**Basics of p-value and limit calculation**

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# 1 PDF, Likelihood and test statistics

## 1.1 Example PDF: Gaussian signal + exponential background

Gaussian signal PDF (on $n_s$)

$$f_s(x|\theta_s = \mu_x, \sigma_x) = \frac{1}{\sigma_x\sqrt{2\pi}} e^{-\frac{(x-\mu_x)^2}{2\sigma_x^2}} \tag{1}$$

where

- $\mu_x = 2.5$ (fixed)
- $\sigma_x = 0.2$ (fixed)

Exponential background PDF (on $n_b$)

$$f_b(x|\theta_b = \lambda) = \frac{1}{\lambda} e^{-\frac{x}{\lambda}} \tag{2}$$

where

- $\lambda = 1[0..5]$ floating

Observed events

$$\langle n \rangle = \langle n_s \rangle + \langle n_b \rangle = \mu s + \mu_b b \tag{3}$$

where

- $\mu$ = signal strenth = 1 [-10..10] floating.
- $s$ = signal yield = 100 (fixed)
- $\mu_b$ = background strength = 1 [-10..10] floating.
- $b$ = background yield = 1000 (fixed)

Total (signal + background) PDF on $n$

$$f(x|\mu, \theta) = f(x|\mu, \mu_b, \theta_s + \theta_b) = f(\mu, \mu_b, \mu_x, \sigma_x, \lambda) \tag{4}$$

$$= \frac{\mu s f_s(x|\mu_x, \sigma_x) + \mu_b b f_b(x|\lambda)}{\mu s + \mu_b b} \tag{5}$$

### 1.2 Likelihood

Liklihood

$$L(x|\mu,\theta) = L(x|\mu,\mu_b,\mu_x,\sigma_x,\lambda) = \text{Pois}(n,\langle n\rangle)\prod_{j=1}^{n} f(x_j|\mu,\mu_b,\mu_x,\sigma_x,\lambda) \tag{6}$$

Likelihood with Gaussian constraint on $\lambda$

$$L(x|\mu,\theta) = \text{Pois}(n,\langle n\rangle)\prod_{j=1}^{n} f(x_j|\mu,\mu_b,\mu_x,\sigma_x,\lambda)\cdot\frac{1}{\sigma_\lambda\sqrt{2\pi}}e^{-\frac{(\lambda-\mu_\lambda)^2}{2\sigma_\lambda^2}} \tag{7}$$

where

- $\mu$ = signal strength: free parameter
- $\mu_b$: free
- $\mu_x = 2.5$: fixed
- $\sigma_x = 0.2$: fixed
- $\lambda$: Gaussian constrained
- $\mu_\lambda = 1.0$: fixed
- $\sigma_\lambda = 0.01$: fixed

### 1.3 Test statictics

Test statistics = profile Likelihood ratio

$$\lambda(\mu) = \frac{L(\mu,\hat{\hat{\theta}})}{L(\hat{\mu},\hat{\theta})} \qquad (\hat{\mu} \geq \mu) \tag{8}$$

$$\lambda(\mu) = \frac{L(\mu,\hat{\hat{\theta}})}{L(0,\hat{\theta})} \qquad (\hat{\mu} < \mu) \tag{9}$$

Or,

$$q = -2\ln\lambda(\mu) = \begin{cases} 2[\ln L(0,\hat{\theta}) - \ln L(\mu,\hat{\hat{\theta}})] & (\hat{\mu} < 0) \\ 2[\ln L(\hat{\mu},\hat{\theta}) - \ln L(\mu,\hat{\hat{\theta}})] & (0 \leq \hat{\mu} \leq \mu) \\ 0 & (\hat{\mu} > \mu) \end{cases} \tag{10}$$

## 2 P-value for null hypothesis

Generate data using $f(x|\mu=0,\mu_b,\lambda)$ with $n = 1000$ ($\mu = 0, s = 100, \mu_b = 1, b = 1000$). This is your observed data.

## 2.1 Calculation of test statistics

Fit the data by $f(x|\mu, \mu_b, \lambda)$ to get

- $\mu = \widehat{\mu}$
- $\mu_b = \widehat{\mu_b}$
- $\lambda = \widehat{\lambda}$

and plug in these to get

- $f = f(x|\widehat{\mu}, \widehat{\mu_b}, \widehat{\lambda})$

Fit the data with $f(x|\mu = 0, \mu_b, \lambda)$ to get

- $\mu_b = \widehat{\widehat{\mu_b}}$
- $\lambda = \widehat{\widehat{\lambda}}$

and plug in these to get

- $f = f(x|\mu = 0, \widehat{\widehat{\mu_b}}, \widehat{\widehat{\lambda}})$

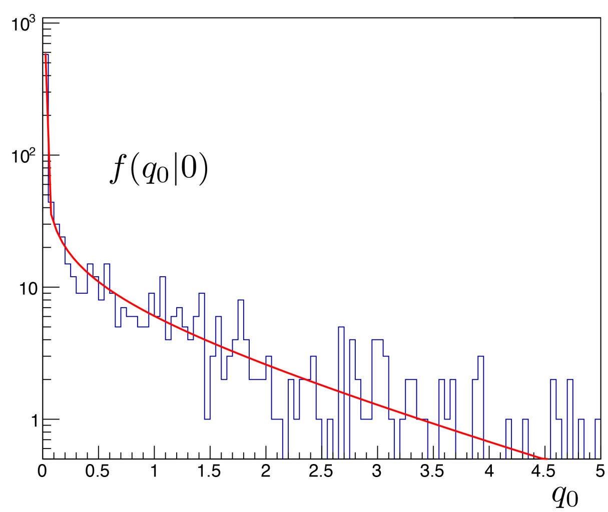
We can calculate the test statistics

$$q_0 = -2 \ln \lambda(0) = 2 \left[ \ln L(\widehat{\mu}, \widehat{\mu_b}, \widehat{\lambda}) - \ln L(0, \widehat{\widehat{\mu_b}}, \widehat{\widehat{\lambda}}) \right] \tag{11}$$

This $q_0$ is the observed one: $q_0^{obs}$.

## 2.2 Obtain $q_0$ distribution

To get $q_0$ distribution, use toy MC. $n_{toy} = 10,000$.
Generate toy data using $f(x|\mu = 0, \mu_b, \lambda)$ ($\mu_b = 1, b = 1000$) by varying $n$ with Poisson random number, which has a mean $n = 1,000$.
Then, calculate $q_0$ for each toy.
Repeat this $n_{toy}$ times to get $f(q_0|\mu = 0)$.



### 2.3 Get p-value

For observed $q_0^{obs}$, the p-value for the null hypothesis is given by

$$p_0 = \int_{q_0^{obs}}^{\infty} f(q_0|0) dq_0 \tag{12}$$

# 3 Limit of Signal Strength ($\mu$)

Generate data using $f(x, \mu, \mu_b, \lambda)$ with fixed $\mu$ ($\mu = 0$ in this example) with $n = 1005$ ($\mu = 0.05, s = 100, \mu_b = 1, b = 1000$). This is your observed data.

## 3.1 Calculate $p_\mu$ for given $\mu$

### 3.1.1 Calculation of $q_\mu$

Then, we scan over $\mu$ to get upper limit.
We start from $\mu = 0.05$.
Fit the data by $f(x|\mu, \mu_b, \lambda)$ to get

- $\mu = \widehat{\mu}$
- $\mu_b = \widehat{\mu_b}$
- $\lambda = \widehat{\lambda}$

Fit the data with fixed $\mu$ with $f(x|\mu = 0.05, \mu_b, \lambda)$ to get

- $\mu_b = \widehat{\widehat{\mu_b}}$
- $\lambda = \widehat{\widehat{\lambda}}$

This gives

$$q_\mu = -2 \ln \lambda(\mu) = 2 \left[ \ln L(\widehat{\mu}, \widehat{\mu_b}, \widehat{\lambda}) - \ln L(\mu, \widehat{\widehat{\mu_b}}, \widehat{\widehat{\lambda}}) \right] \tag{13}$$

This is your observed $q_\mu^{obs}$ with $\mu = 0.05$.

### 3.1.2 Get $q_\mu$ distribution using toy experiments

Generate toys for the fixed $\mu = 0.05$ by varying $n$.
Fit to the toy to get $q_\mu$ for the toy.
Repeat this $n_{toy}$ times to get $f(q|\mu)$ distribution for the fixed $\mu = 0.05$.

### 3.1.3 Get p-value

Then, calculate p-value:

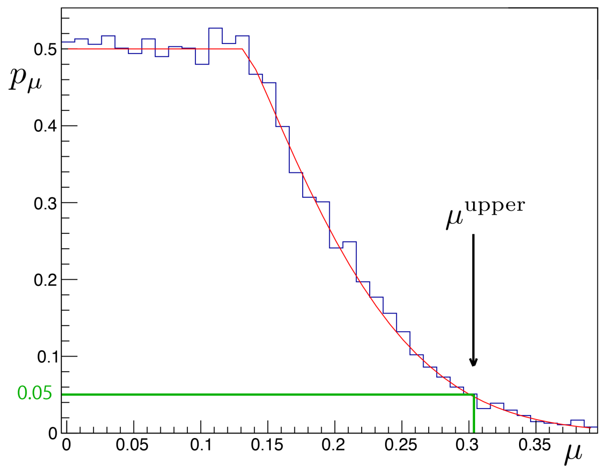
$$p_\mu = \int_{q_\mu^{obs}}^{\infty} f(q|\mu) dq \tag{14}$$

### 3.2 Scan over $\mu$ to get $p_\mu$ distribution

Repeat this for example, $n_\mu = 40$ times, starting from $\mu = 0.05$ with $\Delta_\mu = 0.01$, which means

$$\mu = 0.05, 0.015, 0.025, ..., 0.045$$

to get $p_\mu$ distribution w.r.t. $\mu$.
The 95% confidence level (CL) upper limit of the $\mu$ is given by the $\mu$ value at $p_\mu = 0.05$.




# 4 Expected limit and bands

Generate data' = background only toy MC based on $f(x|\mu = 0, \hat{\hat{\theta}}(0, \text{obs}))$.
Calculate upper limit for the data': $\mu_{up}(\text{data'})$.
Repeat this $n_{exp}$ =? times to get the distribution of the upper limits: $f(\mu_{up}|\mu = 0, \hat{\hat{\theta}}(0, \text{obs}))$
Expected limit = medium of the $f(\mu_{up}|\mu = 0, \hat{\hat{\theta}}(0, \text{obs}))$ distribution.
$\pm 1\sigma$ and $\pm 2\sigma$ bands = 68% and 95% bans of the $f(\mu_{up}|\mu = 0, \hat{\hat{\theta}}(0, \text{obs}))$ distribution.

# 5 Significance

With a give p-value, $p$, its significance, $Z$, is given by

$$Z = \Phi^{-1}(1 - p) \tag{15}$$

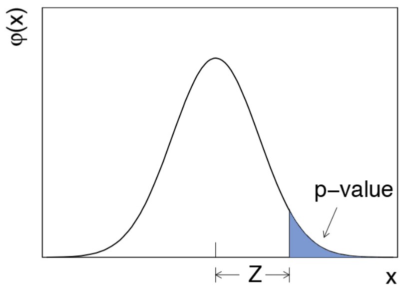
or

$$1 - p = \Phi(Z) \tag{16}$$

where

$$\Phi(x) = \int_{-\infty}^{x} \phi(x)dx \tag{17}$$

and $\phi(x)$ is the PDF.




| $Z(\sigma)$ | p-value | Chance |
|---|---|---|
| 1 | $1.587 \times 10^{-1}$ | 1/6 (16.7%) |
| 2 | $2.275 \times 10^{-2}$ | 1/44 (2.5%) |
| 3 | $1.349 \times 10^{-3}$ | 1/741 (0.1%) |
| 4 | $3.167 \times 10^{-5}$ | 1/31574 (0.003%) |
| 5 | $2.867 \times 10^{-7}$ | 1/3488556 (0.00003%) |

# 6 Asymptotic Formula

The function $f(q|\mu)$ and the relation between $p_\mu$ and $\mu$ were obtained from toy MC above. But they can be derived analytically using an approximation.
Those are called "Asymptotic Formula" and given as red lines in the above two plots.
Test statistics is

$$q_\mu = \frac{\mu^2}{\sigma^2} - \frac{2\mu\widehat{\mu}}{\sigma^2} \qquad (\widehat{\mu} < 0) \tag{18}$$

$$q_\mu = \frac{(\mu - \widehat{\mu})^2}{\sigma^2} \qquad (0 \le \widehat{\mu} \le \mu) \tag{19}$$

$$q_\mu = 0 \qquad (\widehat{\mu} > \mu) \tag{20}$$

PDF is

$$f(q|\mu) = \frac{1}{2}\delta(q) + \frac{1}{2}\frac{1}{\sqrt{2\pi}}\frac{1}{\sqrt{q}}e^{-q/2} \qquad \left(0 < q < \frac{\mu^2}{\sigma^2}\right) \tag{21}$$

$$f(q|\mu) = \frac{1}{2}\delta(q) + \frac{1}{\sqrt{2\pi}(2\mu/\sigma)}e^{-\frac{1}{2}\frac{(q+\mu^2/\sigma^2)^2}{(2\mu/\sigma)^2}} \qquad \left(q > \frac{\mu^2}{\sigma^2}\right) \tag{22}$$

The standard deviation, $\sigma$, of $\widehat{\mu}$, under assumption of a signal strength $\mu$ can be found by generated toy dataset

$$\sigma \sim \frac{\mu}{\sqrt{q}} \tag{23}$$

The cumultive distribution is

$$F(q|\mu) = \Phi\left(\sqrt{q}\right) \qquad \left(0 < q < \frac{\mu^2}{\sigma^2}\right) \tag{24}$$

$$F(q|\mu) = \Phi\left(\frac{q + \mu^2/\sigma^2}{2\mu/\sigma}\right) \qquad \left(q > \frac{\mu^2}{\sigma^2}\right) \tag{25}$$

p-value is

$$p_\mu = 1 - F(q|\mu) \tag{26}$$

Significance is

$$Z_\mu = \sqrt{q} \qquad \left(0 < q < \frac{\mu^2}{\sigma^2}\right) \tag{27}$$

$$Z_\mu = \frac{q + \mu^2/\sigma^2}{2\mu/\sigma} \qquad \left(q > \frac{\mu^2}{\sigma^2}\right) \tag{28}$$

Upper limit at confidence level $1 - \alpha$

$$\mu^{\text{upper}} = \widehat{\mu} + \sigma\Phi^{-1}(1 - \alpha) \tag{29}$$