

upper limit,exclusion&discovery

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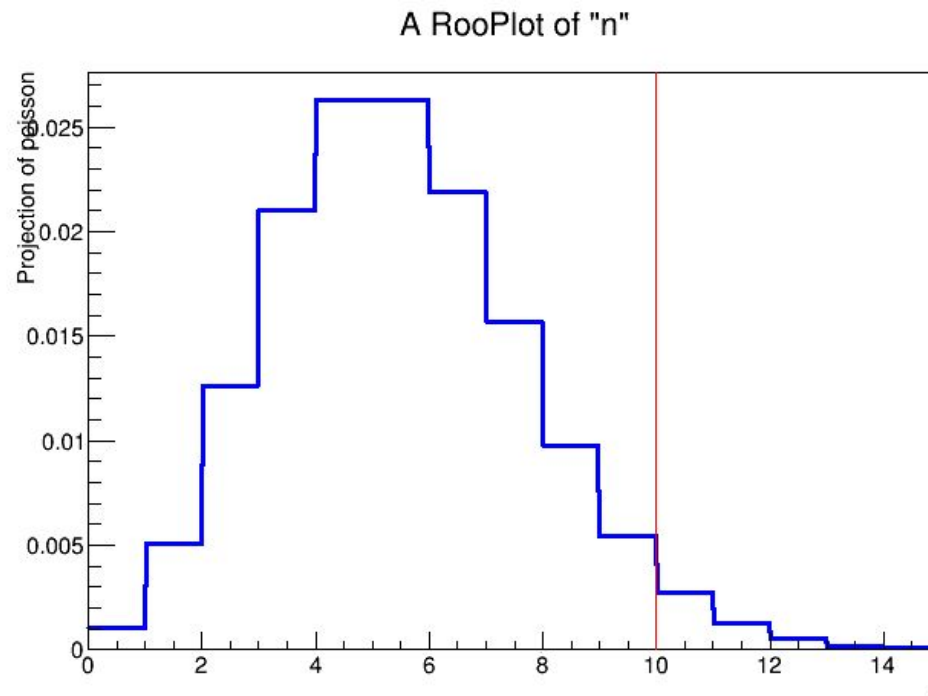
9.3

abstract

- upper limit and exclusion
(what I understand before)
- discovery and their significance
(what we talked about last week ,a little confused)
- I won't talk about any RooStat code here
- we can skip some basic knowledge about probability and hypothesis test here

upper limit

- upper limit means $p(\mu < \mu_{\text{up}}) = 0.95$
- consider a poisson distribution: $b = 4.5, n_{\text{obs}} = 10$, what is the upper limit of s ?
- we scan the value of μ and when the area on the right of the red line is 0.05, we can get the upper limit.



a simple method-PLR fit

Expand $\ln L(\theta)$ about its maximum:

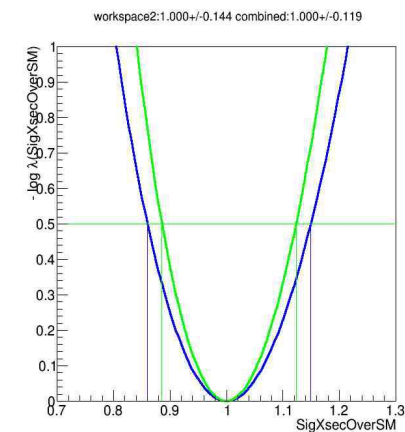
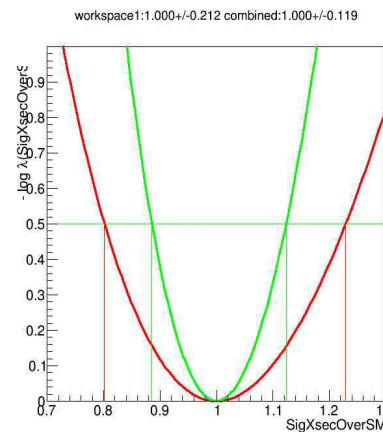
$$\ln L(\theta) = \ln L(\hat{\theta}) + \left[\frac{\partial \ln L}{\partial \theta} \right]_{\theta=\hat{\theta}} (\theta - \hat{\theta}) + \frac{1}{2!} \left[\frac{\partial^2 \ln L}{\partial \theta^2} \right]_{\theta=\hat{\theta}} (\theta - \hat{\theta})^2 +$$

$$\ln L(\theta) \approx \ln L_{\max} - \frac{(\theta - \hat{\theta})^2}{2\hat{\sigma}_{\hat{\theta}}^2}$$

$$\ln L(\hat{\theta} \pm \hat{\sigma}_{\hat{\theta}}) \approx \ln L_{\max} - \frac{1}{2}$$

$$\ln L(\hat{\theta} \pm 2\hat{\sigma}_{\hat{\theta}}) \approx \ln L_{\max} - 2$$

$$- \ln \frac{L(\hat{\theta} \pm 2\hat{\sigma}_{\hat{\theta}})}{L_{\max}} \approx 2$$



- so when $-\ln \lambda(\mu)=2$, upper limit can be obtained

general method

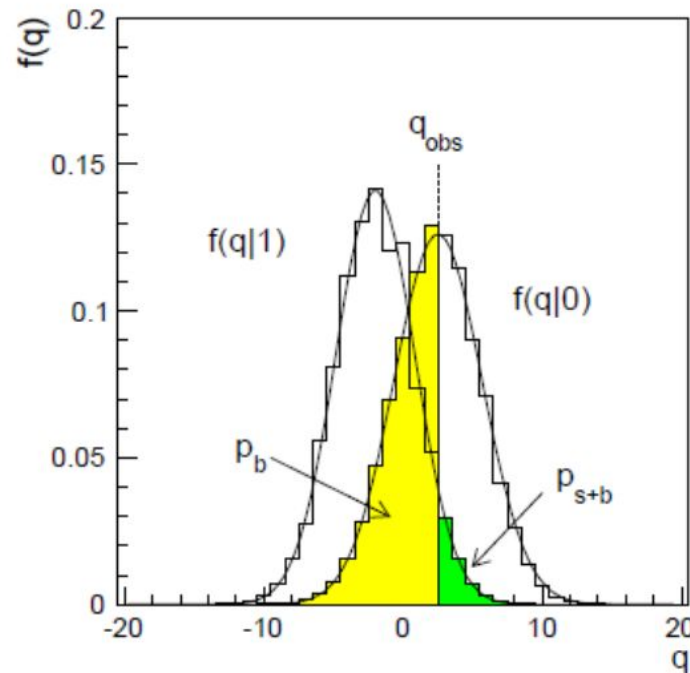
- Null hypo: $\mu=0$, alternate hypo: $\mu=1$
- probability of x given θ : $f(x|\theta)$
- test statistic: $q_\mu = -2Ln \frac{L(\mu, \hat{\theta})}{L(\hat{\mu}, \hat{\theta})}$ if $\mu^{\text{hat}} > 0$
- parameters with one hat mean the best fit,
- μ is a variable and parameters with two hat is the best fit for a certain given μ

upper limit

- q_{obs} is calculated from data, q_{expect} is the median of background-only hypothesis
- I put Xiaohu's slides here.....

Test statistic $\rightarrow$ exclusion or upper limit

- Calculate the test statistic of S+B hypo based on its p-value
- The signal model is regarded as excluded at a confidence level of $1 - \alpha = 95\%$ if one finds



$$p_{s+b} < \alpha$$

$$1 - \alpha = 95\%$$

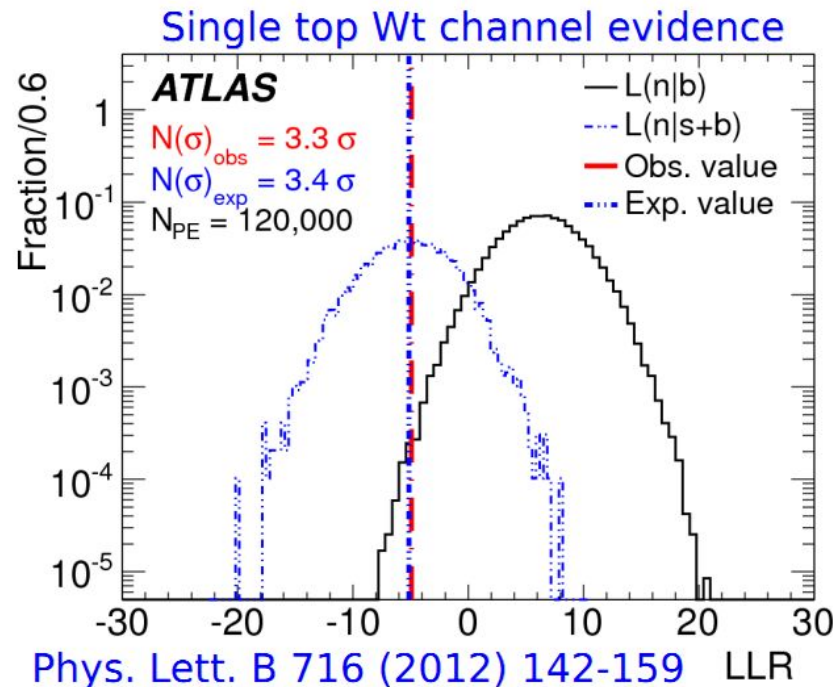
$$\text{confidence level CL} = 1 - \alpha$$

NOTE: in another word, the signal rate s under which the 5% p_{s+b} reaches, can be regarded as a upper limit s_{up} , for which signal is not excluded.

So the interval $[0, s_{up}]$ covers s with a probability of at least 95%

Test statistic $\rightarrow$ discovery

- Calculate the test statistic of B hypo based on its p-value: p_b
- Convert p-value into standard deviation (XX sigma)
- 3 sigma $\rightarrow$ evidence; 5 sigma $\rightarrow$ discovery
- The background-only model is regarded as rejected if 5 sigma



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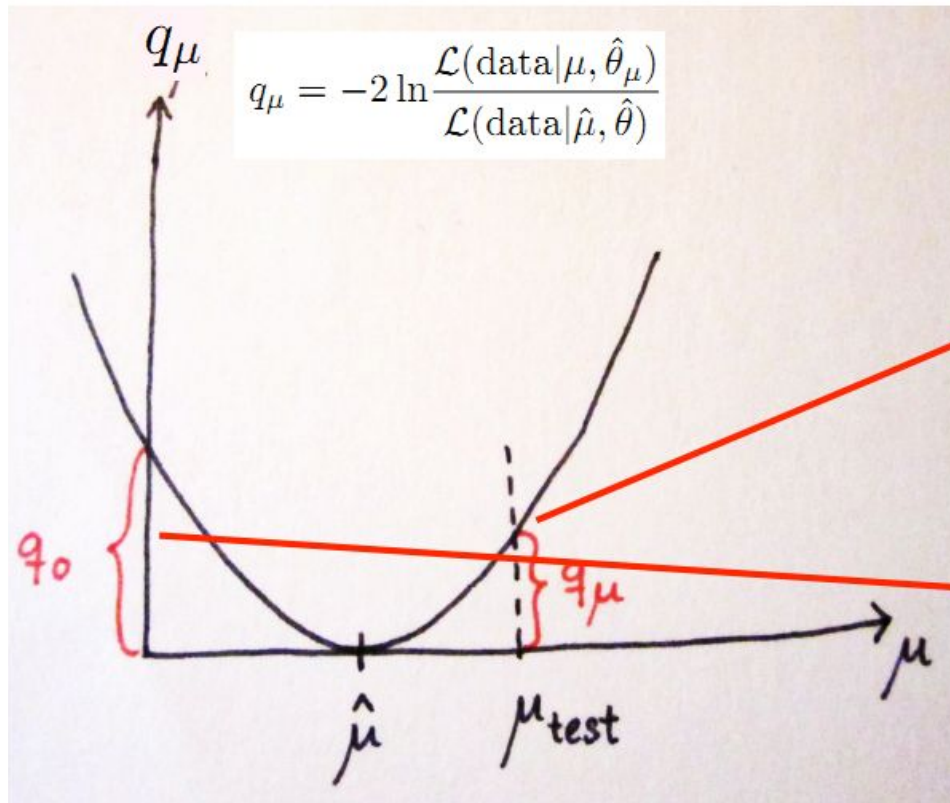
discovery

- if significance is 5 sigma or p-value $< 2.9e-7$, a new particle is discovered---it is to say we have probability of $1-p$ to reject null hypo.

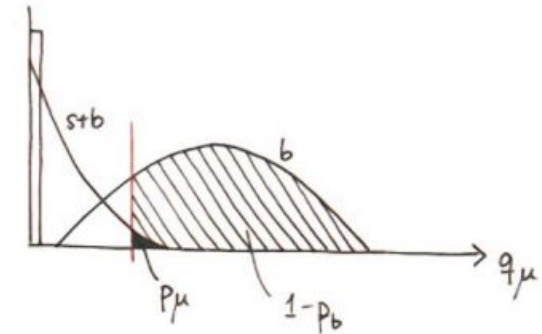
- test statistic: $q_0 = -2Ln \frac{L(0, \hat{\theta})}{L(\hat{\mu}, \hat{\theta})}$ if $\mu^{\text{hat}} > 0$

- also parameters with one hat are the best fit and parameters with two hat is the best fit with $\mu=0$
- so q_0 is only decided by dataset x and $f(x|\mu, \theta)$

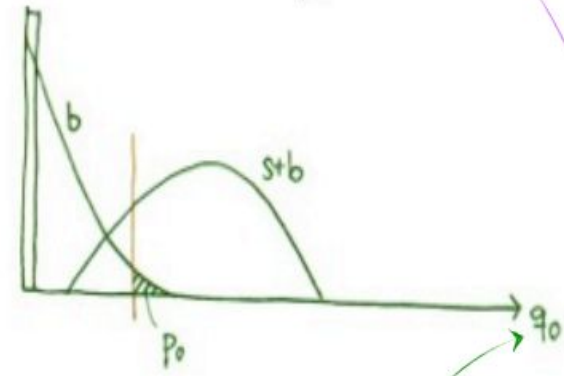
if I am right...



exclusion
test "s+b"



discovery
test "b-only"



- where is the line s+b in lower right plot from?

- anyway, we can calculate p-value as usual

$$p_{obs} = \int_{q_{obs}}^{\infty} f(q_0 | 0) dq_0$$

$$p_{expect} = \int_{q_{expect}}^{\infty} f(q_0 | 0) dq_0$$

significance

$$Z = \Phi^{-1}(1 - p), \Phi(x) = \int_{-\infty}^x \text{Gaussian}(y, 0, 1) dy$$

In large sample limit, $q_0 \sim$ "half chi-2 distribution" (from Cowan's lecture)

$$f(q_0|0) = \frac{1}{2} \delta(q_0) + \frac{1}{2} \frac{1}{\sqrt{2\pi}} \frac{1}{\sqrt{q_0}} e^{-q_0/2}$$

CDF of q_0 $F(q_0|0) = \Phi(\sqrt{q_0})$ p-value $p_0 = 1 - F(q_0|0)$

So Z can be calculate $Z = \Phi^{-1}(1 - p_0) = \sqrt{q_0}$

the following three pages are copied from Cowan's lecture.

$s/\sqrt{b}$ for expected discovery significance

For large $s + b$, $n \rightarrow x \sim \text{Gaussian}(\mu, \sigma)$, $\mu = s + b$, $\sigma = \sqrt{s + b}$.

For observed value x_{obs} , p -value of $s = 0$ is $\text{Prob}(x > x_{\text{obs}} | s = 0)$,:

$$p_0 = 1 - \Phi\left(\frac{x_{\text{obs}} - b}{\sqrt{b}}\right)$$

Significance for rejecting $s = 0$ is therefore

$$Z_0 = \Phi^{-1}(1 - p_0) = \frac{x_{\text{obs}} - b}{\sqrt{b}}$$

Expected (median) significance assuming signal rate s is

$$\text{median}[Z_0 | s + b] = \frac{s}{\sqrt{b}}$$

Better approximation for significance

Poisson likelihood for parameter s is

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

For now
no nuisance
params.

To test for discovery use profile likelihood ratio:

$$q_0 = \begin{cases} -2 \ln \lambda(0) & \hat{s} \geq 0, \\ 0 & \hat{s} < 0. \end{cases} \quad \lambda(s) = \frac{L(s, \hat{\hat{\theta}}(s))}{L(\hat{s}, \hat{\theta})}$$

So the likelihood ratio statistic for testing $s = 0$ is

$$q_0 = -2 \ln \frac{L(0)}{L(\hat{s})} = 2 \left(n \ln \frac{n}{b} + b - n \right) \quad \text{for } n > b, \quad 0 \text{ otherwise}$$

Approximate Poisson significance (continued)

For sufficiently large $s + b$, (use Wilks' theorem),

$$Z = \sqrt{2 \left(n \ln \frac{n}{b} + b - n \right)} \quad \text{for } n > b \text{ and } Z = 0 \text{ otherwise.}$$

To find $\text{median}[Z|s]$, let $n \rightarrow s + b$ (i.e., the Asimov data set):

$$Z_A = \sqrt{2 \left((s + b) \ln \left(1 + \frac{s}{b} \right) - s \right)}$$

This reduces to $s/\sqrt{b}$ for $s \ll b$.

$$Z_A = \sqrt{2 \left((s+b) \ln \left(1 + \frac{s}{b} \right) - s \right)}$$

- if $s \ll b, \ln(1 + \frac{s}{b}) \sim \frac{s}{b} - \frac{s^2}{2b^2}$

$$\begin{aligned} (s+b) \left(\frac{s}{b} - \frac{s^2}{2b^2} \right) - s &= \frac{s^2}{b} - \frac{s^3}{2b^2} + s - \frac{s^2}{2b} - s \\ &= \frac{s^2}{2b} - \frac{s^3}{2b^2} \sim \frac{s^2}{2b} \end{aligned}$$

- $Z \sim \frac{s}{\sqrt{b}}$

back up

Test statistic for discovery

Try to reject background-only ($\mu = 0$) hypothesis using

$$q_0 = \begin{cases} -2 \ln \lambda(0) & \hat{\mu} \geq 0 \\ 0 & \hat{\mu} < 0 \end{cases}$$

Here data in critical region (high q_0) only when estimated signal strength $\hat{\mu}$ is positive.

Could also want two-sided critical region, e.g., if presence of signal process could lead to suppression (and/or enhancement) in number of events.

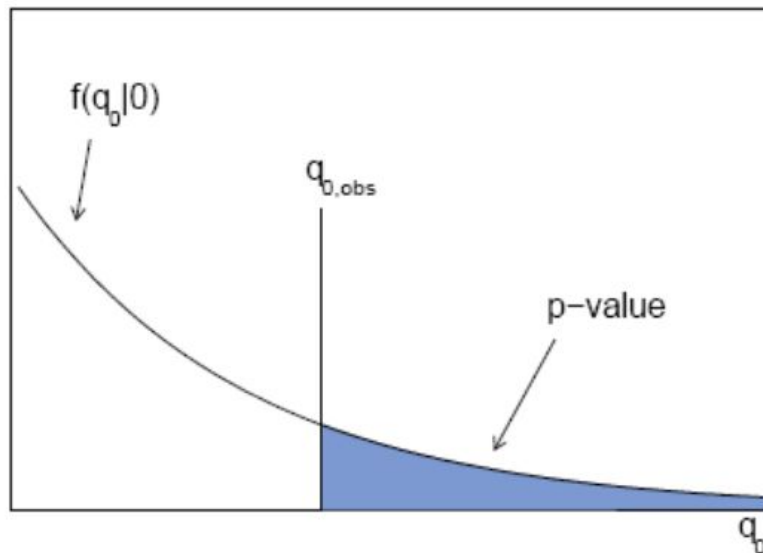
Note that even if physical models have $\mu \geq 0$, we allow $\hat{\mu}$ to be negative. In large sample limit its distribution becomes Gaussian, and this will allow us to write down simple expressions for distributions of our test statistics.

p-value for discovery

Large q_0 means increasing incompatibility between the data and hypothesis, therefore *p*-value for an observed $q_{0,\text{obs}}$ is

$$p_0 = \int_{q_{0,\text{obs}}}^{\infty} f(q_0|0) dq_0$$

will get formula for this later

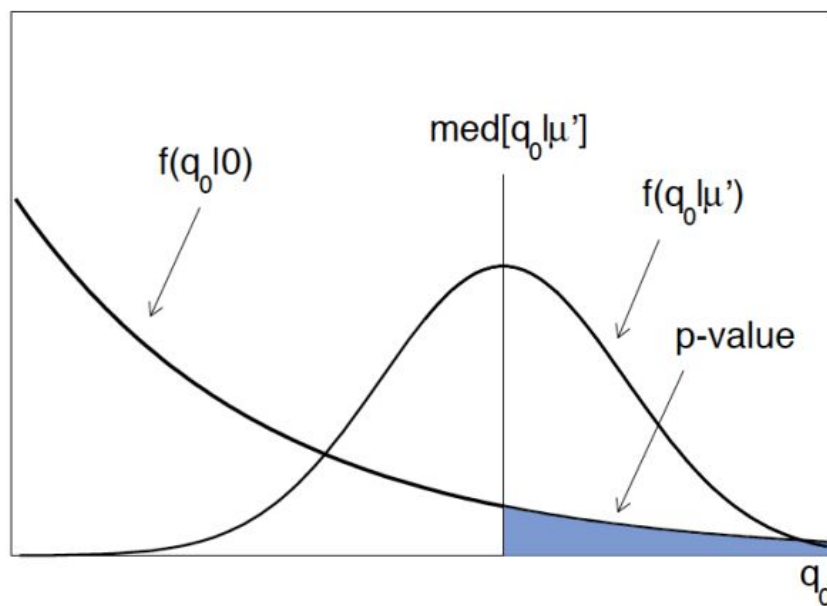


From *p*-value get equivalent significance,

$$Z = \Phi^{-1}(1 - p)$$

Expected (or median) significance / sensitivity

When planning the experiment, we want to quantify how sensitive we are to a potential discovery, e.g., by given median significance assuming some nonzero strength parameter μ' .



So for p -value, need $f(q_0|0)$, for sensitivity, will need $f(q_0|\mu')$,