Using the Profile Likelihood in Searches for New Physics

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Outline

Prototype search analysis for LHC

Test statistics based on profile likelihood ratio

Systematics covered via nuisance parameters

Sampling distributions to get significance/sensitivity

Asymptotic formulae from Wilks/Wald

Examples:

$n \sim$ Poisson $(\mu s + b)$, $m \sim$ Poisson(τb)

Shape analysis

Conclusions

Prototype search analysis

Search for signal in a region of phase space; result is histogram of some variable x giving numbers:

$$\mathbf{n} = (n_1, \ldots, n_N)$$

Assume the n_i are Poisson distributed with expectation values

$$E[n_i] = \mu s_i + b_i$$

strength parameter

where

$$s_i = s_{\rm tot} \int_{\text{bin } i} f_s(x; \boldsymbol{\theta}_s)\, dx \,, \qquad b_i = b_{\rm tot} \int_{\text{bin } i} f_b(x; \boldsymbol{\theta}_b)\, dx \,.$$

signal

background

Prototype analysis (II)

Often also have a subsidiary measurement that constrains some of the background and/or shape parameters:

$$\mathbf{m} = (m_1, \ldots, m_M)$$

Assume the m_i are Poisson distributed with expectation values

$$E[m_i] = u_i(\boldsymbol{\theta})$$

nuisance parameters ($\boldsymbol{\theta}_s$, $\boldsymbol{\theta}_b$,b_{tot})

Likelihood function is

$$L(\mu, \boldsymbol{\theta}) = \prod_{j=1}^{N} \frac{(\mu s_j + b_j)^{n_j}}{n_j!} e^{-(\mu s_j + b_j)} \prod_{k=1}^{M} \frac{u_k^{m_k}}{m_k!} e^{-u_k}$$

The profile likelihood ratio

Base significance test on the profile likelihood ratio:

maximizes L for specified μ

$$\lambda(\mu) = \frac{L(\mu, \hat{\hat{\boldsymbol{\theta}}})}{L(\hat{\mu}, \hat{\boldsymbol{\theta}})}$$

maximize L

The likelihood ratio of point hypotheses gives optimum test (Neyman-Pearson lemma).

The profile LR hould be near-optimal in present analysis with variable μ and nuisance parameters $\boldsymbol{\theta}$.

Test statistic for discovery

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

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

i.e. here only regard upward fluctuation of data as evidence against the background-only hypothesis.

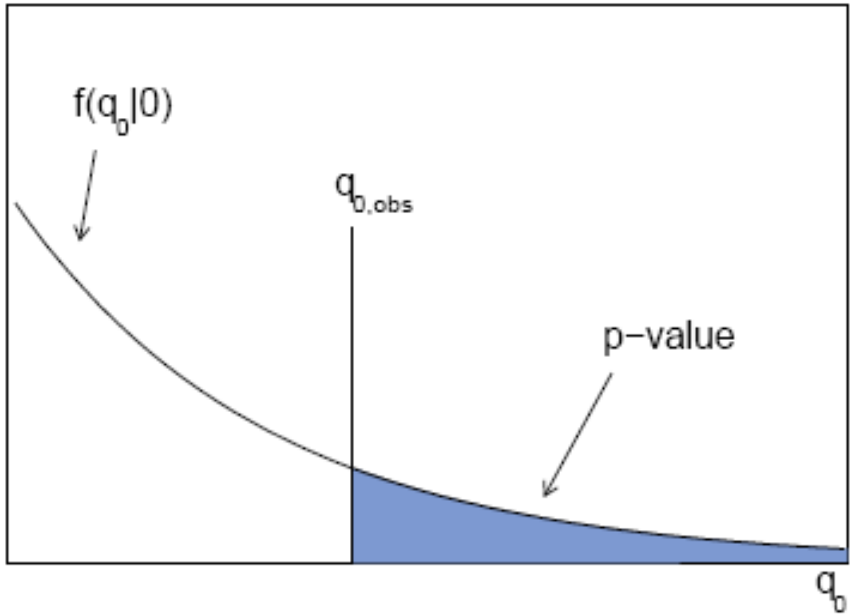
Note that even though here physically $\mu \geq 0$, we allow $\hat{\mu}$ to be negative. In large sample limit its distribution becomes Gaussian, and this will allow us to write down simple expressions for distributions of our test statistics.

p-value for discovery

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

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

will get formula for this later

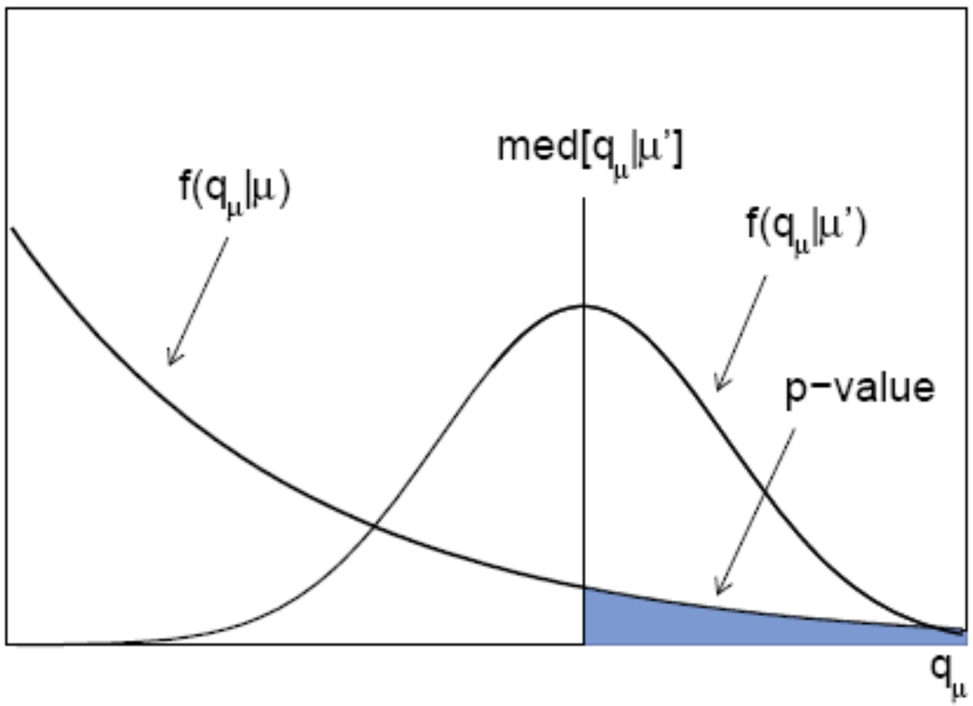


From p-value get equivalent significance,

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

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 $f(q_0|\mu')$,

Wald approximation for profile likelihood ratio

To find *p*-values, we need: $f(q_0|0), \quad f(q_\mu|\mu)$

For median significance under alternative, need: $f(q_\mu|\mu')$

Use approximation due to Wald (1943)

$$-2\ln\lambda(\mu) = \frac{(\mu - \hat{\mu})^2}{\sigma^2} + \mathcal{O}(1/\sqrt{N})$$

sample size

$$\hat{\mu} \sim \ \text{Gaussian}(\mu', \sigma)$$

$$\text{i.e.,} \ \ E[\hat{\mu}] = \mu'$$

σ from covariance matrix V, use, e.g.,

$$V^{-1} = -E\left[\frac{\partial^2 \ln L}{\partial\theta_i \partial\theta_j}\right]$$

Noncentral chi-square for $-2\ln\lambda(\mu)$

If we can neglect the $O(1/\sqrt{N})$ term, $-2\ln\lambda(\mu)$ follows a noncentral chi-square distribution for one degree of freedom with noncentrality parameter

$$\Lambda = \frac{(\mu - \mu')^2}{\sigma^2}$$

As a special case, if $\mu' = \mu$ then $\Lambda = 0$ and $-2\ln\lambda(\mu)$ follows a chi-square distribution for one degree of freedom (Wilks).

Distribution of q_0

Assuming the Wald approximation, we can write down the full distribution of q_0 as

$$f(q_0|\mu') = \left(1 - \Phi\left(\frac{\mu'}{\sigma}\right)\right)\delta(q_0) + \frac{1}{2}\frac{1}{\sqrt{2\pi}}\frac{1}{\sqrt{q_0}}\exp\left[-\frac{1}{2}\left(\sqrt{q_0} - \frac{\mu'}{\sigma}\right)^2\right]$$

The special case $\mu' = 0$ is a "half chi-square" distribution:

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

Cumulative distribution of q_0, significance

From the pdf, the cumulative distribution of q_0 is found to be

$$F(q_0|\mu') = \Phi\left(\sqrt{q_0} - \frac{\mu'}{\sigma}\right)$$

The special case $\mu' = 0$ is

$$F(q_0|0) = \Phi\left(\sqrt{q_0}\right)$$

The p-value of the $\mu = 0$ hypothesis is

$$p_0 = 1 - F(q_0|0)$$

Therefore the discovery significance Z is simply

$$\boxed{Z = \Phi^{-1}(1 - p_0) = \sqrt{q_0}}$$

The Asimov data set

To estimate median value of $-2\ln\lambda(\mu)$, consider special data set where all statistical fluctuations suppressed and n_i, m_i are replaced by their expectation values (the "Asimov" data set):

$$
\begin{aligned}
n_i &= \mu' s_i + b_i \\
m_i &= u_i
\end{aligned}
$$

$$\rightarrow \quad \hat{\mu} = \mu' \qquad \hat{\boldsymbol{\theta}} = \boldsymbol{\theta}$$

$$\lambda_{\mathrm{A}}(\mu) = \frac{L_{\mathrm{A}}(\mu, \hat{\hat{\boldsymbol{\theta}}})}{L_{\mathrm{A}}(\hat{\mu}, \hat{\boldsymbol{\theta}})} = \frac{L_{\mathrm{A}}(\mu, \hat{\hat{\boldsymbol{\theta}}})}{L_{\mathrm{A}}(\mu', \boldsymbol{\theta})}$$

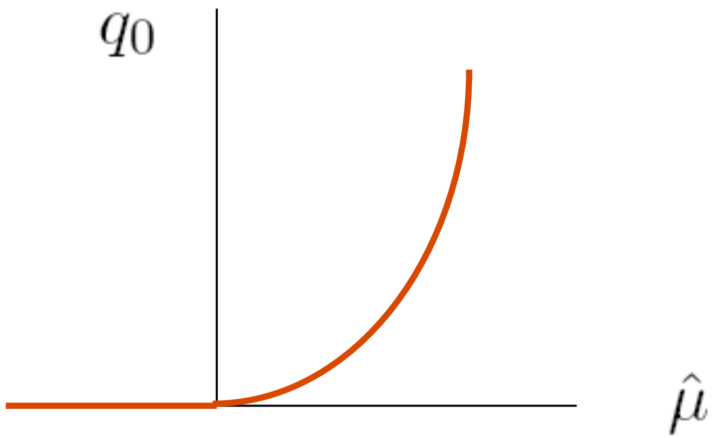
$$-2\ln\lambda_{\mathrm{A}}(\mu) = \frac{(\mu - \mu')^2}{\sigma^2} = \Lambda$$

Asimov value of $-2\ln\lambda(\mu)$ gives non-centrality param. Λ, or equivalently, σ

Relation between test statistics and $\hat{\mu}$

Assuming Wald approximation, the relation between q_0 and $\hat{\mu}$ is

$$q_0 = \begin{cases} \hat{\mu}^2/\sigma^2 & \hat{\mu} \geq 0 \\ 0 & \hat{\mu} < 0 \end{cases}$$



Monotonic, therefore quantiles of $\hat{\mu}$ map one-to-one onto those of q_0, e.g.,

$$\mathrm{med}[q_0] = q_0(\mathrm{med}[\hat{\mu}]) = q_0(\mu') = \frac{\mu'^2}{\sigma^2} = -2\ln\lambda_{\mathrm{A}}(0)$$

$$\mathrm{med}[Z_0] = \sqrt{-2\ln\lambda_{\mathrm{A}}(0)}$$

Profile likelihood ratio for upper limits

For purposes of setting an upper limit on μ use

$$q_\mu = \begin{cases} -2\ln\lambda(\mu) & \hat{\mu} \le \mu \\ 0 & \hat{\mu} > \mu \end{cases} \qquad \text{where} \qquad \lambda(\mu) = \frac{L(\mu, \hat{\hat{\boldsymbol{\theta}}})}{L(\hat{\mu}, \hat{\boldsymbol{\theta}})}$$

Note for purposes of setting an upper limit, one does not regard an upwards fluctuation of the data as representing incompatibility with the hypothesized μ.

Note also here we allow the estimator for μ be negative (but $\hat{\mu} s_i + b_i$ must be positive).

Alternative test statistic for upper limits

Assume physical signal model has $\mu > 0$, therefore if estimator for μ comes out negative, the closest physical model has $\mu = 0$.

Therefore could also measure level of discrepancy between data and hypothesized μ with

$$\tilde{\lambda}(\mu) = \begin{cases} \dfrac{L(\mu, \hat{\hat{\boldsymbol{\theta}}}(\mu))}{L(\hat{\mu}, \hat{\boldsymbol{\theta}})} & \hat{\mu} \geq 0, \\[2ex] \dfrac{L(\mu, \hat{\hat{\boldsymbol{\theta}}}(\mu))}{L(0, \hat{\hat{\boldsymbol{\theta}}}(0))} & \hat{\mu} < 0 \,. \end{cases} \qquad \tilde{q}_\mu = \begin{cases} -2 \ln \tilde{\lambda}(\mu) & \hat{\mu} \leq \mu \\ 0 & \hat{\mu} > \mu \end{cases}$$

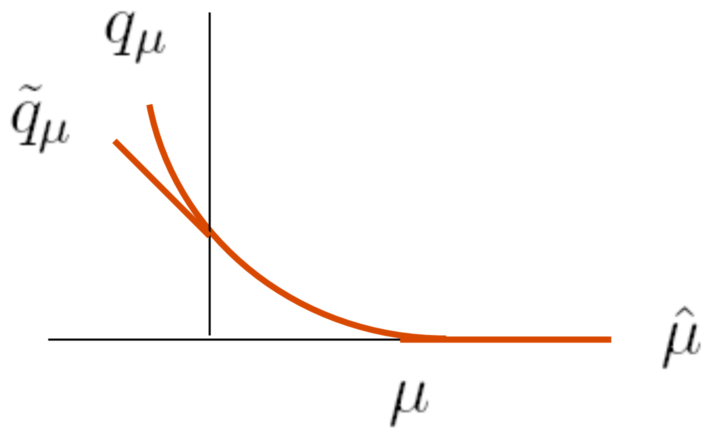
Performance not identical to but very close to q_μ (of previous slide).

q_μ is simpler in important ways.

Relation between test statistics and $\hat{\mu}$

Assuming the Wald approximation for $-2\ln\lambda(\mu)$, q_μ and $\tilde{q}_\mu$ both have monotonic relation with μ.

$$q_\mu = \begin{cases} \frac{(\mu-\hat{\mu})^2}{\sigma^2} & \hat{\mu} < \mu \\ 0 & \hat{\mu} > \mu \end{cases}$$



$$\tilde{q}_\mu = \begin{cases} \frac{\mu^2}{\sigma^2} - \frac{2\mu\hat{\mu}}{\sigma^2} & \hat{\mu} < 0 \\ \frac{(\mu-\hat{\mu})^2}{\sigma^2} & 0 \le \hat{\mu} \le \mu \\ 0 & \hat{\mu} > \mu \; , \end{cases}$$

And therefore quantiles of q_μ, $\tilde{q}_\mu$ can be obtained directly from those of $\hat{\mu}$ (which is Gaussian).

Distribution of q_μ

Similar results for q_μ

$$f(q_\mu|\mu') = \Phi\left(\frac{\mu' - \mu}{\sigma}\right)\delta(q_\mu) + \frac{1}{2}\frac{1}{\sqrt{2\pi}}\frac{1}{\sqrt{q_\mu}}\exp\left[-\frac{1}{2}\left(\sqrt{q_\mu} - \frac{(\mu - \mu')}{\sigma}\right)^2\right]$$

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

$$F(q_\mu|\mu') = \Phi\left(\sqrt{q_\mu} - \frac{(\mu - \mu')}{\sigma}\right)$$

$$p_\mu = 1 - F(q_\mu|\mu) = 1 - \Phi\left(\sqrt{q_\mu}\right)$$

Distribution of $\tilde{q}_\mu$

Similar results for $\tilde{q}_\mu$

$$f(\tilde{q}_\mu|\mu') = \Phi\left(\frac{\mu'-\mu}{\sigma}\right)\delta(\tilde{q}_\mu)$$

$$+ \begin{cases} \frac{1}{2}\frac{1}{\sqrt{2\pi}}\frac{1}{\sqrt{\tilde{q}_\mu}}\exp\left[-\frac{1}{2}\left(\sqrt{\tilde{q}_\mu}-\frac{\mu-\mu'}{\sigma}\right)^2\right] & 0 < \tilde{q}_\mu \le \mu^2/\sigma^2\,, \\ \frac{1}{\sqrt{2\pi}(2\mu/\sigma)}\exp\left[-\frac{1}{2}\frac{(\tilde{q}_\mu-(\mu^2-2\mu\mu')/\sigma^2)^2}{(2\mu/\sigma)^2}\right] & \tilde{q}_\mu > \mu^2/\sigma^2\,. \end{cases}$$

$$F(\tilde{q}_\mu|\mu') = \begin{cases} \Phi\left(\sqrt{\tilde{q}_\mu}-\frac{(\mu-\mu')}{\sigma}\right) & 0 < \tilde{q}_\mu \le \mu^2/\sigma^2\,, \\ \Phi\left(\frac{\tilde{q}_\mu-(\mu^2-2\mu\mu')/\sigma^2}{2\mu/\sigma}\right) & \tilde{q}_\mu > \mu^2/\sigma^2\,. \end{cases}$$

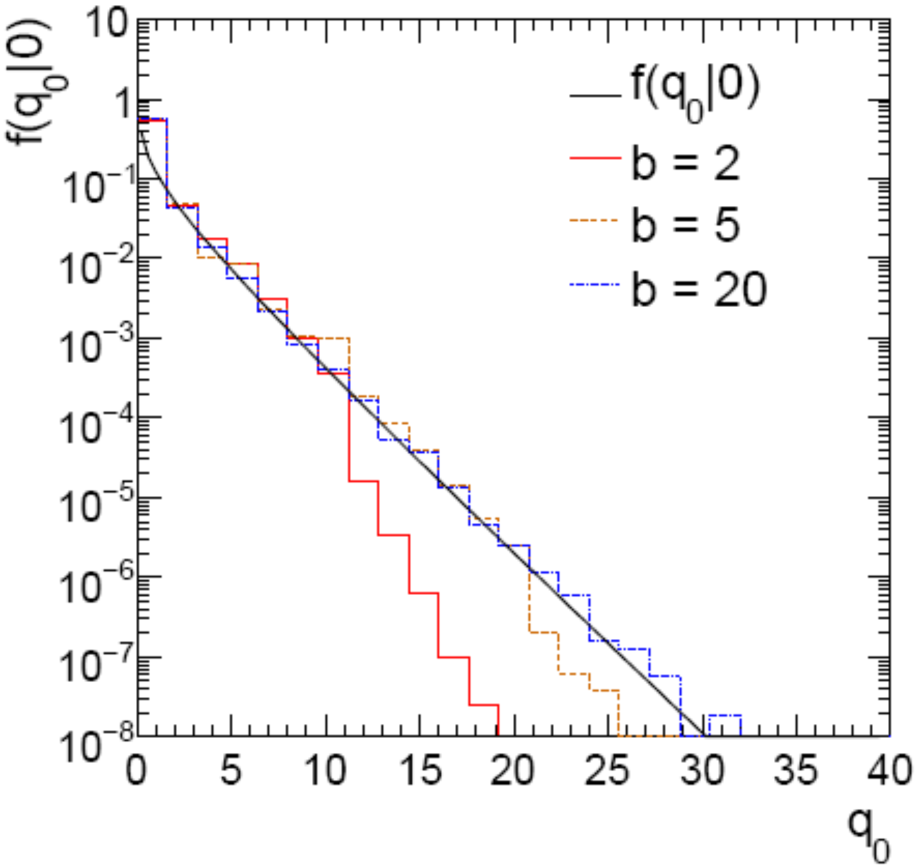
Monte Carlo test of asymptotic formula

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

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

Here take $\tau = 1$.

Asymptotic formula is good approximation to 5σ level ($q_0 = 25$) already for $b \sim 20$.

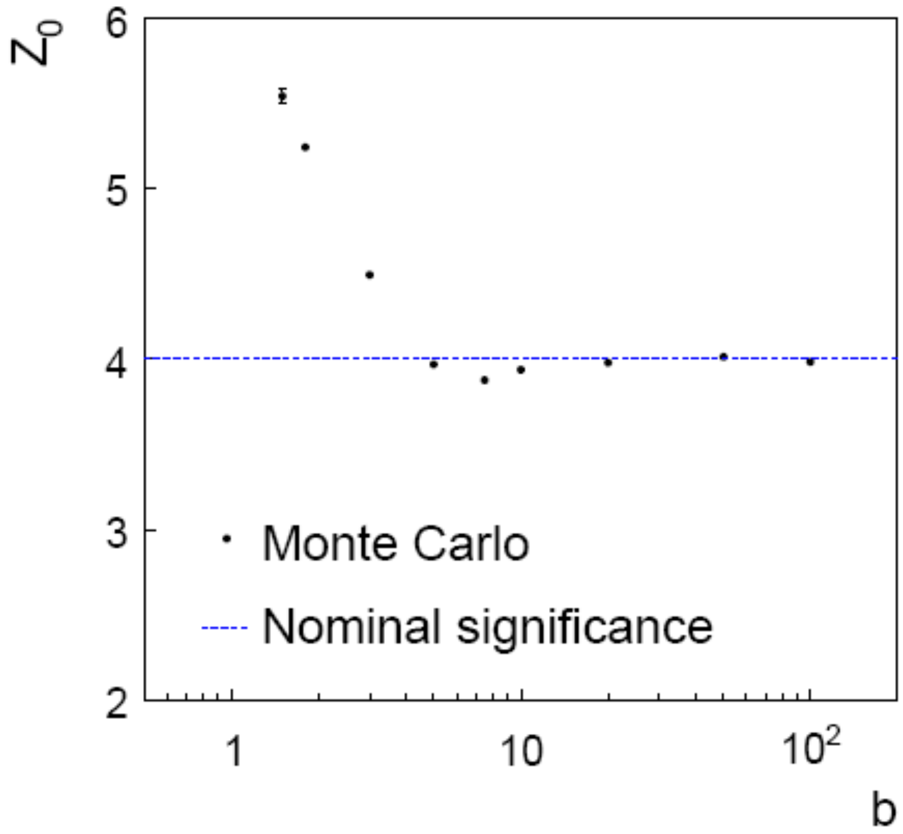


Monte Carlo test of asymptotic formulae

Significance from asymptotic formula, here $Z_0 = \sqrt{q_0} = 4$, compared to MC (true) value.

For very low b, asymptotic formula underestimates Z_0.

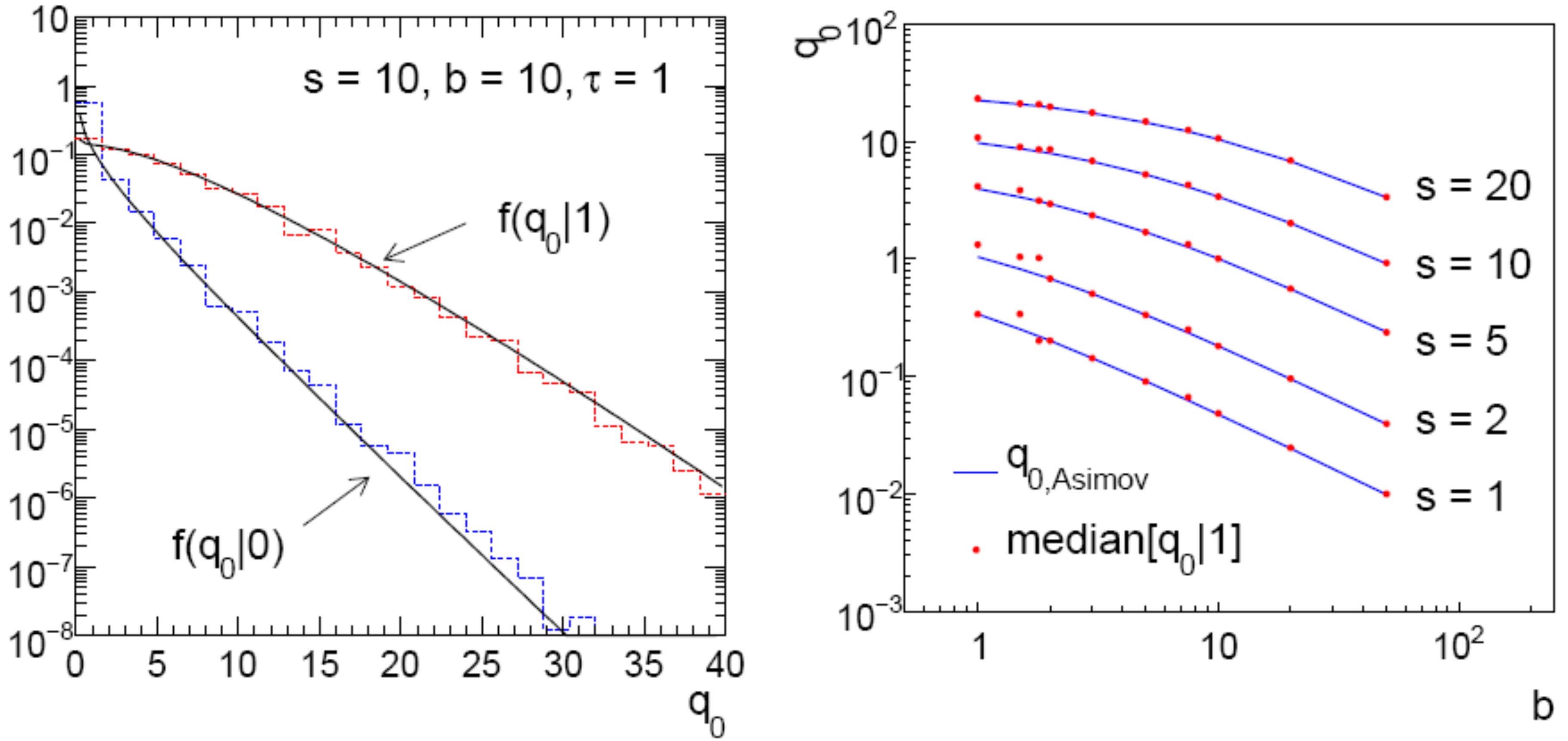
Then slight overshoot before rapidly converging to MC value.



Monte Carlo test of asymptotic formulae

Asymptotic $f(q_0|1)$ good already for fairly small samples.

Median$[q_0|1]$ from Asimov data set; good agreement with MC.



Monte Carlo test of asymptotic formulae

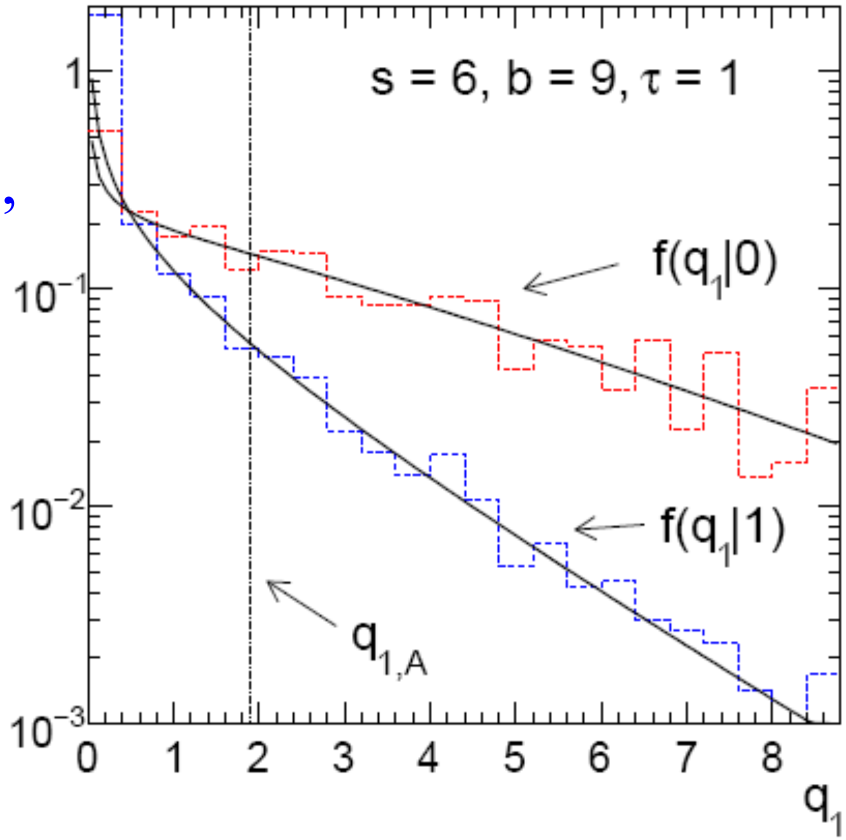
Consider again $n \sim$ Poisson $(\mu s + b)$, $m \sim$ Poisson(τb)
Use q_μ to find p-value of hypothesized μ values.

E.g. $f(q_1|1)$ for p-value of $\mu = 1$.

Typically interested in 95% CL, i.e., p-value threshold = 0.05, i.e., $q_1 = 2.69$ or $Z_1 = \sqrt{q_1} = 1.64$.

Median$[q_1|0]$ gives "exclusion sensitivity".

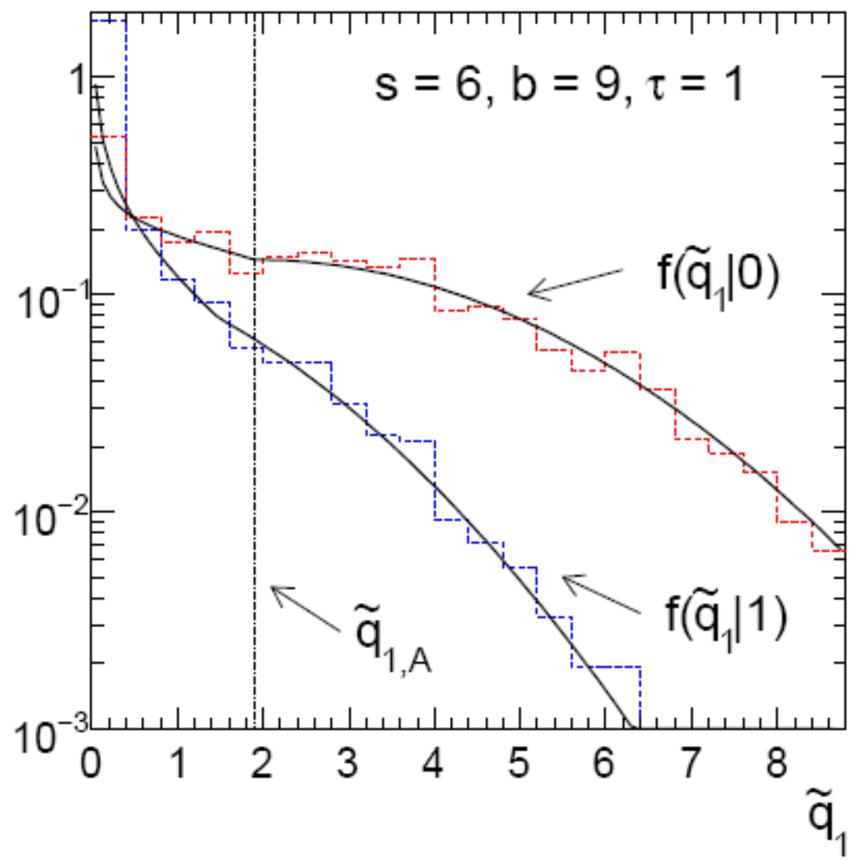
Here asymptotic formulae good for $s = 6$, $b = 9$.



Monte Carlo test of asymptotic formulae

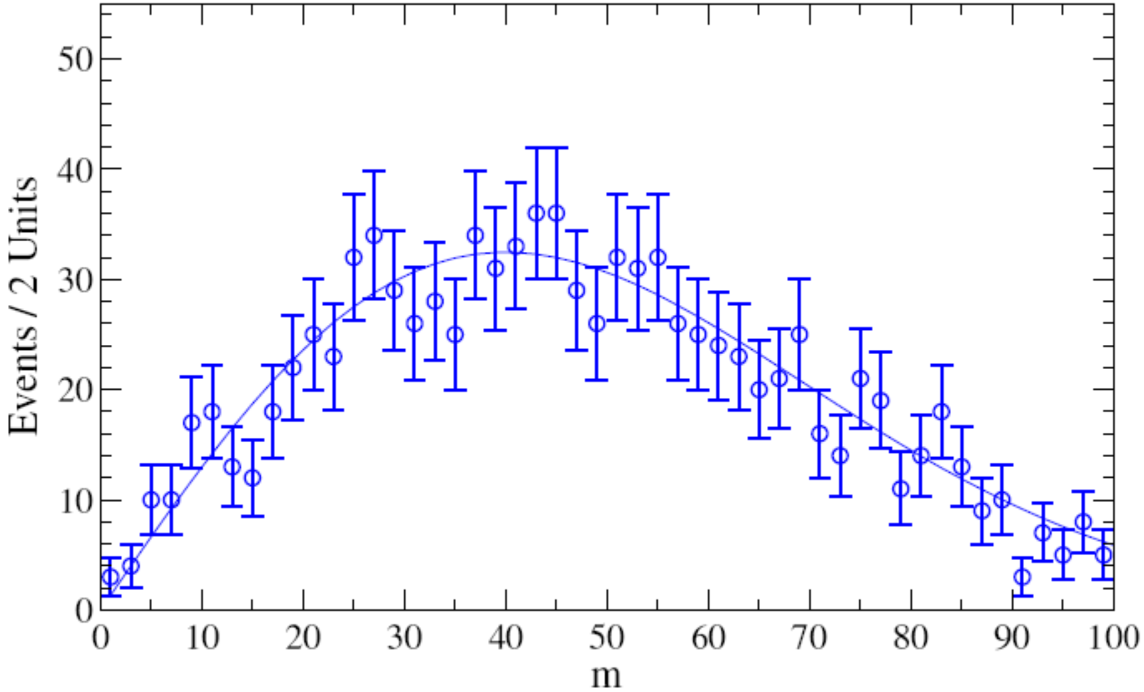
Same message for test based on $\tilde{q}_\mu$.

q_μ and $\tilde{q}_\mu$ give similar tests to the extent that asymptotic formulae are valid.



Example 2: Shape analysis

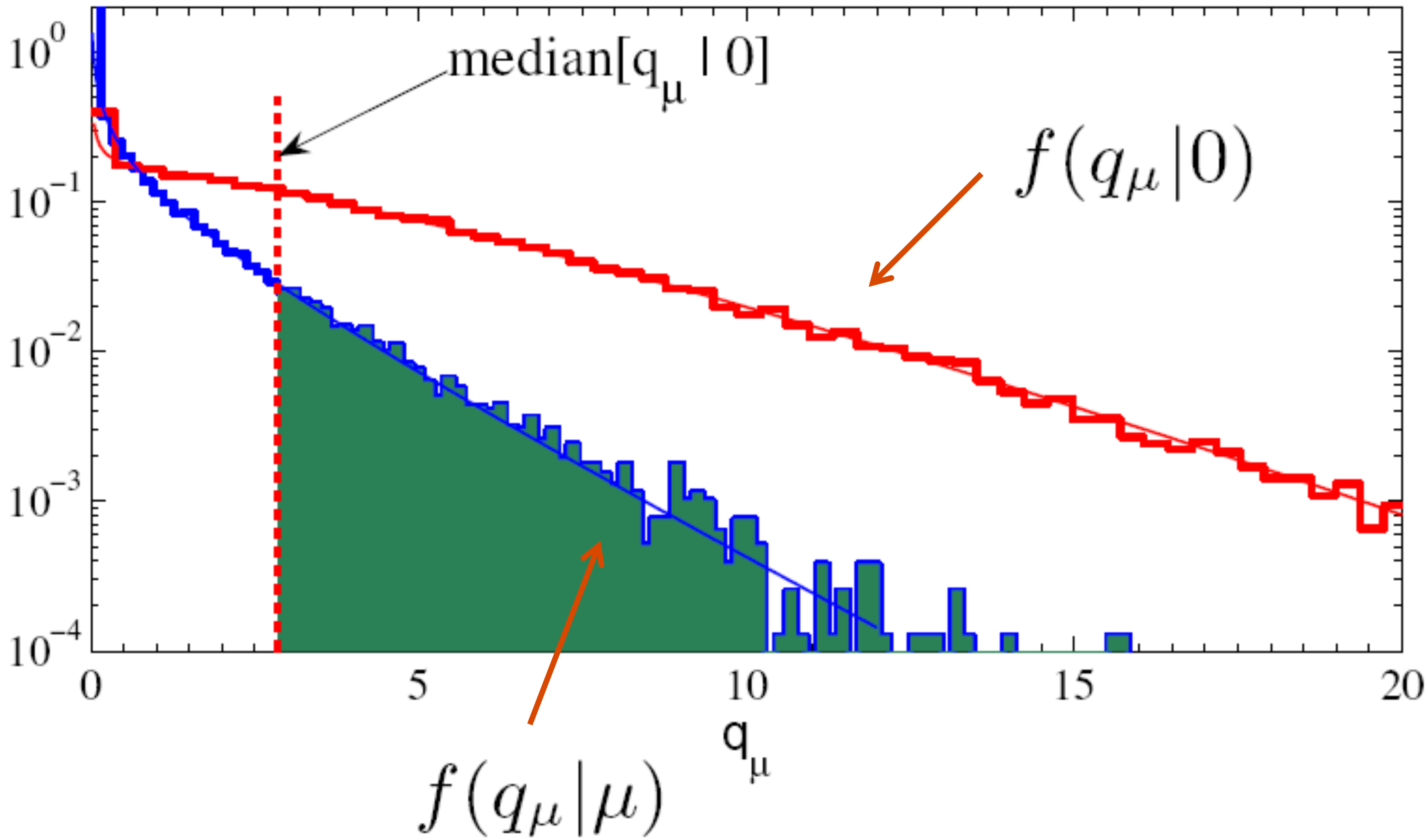
Look for a Gaussian bump sitting on top of:



$$L(\mu, \theta) = \prod_{i=1}^{N} \frac{(\mu s_i + \theta f_{\mathrm{b},i})^{n_i}}{n_i!} e^{-(\mu s_i + \theta f_{\mathrm{b},i})}$$

Monte Carlo test of asymptotic formulae

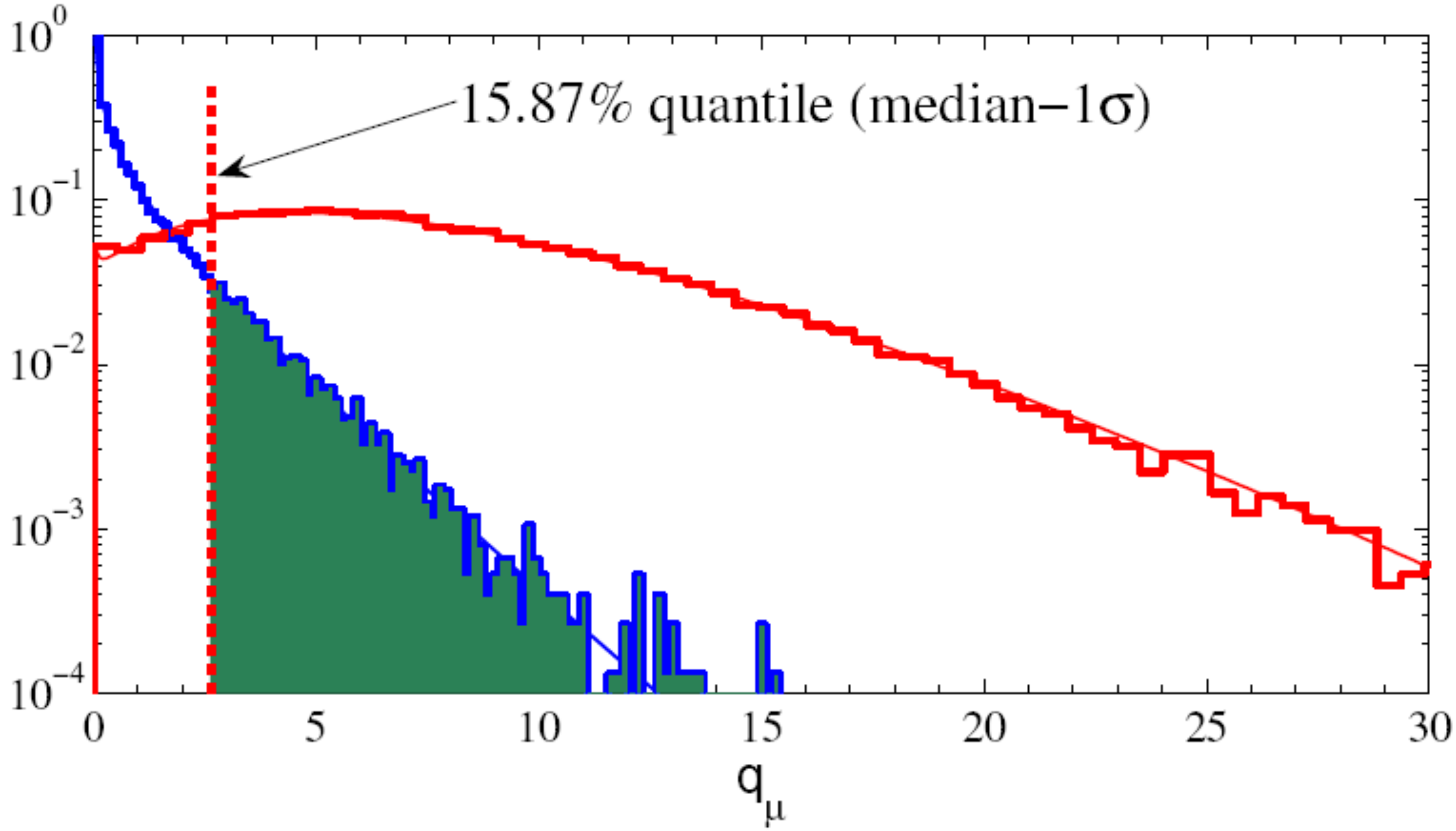
Distributions of q_μ here for μ that gave $p_\mu = 0.05$.



Using $f(q_\mu|0)$ to get error bands

We are not only interested in the median[q_μ|0]; we want to know how much statistical variation to expect from a real data set.

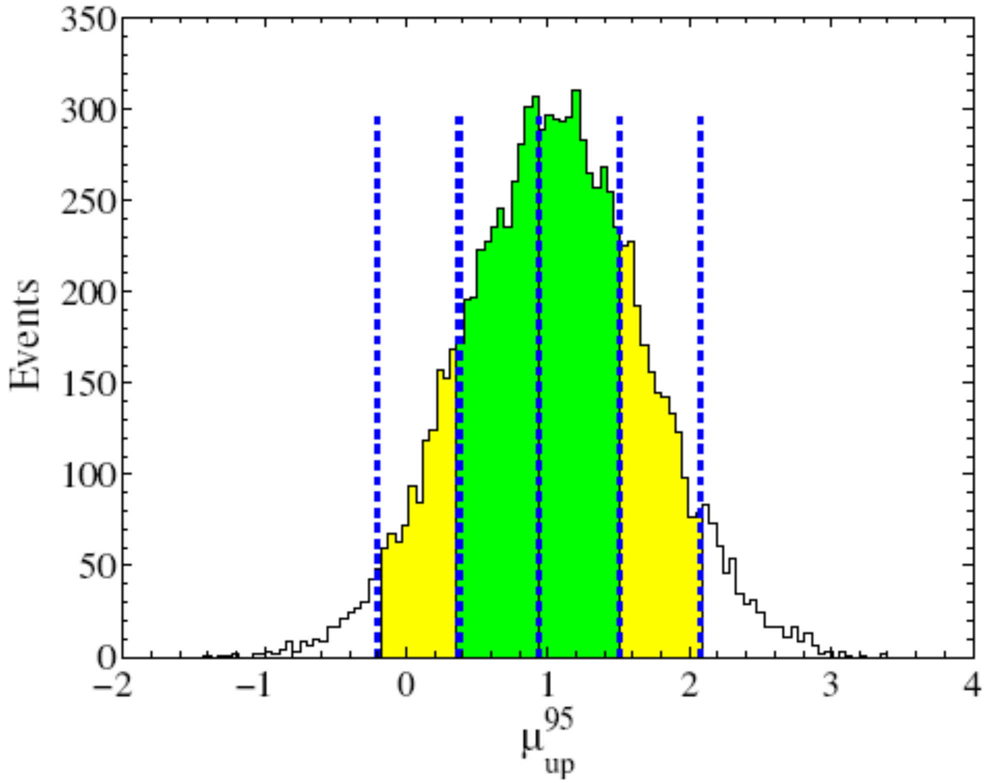
But we have full $f(q_\mu|0)$; we can get any desired quantiles.



Distribution of upper limit on μ

$\pm 1\sigma$ (green) and $\pm 2\sigma$ (yellow) bands from MC;

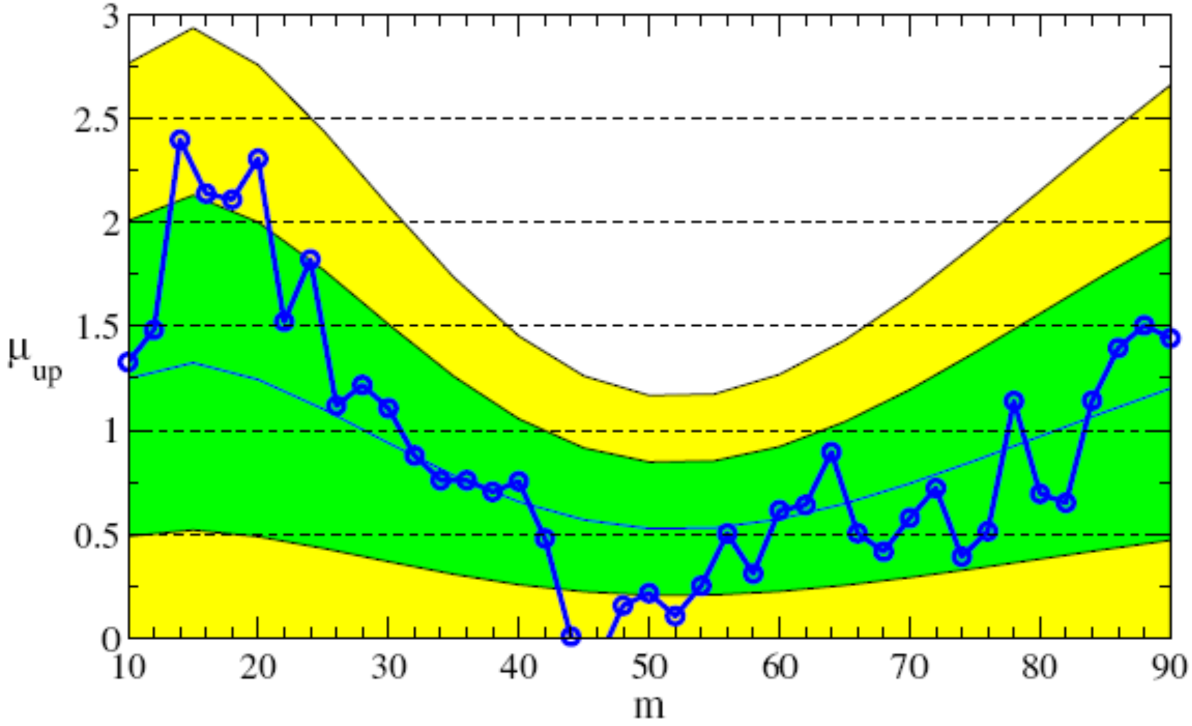
Vertical lines from asymptotic formulae



Limit on μ versus peak position (mass)

$\pm 1\sigma$ (green) and $\pm 2\sigma$ (yellow) bands from asymptotic formulae;

Points are from a single arbitrary data set.



Using likelihood ratio L_{s+b}/L_b

Many searches at the Tevatron have used the statistic

$$q = -2\ln\frac{L_{s+b}}{L_b}$$

likelihood of $\mu = 1$ model (s+b)

likelihood of $\mu = 0$ model (bkg only)

This can be written

$$q = -2\ln\frac{L(\mu = 1, \hat{\hat{\boldsymbol{\theta}}}(1))}{L(\mu = 0, \hat{\hat{\boldsymbol{\theta}}}(0))} = -2\ln\lambda(1) + 2\ln\lambda(0)$$

Wald approximation for L_{s+b}/L_b

Assuming the Wald approximation, q can be written as

$$q = \frac{(\hat{\mu} - 1)^2}{\sigma^2} - \frac{\hat{\mu}^2}{\sigma^2} = \frac{1 - 2\hat{\mu}}{\sigma^2}$$

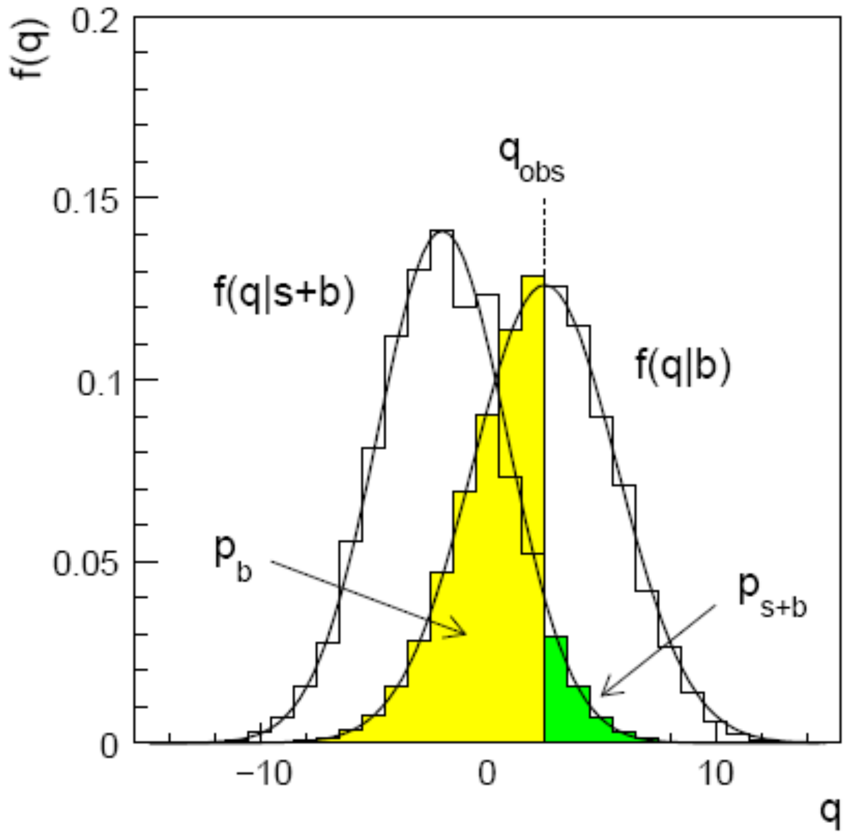
i.e. q is Gaussian distributed with mean and variance of

$$E[q] = \frac{1 - 2\mu}{\sigma^2} \qquad V[q] = \frac{4}{\sigma^2}$$

To get σ^2 use 2nd derivatives of $\ln L$ with Asimov data set.

Example with L_{s+b}/L_b

Consider again $n \sim$ Poisson ($\mu s + b$), $m \sim$ Poisson(τb)
$b = 20$, $s = 10$, $\tau = 1$.



So even for smallish data sample, Wald approximation can be useful; no MC needed.

Summary

Asymptotic distributions of profile LR applied to an LHC search.

Wilks: $f(q_\mu|\mu)$ for p-value of μ.

Wald approximation for $f(q_\mu|\mu')$.

"Asimov" data set used to estimate median q_μ for sensitivity.

Gives σ of distribution of estimator for μ.

Asymptotic formulae especially useful for estimating sensitivity in high-dimensional parameter space.

Can always check with MC for very low data samples and/or when precision crucial.

Implementation in RooStats (ongoing).

Thanks to Louis Fayard, Nancy Andari, Francesco Polci, Marumi Kado for their observations related to allowing a negative estimator for μ.

Extra slides

Discovery significance for $n \sim \text{Poisson}(s + b)$

Consider again the case where we observe n events , model as following Poisson distribution with mean $s + b$ (assume b is known).

1) For an observed n, what is the significance Z_0 with which we would reject the $s = 0$ hypothesis?

2) What is the expected (or more precisely, median) Z_0 if the true value of the signal rate is s?

Gaussian approximation for Poisson significance

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

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

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

Significance for rejecting $s = 0$ is therefore

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

Expected (median) significance assuming signal rate s is

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

Better approximation for Poisson significance

Likelihood function for parameter *s* is

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

or equivalently the log-likelihood is

$$\ln L(s) = n \ln(s+b) - (s+b) - \ln n!$$

Find the maximum by setting $\frac{\partial \ln L}{\partial s} = 0$

gives the estimator for *s*: $\hat{s} = n - b$

Approximate Poisson significance (continued)

The likelihood ratio statistic for testing $s = 0$ is

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

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

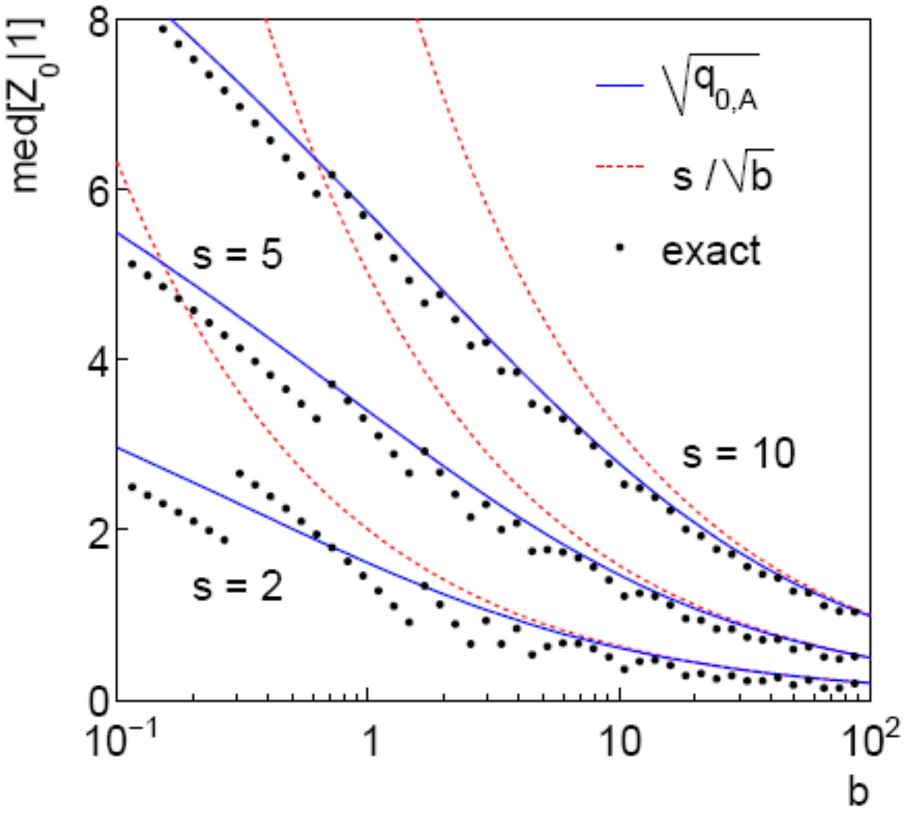
$$Z_0 \approx \sqrt{q_0} = \sqrt{2 \left(n \ln \frac{n}{b} + b - n \right)} \quad \text{for } n > b, \; 0 \text{ otherwise}$$

To find median[$Z_0|s+b$], let $n \to s + b$ (i.e., the Asimov data set):

$$\boxed{\text{median}[Z_0|s+b] \approx \sqrt{2\left((s+b)\ln(1+s/b) - s\right)}}$$

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

$n \sim$ Poisson($\mu\, s$+b), median significance, assuming $\mu = 1$, of the hypothesis $\mu = 0$



"Exact" values from MC, jumps due to discrete data.

Asimov $\sqrt{q_{0,\mathrm{A}}}$ good approx. for broad range of s, b.

$s/\sqrt{b}$ only good for $s \ll b$.

Profile likelihood ratio for unified interval

We can also use directly

$$t_\mu = -2 \ln \lambda(\mu) \qquad \text{where} \qquad \lambda(\mu) = \frac{L(\mu, \hat{\hat{\boldsymbol{\theta}}})}{L(\hat{\mu}, \hat{\boldsymbol{\theta}})}$$

as a test statistic for a hypothesized μ.

Large discrepancy between data and hypothesis can correspond either to the estimate for μ being observed high or low relative to μ.

Distribution of t_μ

Using Wald approximation, $f(t_\mu|\mu')$ is noncentral chi-square for one degree of freedom:

$$f(t_\mu|\mu') = \frac{1}{2\sqrt{t_\mu}} \frac{1}{\sqrt{2\pi}} \left[\exp\left(-\frac{1}{2} \left(\sqrt{t_\mu} + \frac{\mu - \mu'}{\sigma} \right)^2 \right) + \exp\left(-\frac{1}{2} \left(\sqrt{t_\mu} - \frac{\mu - \mu'}{\sigma} \right)^2 \right) \right]$$

Special case of $\mu = \mu'$ is chi-square for one d.o.f. (Wilks).

The p-value for an observed value of t_μ is

$$p_\mu = 1 - F(t_\mu|\mu) = 2\left(1 - \Phi\left(\sqrt{t_\mu}\right)\right)$$

and the corresponding significance is

$$Z_\mu = \Phi^{-1}(1 - p_\mu) = \Phi^{-1}\left(2\Phi\left(\sqrt{t_\mu}\right) - 1\right)$$

Combination of channels

For a set of independent decay channels, full likelihood function is product of the individual ones:

$$L(\mu, \boldsymbol{\theta}) = \prod_i L_i(\mu, \boldsymbol{\theta}_i)$$

For combination need to form the full function and maximize to find estimators of μ, $\boldsymbol{\theta}$.

→ ongoing ATLAS/CMS effort with RooStats framework

Trick for median significance: estimator for μ is equal to the Asimov value μ' for all channels separately, so for combination,

$$\lambda_{\mathrm{A}}(\mu) = \prod_i \lambda_{\mathrm{A},i}(\mu) \qquad \text{where} \qquad \lambda_{\mathrm{A},i}(\mu) = \frac{L_i(\mu, \hat{\hat{\boldsymbol{\theta}}})}{L_i(\mu', \boldsymbol{\theta})}$$