm^{1.55}_{1.75}$
3	1.74	$6.29\pm^{2.86}_{3.30}$
5	−0.26	$9.15\pm^{2.69}_{2.86}$

$N_{obs} = 1$ Uncert's from 68% quantile.



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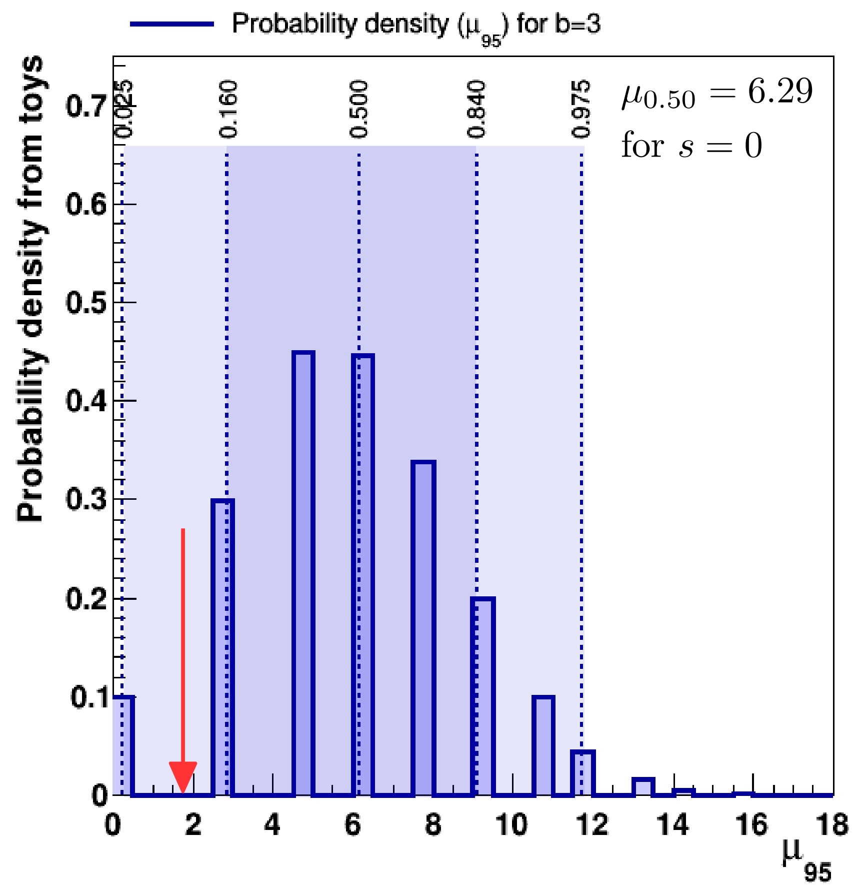

Countermeasures:

- Bayesian limit allows to incorporate prior knowledge about physical boundaries.
- Modify Frequentist limit to prevent exclusion far beyond sensitivity.

Example: 95% CL upper limit on $\mu = b$ in absence of signal for $b = 3$ and using Frequentist limit setting.

Exercise-4: Limits near a boundary

Assume you have an observation of 1 event, were you expect 0, 2, 3, 5 due to already known processes. You want to quote a 95% CL upper limit on the true value μ of the expected events for a Poisson distributed signal model.

a) Use the numerical integration for the Bayesian limit, modify it to incorporate b and complete the table below.

NB: for this exercise modify the macro `GetPosterior.C` or use the macro given below in the same way.

`GetPosteriorWithBackground.C`$(s, b, N) = \alpha(s, N)$

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0	4.74	0	
2	2.74	$4.75\pm^{1.55}_{1.75}$	
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0	4.74	0	4.74
2	2.74	$4.75\pm^{1.55}_{1.75}$	3.80
3	1.74	$6.29\pm^{2.86}_{3.30}$	3.60
5	-0.26	$9.15\pm^{2.69}_{2.86}$	3.45

$N_{obs} = 1$ Uncert's from 68% quantile.

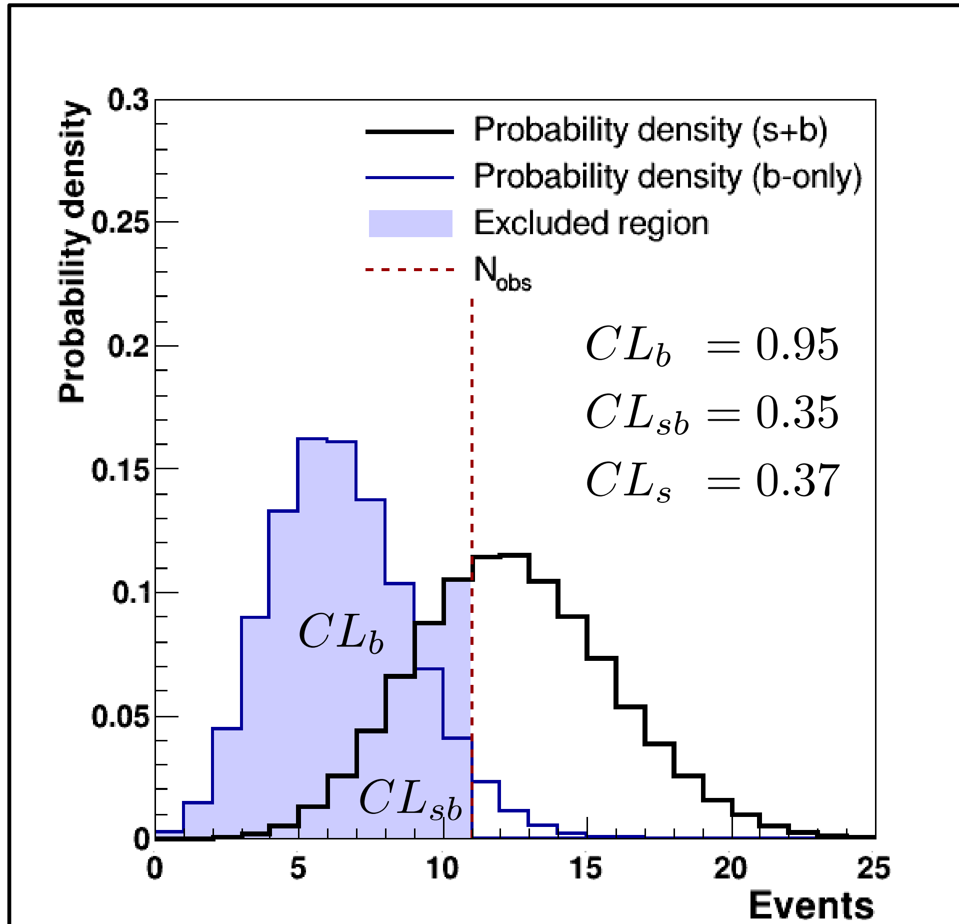
Modified Frequentist limit (CLs)

- Prevent exclusion beyond sensitivity of the experiment ("modified Frequentist limit").

$$CL_s = \frac{CL_{sb}}{CL_b} = \frac{\mathcal{P}(N \leq N_{obs})|_{\mu=s+b}}{\mathcal{P}(N \leq N_{obs})|_{\mu=b}}$$

- $CL_b \leq 1 \quad \Rightarrow C_{sb} \leq CL_s$, i.e. larger signal required to reach the same CL for exclusion.

- Zero signal never excluded.



Example: CLs value for $b = 6$, $s = 6$, $N_{obs} = 11$.

Exercise-4: Limits near a boundary

Assume you have an observation of 1 event, were you expect 0, 2, 3, 5 due to already known processes. You want to quote a 95% CL upper limit on the true value μ of the expected events for a Poisson distributed signal model.

a) Use the numerical integration for the Bayesian limit, modify it to incorporate b and complete the table below.

b) Calculate the limits using the modified Frequentist approach and CLs.

NB: for this exercise use the macro

`GetCLs.C`$(s, b, N) = \alpha(s, N)$

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2	2.74	$4.75 \pm^{1.55}_{1.75}$	3.80	
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Exercise-4: Limits near a boundary

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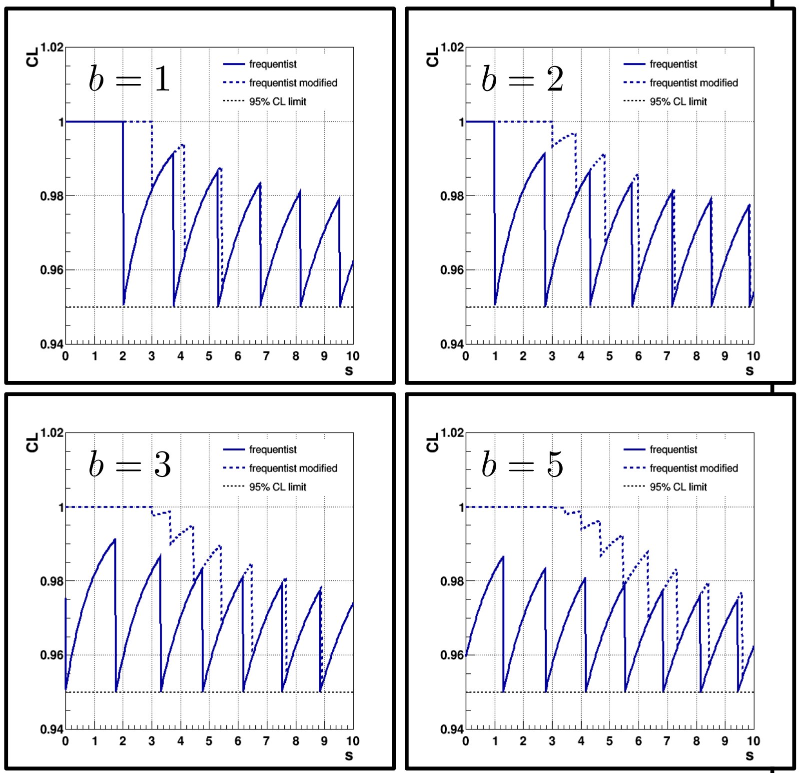
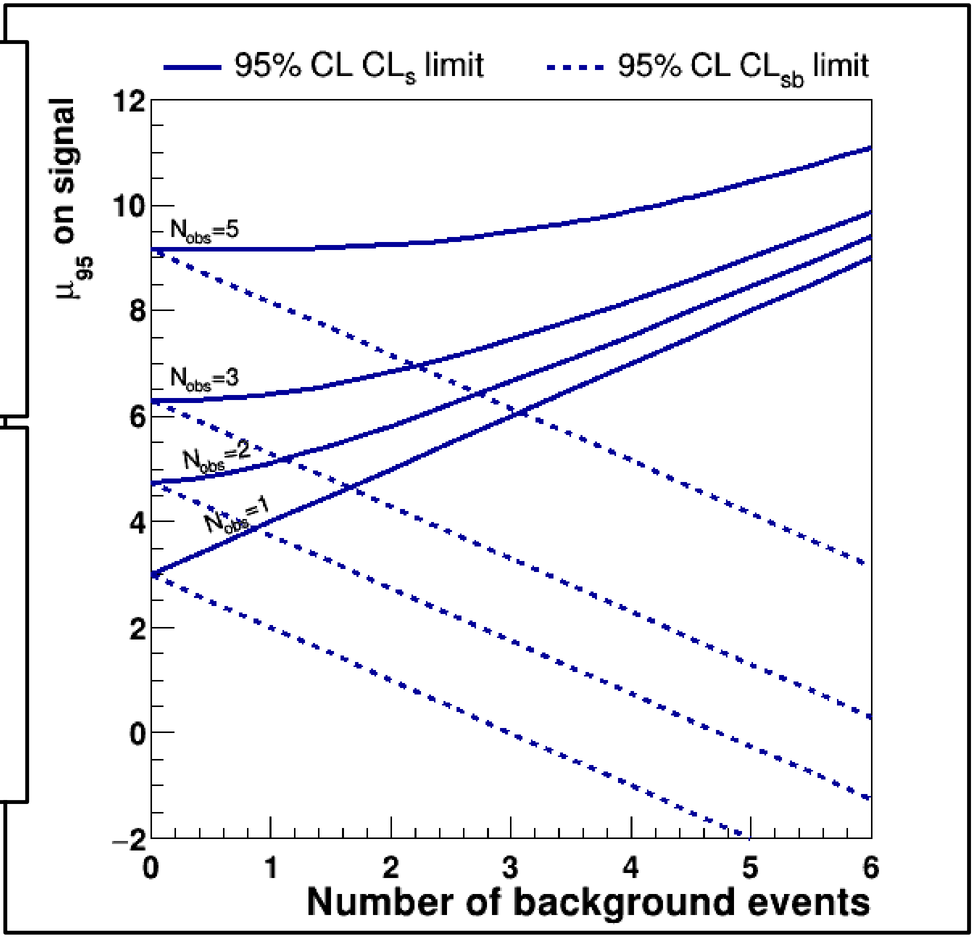
5	-0.26	$9.15\pm^{2.69}_{2.86}$	3.45	3.45

$N_{obs} = 1$ Uncert's from 68% quantile.

Coverage (CLs)

- CLs limit has always over coverage (→ more conservative than pure Frequentist approach).





Summary (lecture part-II)

- Limits for signal on top of a known background.
- Problems of Frequentist approach near physical boundaries.
- Differences between Frequentist and Bayesian limit setting.
- Modified Frequentist limit ($\rightarrow$ CLs).

Limits w/ systematic uncertainties

- Take previous example and extend model by two typical systematic uncertainties:
- Even simple experiments quickly turn into complex multi-parameter problems.

Uncertainty model:

$$\mathcal{L} = \mathcal{L}_{obs} \pm \Delta\mathcal{L}$$

$$b = b_{obs} \pm \Delta b$$

$\Delta\mathcal{L}, \Delta b$ modelled by (truncted) Gaussian's.

Signal model:

$$\mu = \mathcal{L}\,(s+b)$$

$\mathcal{L}$: integrated Luminosity

s : expected signal

b : expected background

Simple likelihood model:

$$\mathcal{P}_{s,\mathcal{L},b}(N_{obs}, \mathcal{L}_{obs}, b_{obs}) = \mathcal{P}_s(N_{obs}, \mathcal{L}_{obs}, b_{obs}) \times \mathcal{P}_{\mathcal{L}}(\mathcal{L}_{obs}, \Delta\mathcal{L}_{obs}) \times \mathcal{P}_b(b_{obs}, \Delta b_{obs})$$

$$\mathcal{P}_s(N_{obs}, \mathcal{L}_{obs}, b_{obs}) = \frac{(\mathcal{L}_{obs}\,(s+b_{obs}))^{N_{obs}}}{N_{obs}!} e^{-\mathcal{L}_{obs}(s+b_{obs})}$$ (counting experiment)

$$\mathcal{P}_{\mathcal{L}}(\mathcal{L}_{obs}, \Delta\mathcal{L}_{obs}) = \frac{1}{\sqrt{2\pi}\Delta\mathcal{L}_{obs}} e^{-\frac{(\mathcal{L}-\mathcal{L}_{obs})^2}{2\,\Delta\mathcal{L}_{ob}^2}}$$ (luminosity estimate)

$$\mathcal{P}_b(b_{obs}, \Delta b_{obs}) = \frac{1}{\sqrt{2\pi}\Delta b_{obs}}\ e^{-\frac{(b-b_{obs})^2}{2\,\Delta b_{ob}^2}}$$ (background estimate)

Limits w/ systematic uncertainties

- Take previous example and extend model by two typical systematic uncertainties:

- Even simple experiments quickly turn into complex multi-parameter problems.

- Here interpret as estimate of three observables $N_{obs}, \mathcal{L}_{obs}, b_{obs}$, based on likelihood function with three parameters (two nuisance parameters $\theta_{\mathcal{L}}, \theta_b$ and one POI μ_s).

- → 3d likelihood!

Bayesian:

Integrate over nuisance parameters and apply Bayesian limit procedure on POI.

Frequentist:

Neyman construction in 6d not feasible.

Integrate over nuisance parameters; apply Neyman construction on POI
(→ hybrid method).

Exercise-5: Limits w/ systematic uncertainties

Karlsruhe Institute of Technology

Assume you have an observation of 1 event, were you expect 0, 2, 3, 5 due to already known processes. You want to quote a 95% CL upper limit on the true value μ of the expected events for a Poisson distributed signal model.

Complete the table below for a limit with 10% uncertainty on the luminosity.

NB: for this exercise use the macro

$\texttt{GetCLsSys.C}(s, b, \Delta\mathcal{L}, N) = \alpha(s, N)$

b	$\mu_{95}^{freq} - b$	$\mu_{exp}^{freq}(s=0)$	$\mu_{95}^{bayes} - b$	$\mu_{95}^{CLs} - b$	$\mu_{95}^{CLs} - b(\Delta\mathcal{L})$
0	4.74	0	4.74	4.75	
2	2.74	$4.74\pm^{1.55}_{1.75}$	3.80	3.81	
3	1.74	$6.29\pm^{2.86}_{3.30}$	3.60	3.65	
5	-0.26	$9.15\pm^{2.69}_{2.86}$	3.45	3.45	

$N_{obs} = 1$ Uncert's from 68% quantile.

Exercise-5: Limits w/ systematic uncertainties

Karlsruhe Institute of Technology

Assume you have an observation of 1 event, were you expect 0, 2, 3, 5 due to already known processes. You want to quote a 95% CL upper limit on the true value μ of the expected events for a Poisson distributed signal model.

Complete the table below for a limit with 10% uncertainty on the luminosity.

NB: for this exercise use the macro

$\texttt{GetCLsSys.C}(s, b, \Delta\mathcal{L}, N) = \alpha(s, N)$

b	$\mu_{95}^{freq} - b$	$\mu_{exp}^{freq}(s=0)$	$\mu_{95}^{bayes} - b$	$\mu_{95}^{CLs} - b$	$\mu_{95}^{CLs} - b(\Delta\mathcal{L})$
0	4.74	0	4.74	4.75	4.84
2	2.74	$4.74\pm^{1.55}_{1.75}$	3.80	3.81	3.96
3	1.74	$6.29\pm^{2.86}_{3.30}$	3.60	3.65	3.84
5	-0.26	$9.15\pm^{2.69}_{2.86}$	3.45	3.45	3.62

$N_{obs} = 1$ Uncert's from 68% quantile.

Limits w/ multiple channels

- Take previous example (for simplicity again w/o uncert's) & extend to multiple channels, e.g. in form of a binned distribution:

Signal + known background (in 25 bins):

$$\mathcal{P}(k_i, \mu_i) = \frac{\mu_i^{k_i}}{k_i!} e^{-\mu_i}$$

$$\mathcal{L}(\{k_i\}, \mu, \{\theta_j\}) = \underbrace{\prod_i \mathcal{P}(k_i, \mu_i(\mu, \{\theta_j\}))}$$

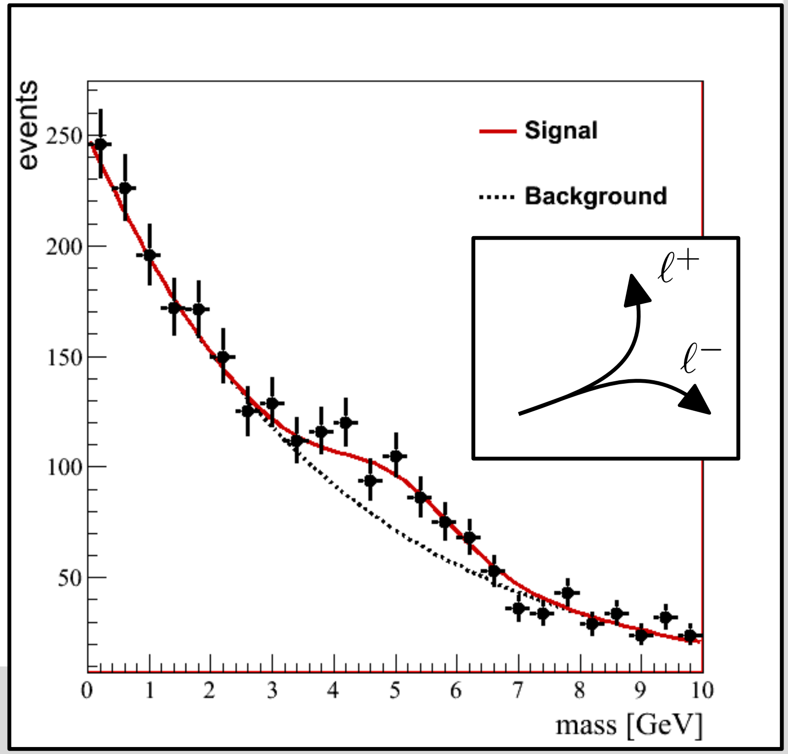
Product of individual probability densities for each bin.

$$\mu_i(\mu, \{\theta_j\}) = \underbrace{\theta_0 \cdot e^{-\theta_1 x_i}}_{\text{background}} + \underbrace{\mu \cdot e^{-(\theta_2 - x_i)^2}}_{\text{signal}}$$

- Neyman construction in (2·25)d not feasible.

- Use appropriate test statistic that maps 25d sample space to $\mathbb{R}$.

$$\Omega^n \rightarrow \mathbb{R}: \quad x \rightarrow f(x)$$



Proper choice of test statistic

- Formally base limit on hypothesis test:

$$H_1: \quad s+b \quad (\text{"signal+SM"})$$
$$H_0: \quad b\text{-only} \ (\text{"SM"})$$

- Best choice for hypothesis separation → likelihood ratio.
- For $q = -2\ln Q$ this ratio turns into a difference.
- Exact form of likelihood ratio used in HEP evolved over time.

Fundamental lemma of Neyman-Pearson:

when performing a test between H_1 and H_0 the *likelihood ratio test*, which rejects H_0 in favor of H_1 when

$$Q = \frac{\mathcal{L}_{H_1}(\{k_i\},\mu,\{\theta_j\})}{\mathcal{L}_{H_0}(\{k_i\},\mu,\{\theta_j\})} \leq \eta$$

$$\mathcal{P}(Q(\{k_i\},\mu,\{\theta_j\}) \leq \eta | H_i) = \alpha$$

is the most powerful test at significance level α for a threshold η.

Example: Higgs searches (LEP ~2000 – 2005)

- Test signal (H_1, for fixed mass, m, and fixed signal strength, μ) vs. background-only (H_0).

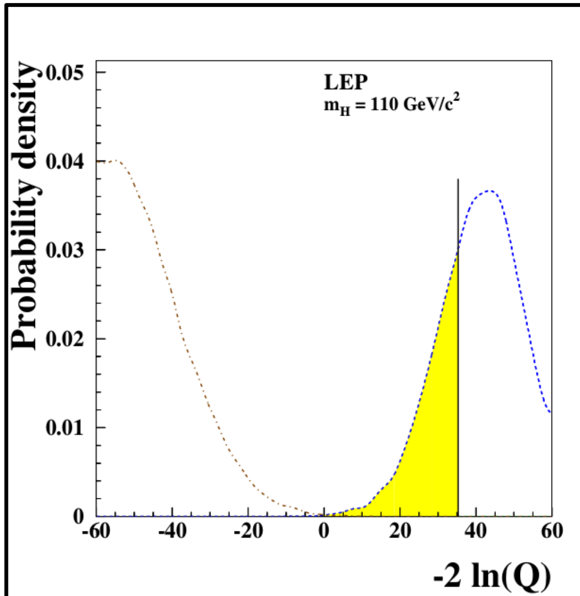
$$\mathcal{L}(\{k_i\}|\,\mu s(\theta_j)+b(\theta_j)) = \prod_i \mathcal{P}(k_i|\mu s_i(\theta_j)+b_i(\theta_j)) \times \prod_j \mathcal{C}(\theta_j|\theta_{j,obs})$$

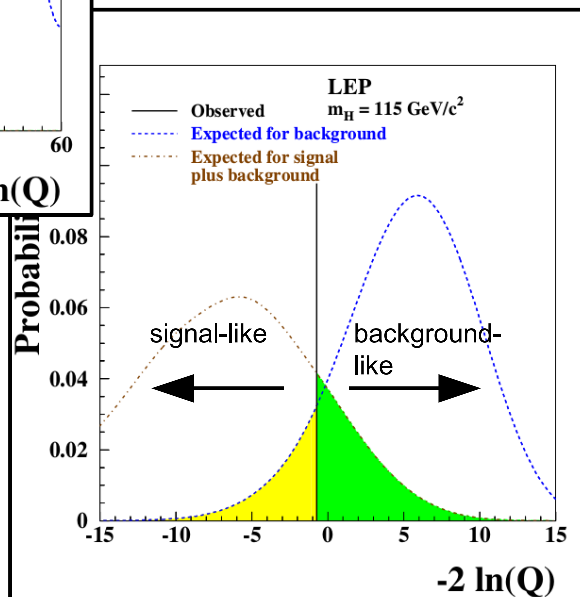
$$q_\mu = -2\ln\left(\frac{\mathcal{L}(n|\mu s+b)}{\mathcal{L}(n|b)}\right), \quad 0 \le \mu$$

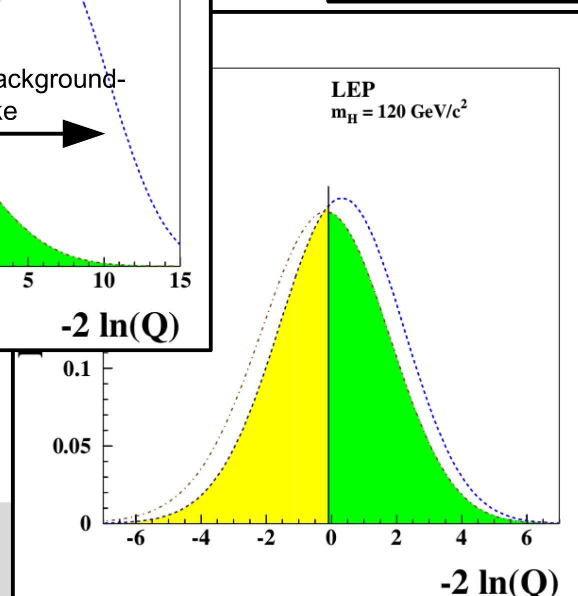
- Interpret $\mathcal{C}(\theta_j|\theta_{j,obs})$ as probability for θ_j given $\theta_{j,obs}$ (like in Bayesian statistics → hybrid method).
- Integrate over all θ_j (→ marginalization) and make Neyman construction.

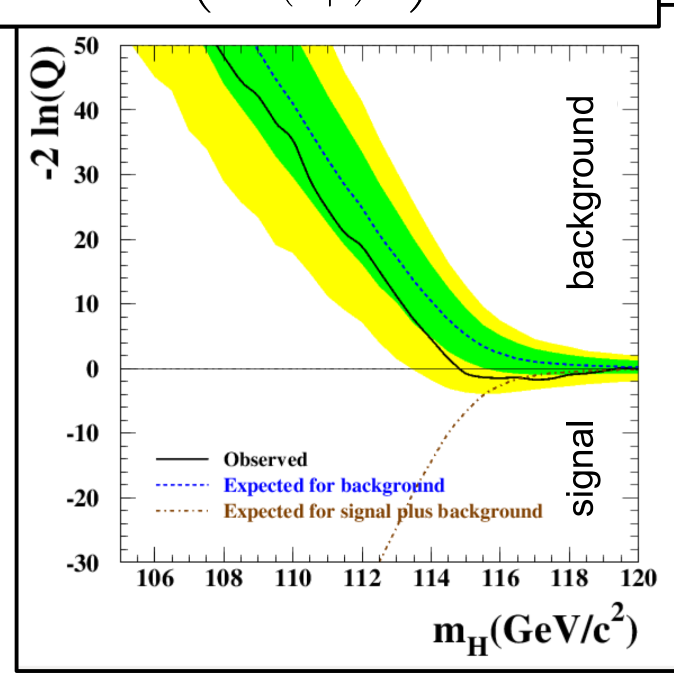
Higgs searches @ LEP

$$q_{\mu} = -2\ln\left(\frac{\mathcal{L}(n|\mu s+b)}{\mathcal{L}(n|b)}\right), \quad 0 \leq \mu$$









- Determine probability densities for $q_{\mu}|_{H_{0,1}}$ (for exp. limits) from toys.

Example: Higgs searches (Tevatron ~2005 – 2010)

- Test signal (H_1, for fixed mass, m, and fixed signal strength, μ) vs. background-only (H_0).

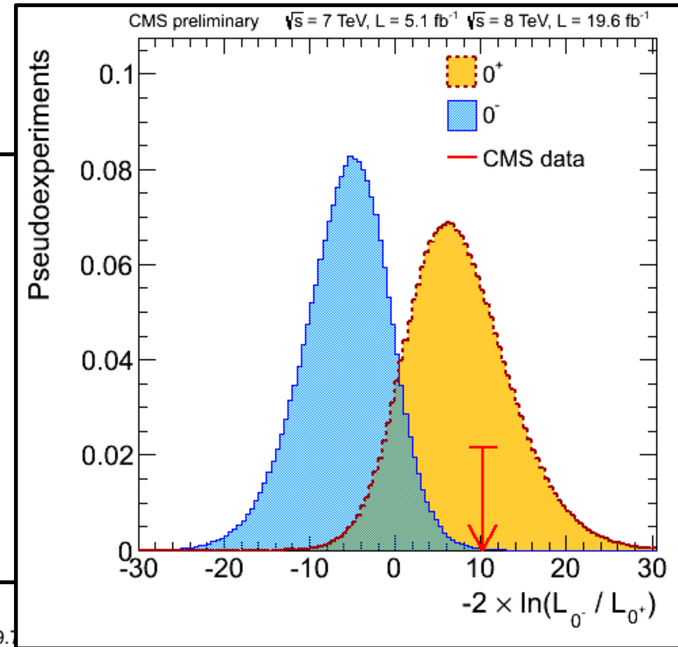
$$\mathcal{L}(\{k_i\}|\,\mu s(\theta_j)+b(\theta_j)) = \prod_i \mathcal{P}(k_i|\mu s_i(\theta_j)+b_i(\theta_j)) \times \prod_j \mathcal{C}(\theta_j|\theta_{j,obs})$$

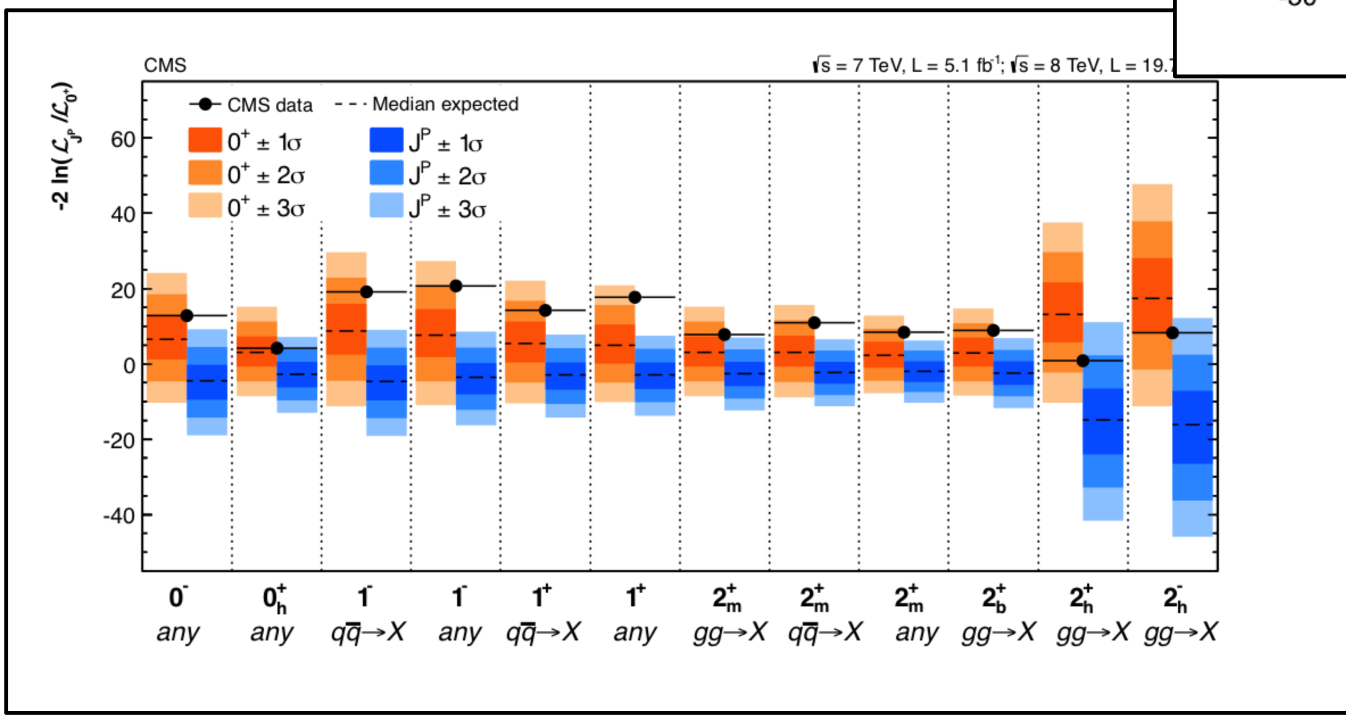
$$q_\mu = -2\ln\left(\frac{\mathcal{L}(\,n|\mu s(\hat{\theta}_\mu)+b(\hat{\theta}_\mu))}{\mathcal{L}(\,n|b(\hat{\theta}_0))}\right), \quad 0 \leq \mu$$

- Interpret $\mathcal{C}(\theta_j|\theta_{j,obs})$ as probability for θ_j given $\theta_{j,obs}$ (like in Bayesian statistics → hybrid method).
- Determine best fit values $\hat{\theta}_j \pm \Delta\hat{\theta}_j$ for all θ_j from initial fit under both hypotheses before marginalization (→ profiling).

J^P hypothesis tests @ LHC

- Test statistic: $q = -2\ln\left(\frac{\mathcal{L}(0^+ + BG)}{\mathcal{L}(J^P + BG)}\right)$.
- Determine probability densities for $q_\mu|_{H_{0,1}}$ (for expected limits) from toys.





Example: Higgs searches (LHC ~2010 – now)

- Test signal (H_1, for fixed mass, m, and fixed signal strength, μ) vs. background-only (H_0).

$$\mathcal{L}(\{k_i\}|\,\mu s(\theta_j)+b(\theta_j)) = \prod_i \mathcal{P}(k_i|\mu s_i(\theta_j)+b_i(\theta_j)) \times \prod_j \mathcal{C}(\theta_j|\theta_{j,obs})$$

$$q_\mu = -2\ln\left(\frac{\mathcal{L}(\,n|\mu s(\hat{\theta}_\mu)+b(\hat{\theta}_\mu))}{\mathcal{L}(\,n|\hat{\mu}s(\hat{\theta}_{\hat{\mu}})+b(\hat{\theta}_{\hat{\mu}}))}\right), \quad 0 \leq \hat{\mu} \leq \mu$$

- Interpret $\mathcal{C}(\theta_j|\theta_{j,obs})$ as probability for θ_j given $\theta_{j,obs}$ (like in Bayesian statistics → hybrid method).
- Profile numerator for fixed μ and denominator for $0 \leq \hat{\mu} \leq \mu$ (→ profile likelihood ratio).

Profile likelihood ratio (→ asymptotic limit)

- Since numerator always smaller than denominator $q_\mu \geq 0$.
- In the large number limit probability density $f(q_\mu|\mu')$ can be approximated by analytical function (→ see arXiv:1007.1727):

$$f(q_\mu|\mu') = \Phi\left(\frac{\mu'-\mu}{\sigma}\right)\delta(q_\mu) + \begin{cases} \frac{1}{2\sqrt{2\pi}\sqrt{q_\mu}}\exp\left(-\frac{1}{2}\left(\sqrt{q_\mu}-\frac{\mu-\mu'}{\sigma}\right)^2\right) & 0 < q \leq \mu^2/\sigma^2 \\ \frac{1}{2\sqrt{2\pi}\sqrt{\mu/\sigma}}\exp\left(-\frac{1}{2}\left(\frac{q_\mu-\left(\mu^2-2\mu\mu'\right)/\sigma^2)^2}{4(\mu/\sigma)^2}\right)\right) & q > \mu^2/\sigma^2 \end{cases}$$

μ : μ value for model in question

μ' : True value of POI that leads to global likelihood maximum in denominator

σ : Uncertainty on μ'

- σ can be estimated from Asimov dataset of b-only hypothesis to be $\sigma^2 = \mu^2/q_A$.

Asimov dataset

- Defined such that when one uses it to evaluate the estimators for all parameters $\{\hat{\theta}_j\}, \hat{\mu}$ one obtains the true parameter values.

- In practice obtain Asimov dataset by adding all MC templates with nuisance parameters at expected values to obtain exact expectation (→ assume no biases).

$$f(q_\mu|\mu') = \Phi\left(\left(\frac{\mu'}{\mu} - 1\right) q_A\right) \delta(q_\mu) + \begin{cases} \frac{1}{2\sqrt{2\pi}\sqrt{q_\mu}} \exp\left(-\frac{1}{2}\left(\sqrt{q_\mu} - \sqrt{q_A}\frac{\mu-\mu'}{\mu}\right)^2\right) & 0 < q \leq q_A \\ \frac{1}{2\sqrt{2\pi}\sqrt{q_A}} \exp\left(-\frac{1}{2}\left(\frac{\left(q_\mu - q_A\left(\mu^2 - 2\mu\mu'\right)/\mu^2\right)^2}{4q_A}\right)\right) & q > q_A \end{cases}$$

$$f(q_\mu|\mu' = \mu) = \frac{1}{2} q_A \quad \delta(q_\mu) + \begin{cases} \frac{1}{2\sqrt{2\pi}\sqrt{q_\mu}} \exp\left(-\frac{1}{2} q_\mu\right) = \frac{1}{2}\chi^2(q_\mu, 1) & 0 < q \leq q_A \\ \frac{1}{2\sqrt{2\pi}\sqrt{q_A}} \exp\left(-\frac{1}{2}\frac{(q_\mu + q_A)^2}{4q_A}\right) \approx \frac{1}{2}\chi^2(q_A, 1) & q > q_A \end{cases}$$

$$f(q_\mu|\mu' = 0) = \Phi(-\sqrt{q_A}) \quad \delta(q_\mu) + \begin{cases} \frac{1}{2\sqrt{2\pi}\sqrt{q_\mu}} \exp\left(-\frac{1}{2}\left(\sqrt{q_\mu} - \sqrt{q_A}\right)^2\right) & 0 < q \leq q_A \\ \frac{1}{2\sqrt{2\pi}\sqrt{q_A}} \exp\left(-\frac{1}{2}\frac{(q_\mu - q_A)^2}{4q_A}\right) & q > q_A \end{cases}$$

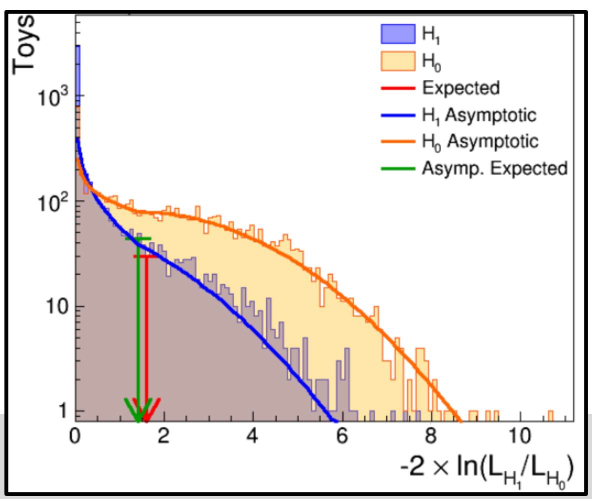
Confidence intervals

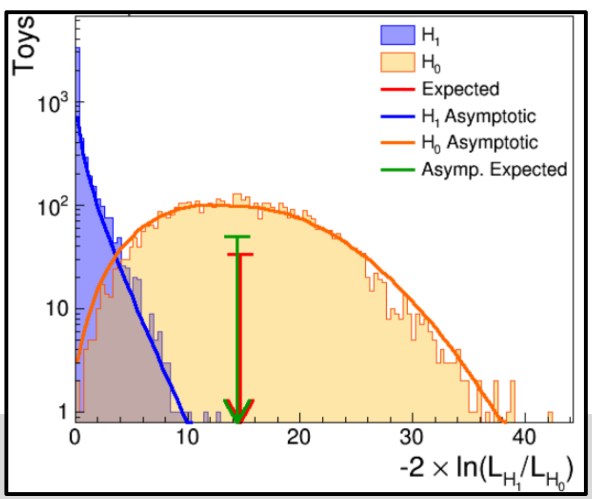
- Confidence intervals obtained from cumulative distribution functions of $f(q_\mu|\mu')$.

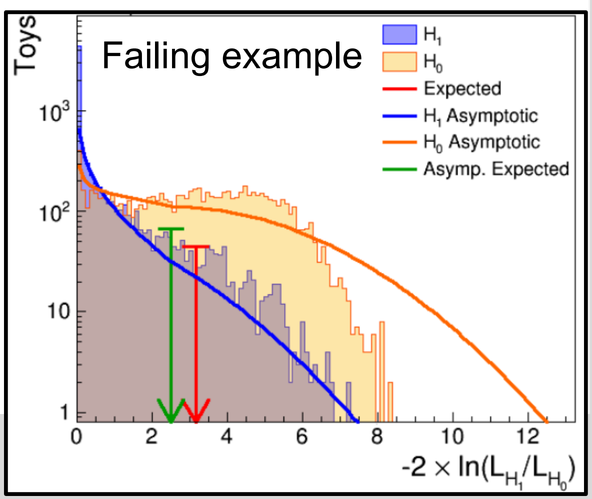
$$CL_{sb} = \begin{cases} 1 - \Phi\left(\sqrt{q_{obs}}\right) & 0 < q \leq q_A \\ 1 - \Phi\left(\frac{q_{obs}+q_A}{2\sqrt{q_A}}\right) & q > q_A \end{cases}$$

$$CL_b = \begin{cases} \Phi\left(\sqrt{q_A} - \sqrt{q_{obs}}\right) & 0 < q \leq q_A \\ 1 - \Phi\left(\frac{q_{obs}-q_A}{2\sqrt{q_A}}\right) & q > q_A \end{cases}$$

- Limit can be obtained from knowledge of q_{obs} and q_A only → no need for toys! Expected limit (for $s = 0$) obtained from quantiles of CLs from q_A .

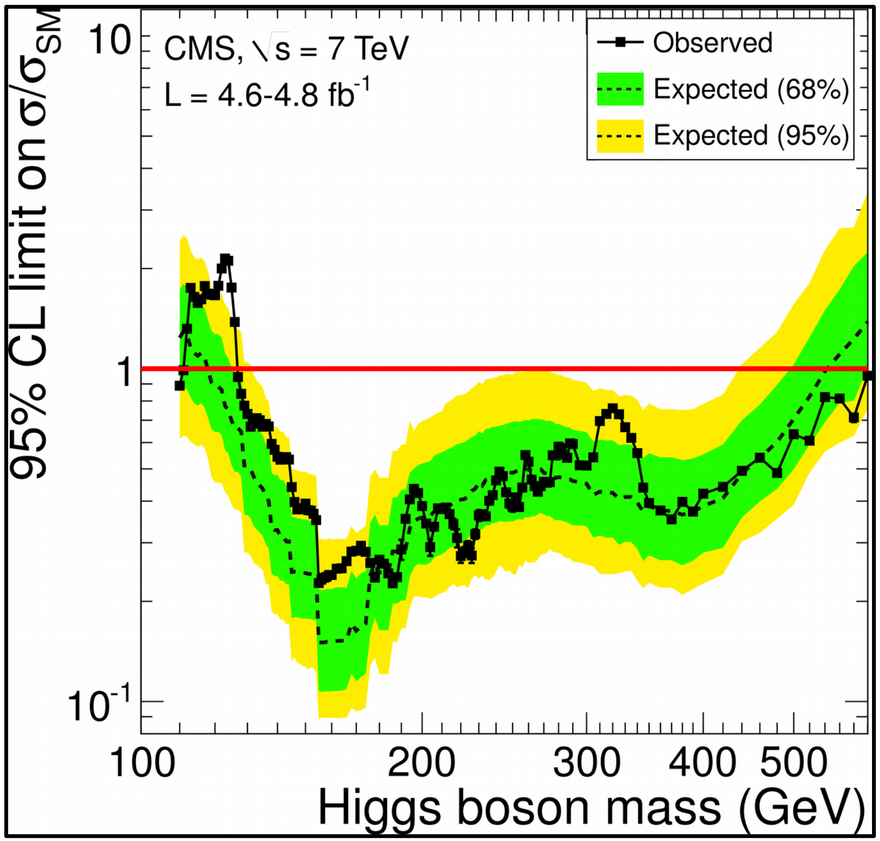






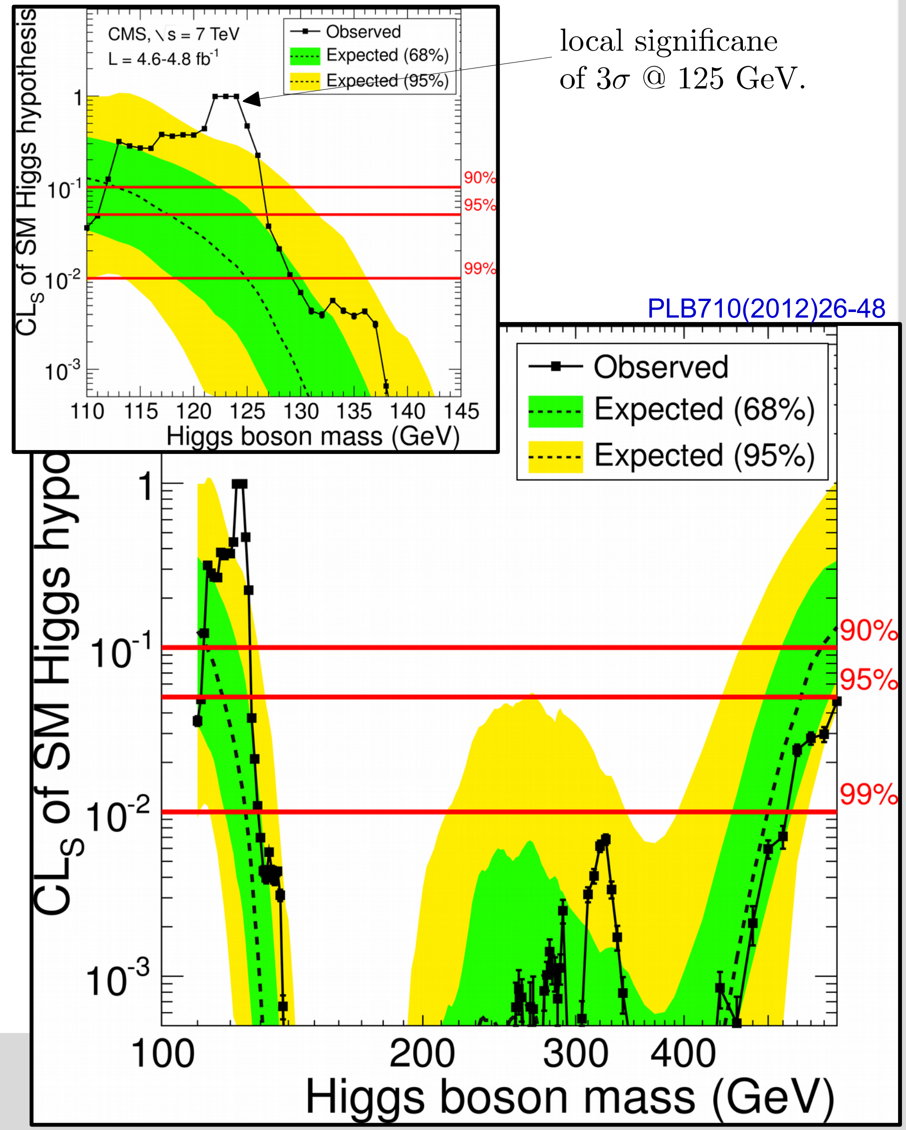
Limits @ the LHC

- Last published limit before Higgs boson discovery (example from CMS):



local significane of 3σ @ 125 GeV.

PLB710(2012)26-48



- Five different final states, O(2500) nuisance parameters.

Summary (lecture part-III)

- Limits for multichannel measurements (e.g. binned distributions).
- Likelihood ratio test.
- Asymptotic approximation.

Backup

Relation between Poisson & χ^2 distribution

- Relation between sum over Poisson terms and χ^2 distribution:

$$\chi^2\left(2\mu, 2(N+1)\right) = \frac{(2\mu)^N e^{-2\mu/2}}{2^{N+1}\Gamma(N+1)} = \frac{1}{2}\frac{\mu^N}{N!}e^{-\mu} = \frac{1}{2}\mathcal{P}(N,\mu)$$

$$\alpha(\mu, N) = \sum_{i=0}^{N} \mathcal{P}(k,\mu) = \int_{2\mu}^{\infty} \chi^2\left(x, 2(N+1)\right) \mathrm{d}x = 2\int_{\mu}^{\infty} \chi^2\left(2\mu', 2(N+1)\right) \mathrm{d}\mu'$$

- Standard root functions for the evaluation of χ^2:

$$\texttt{TMath::Prob}(2\,\mu, 2(N+1)) = \int_{2\mu}^{\infty} \chi^2(x, 2(N+1))\mathrm{d}x = \sum_{i \leq N} \frac{\mu^N}{N!} e^{-\mu} = \alpha(\mu, N)$$

$$\mu_{1-\alpha} = \texttt{TMath::ChisquareQuantile}(1-\alpha, 2\,(N+1))/2.$$

Returns the upper boundary of the integral $\int_0^{2\mu} \chi^2(x, 2(N+1))\mathrm{d}x$ for which the integral has the value $1-\alpha$ (→ quantile to value $1-\alpha$).