

# STATISTICA PER FISICI

1. Calcolo delle probabilità
- 2a. Statistica frequentista
- 2b. Statistica bayesiana
3. Likelihood
4. Fondo e segnale
5. Metodi Bootstrap
6. *Unfolding*

## What is Statistics ?

- *a problem of probability calculus:* if  $p = 1/2$  for having head in tossing a coin, what is the probability to have in 1000 coin tosses less than 450 heads?
- *the same problem in statistics:* if in 1000 coin tosses 450 heads have been obtained, what is the estimate of the true head probability?

**Statistical error:**  $s \approx \sigma$

$$\mu \pm \sigma = 500.0 \pm 15.8 \simeq 500 \pm 16 = [484, 516]$$

$$x \pm s = 450.0 \pm 15.7 \simeq 450 \pm 16 = [434, 466]$$

## Physics and Statistics

- Higgs mass  
(PDG 2000):

$$m > 95.3 \text{ GeV}, CL = 95\%$$

- $W$  mass:

$$m_W = 80.419 \pm 0.056 \text{ GeV}$$

These are  
confidence intervals

# The hystorical path

	<b>FREQUENTISTS</b>	<b>BAYESIANS</b>
1763		Thomas Bayes writes a fundamental paper. <b>Bayesian age</b>
1900	Karl Pearson proposes the $\chi^2$ test	
1910	Robert Fisher invents Maximum Likelihood	
<b>1937</b>	The J. Neyman frequentist interval estimate	
1940	The Hypothesis testing of Pearson. <b>Frequentist age</b> The Popper scheme <b>Frequentist teaching</b>	
1990		rediscovering of the bayesian works of Jeffreys, De Finetti and Jaynes
<b>now</b>	the debate is open: see on Confidence Limits	the CERN Workshop (Geneva 2000) <b>neo-Bayesian age?</b>



**Statistics 1.**

**Frequentist approach**

**Bayesian approach**

## What is Statistics ?

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# Statistics

We have 2 inferences

- **parameter estimation:** to estimate  $p$  from 1000 coin tosses
- **hypothesis testing:** in in two experiments of 1000 coin tosses 450 and 600 tosses have been obtained, how much is probable that the two experiments use two consistent coins?

**Parametric Statistics:** the probability depends on  $\theta$ :

$$\mathcal{E}(\theta) \equiv (S, \mathcal{F}, P_\theta)$$

corresponding to a density

$$P\{X \in A\} = \int_A p(x; \theta) dx$$

## Physics and Statistics

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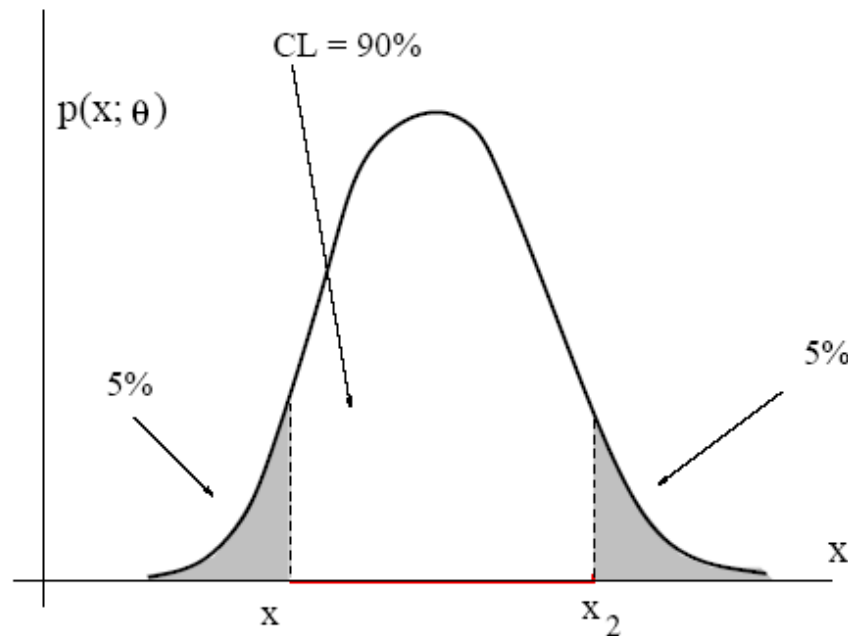
These are  
confidence intervals

# Frequentist Confidence Intervals

One (Neyman, 1937) starts from probability calculus

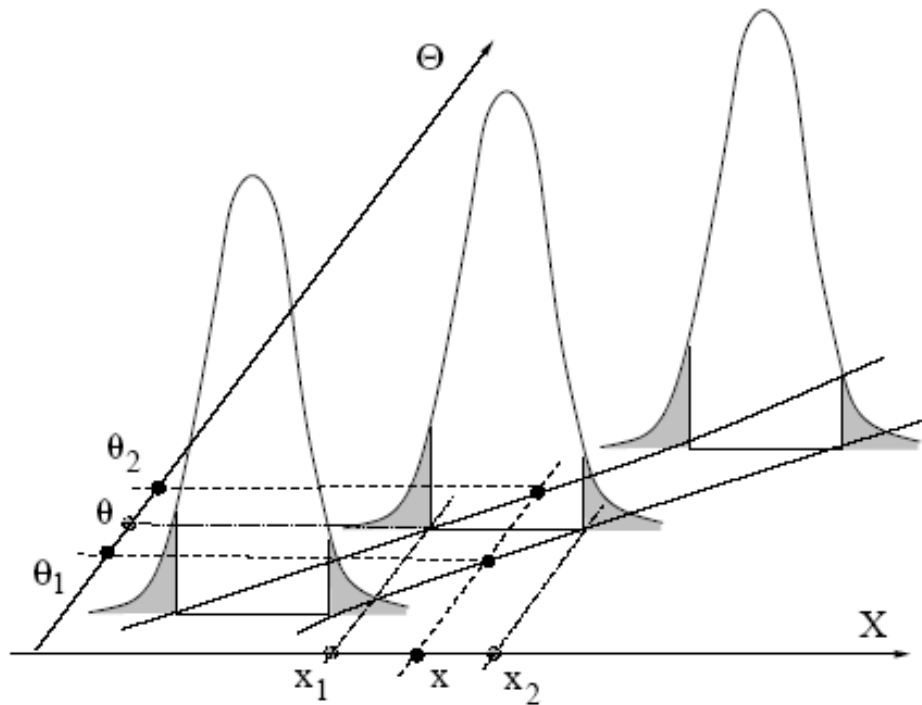
$$\int_{x_1}^{x_2} p(x; \theta) dx = CL$$

and the procedure is repeated



for all the possible  $\theta$  values

# Frequentist confidence intervals



It is possible to show that

$$X \in [x_1, x_2] \text{ iff } \Theta \in [\theta_1, \theta_2]$$

Since

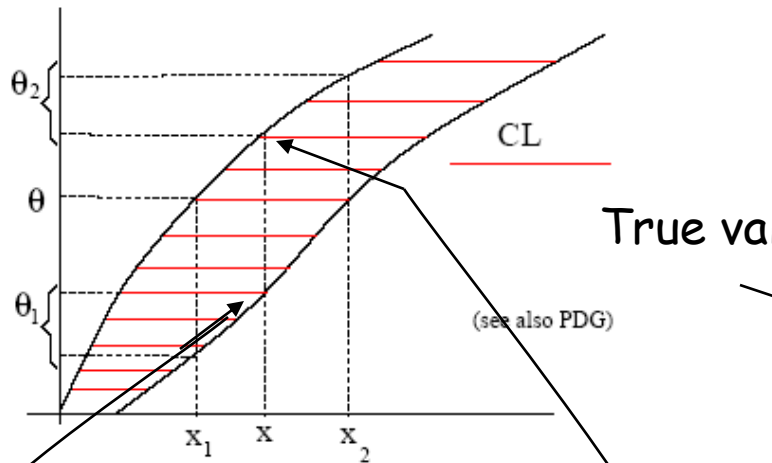
$$P\{X \in [x_1, x_2]\} = CL$$

then

$$P\{\Theta \in [\theta_1, \theta_2]\} = CL$$

**Fundamental Neyman result (1937)**

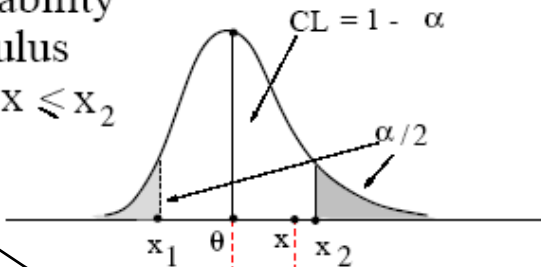
# Cut and top views of the Neyman construction:



$$P\{\theta_1 < \theta < \theta_2\} = P\{x_1 < x < x_2\} = CL$$

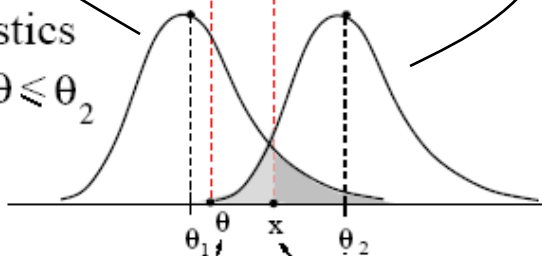
probability calculus

$$x_1 \leq x \leq x_2$$



statistics

$$\theta_1 \leq \theta \leq \theta_2$$



true value

observed value

$$x = x_1 \rightarrow \theta_1 < \theta < \theta$$

interval

$$x = x_2 \rightarrow \theta < \theta < \theta_2$$

$$\theta_1 < \theta < \theta_2 \text{ when } x_1 < x < x_2$$

# Frequentist Confidence Intervals

## mathematical definitions

If  $T_1$  and  $T_2$  are two statistics, the interval

$$I = [T_1, T_2]$$

is a confidence interval for  $\theta$ , with  $0 < CL < 1$  confidence level, if, for all  $\theta \in \Theta$ , the probability that  $I$  contains  $\theta$  (*coverage*) is  $CL$ :

$$P\{T_1 \leq \theta \leq T_2\} = CL .$$

If  $T_1$  e  $T_2$  are discrete variables, the confidence interval satisfies the *minimum overcoverage*

$$P\{T_1 \leq \theta \leq T_2\} \geq CL .$$

**Note:**  $[T_1, T_2]$  are random variables, the  $\theta$  parameter is fixed



# Frequentist C.I.

## right and wrong definitions

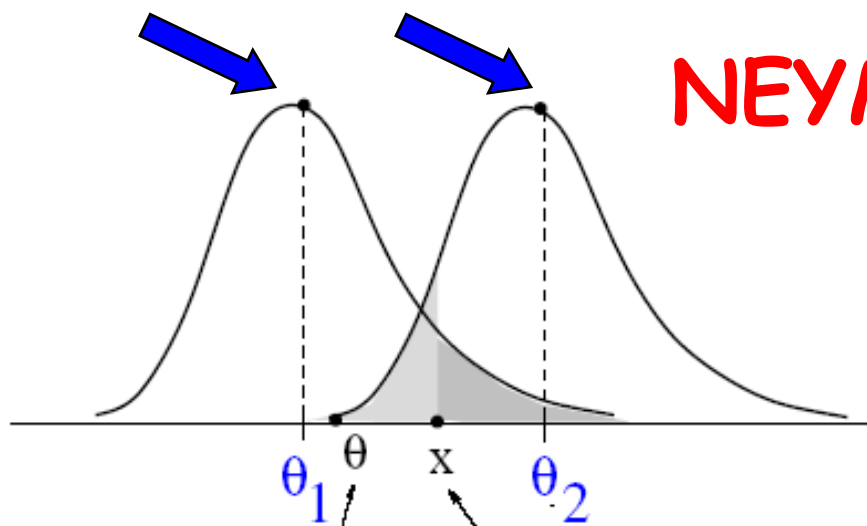
### RIGHT quotations:

- CL is the probability that **the random interval**  $[T_1, T_2]$  **covers** the true value  $\theta$ ;
- in an infinite set of repeated identical experiments, **a fraction equal to CL** will succeed in assigning  $\theta \in [\theta_1, \theta_2]$ ;
- if  $\theta \notin [\theta_1, \theta_2]$ , one can obtain  $\{I = [\theta_1, \theta_2]\}$  in a **fraction of experiments**  $\leq 1 - CL$
- if  $H_0 : \theta \notin [\theta_1, \theta_2]$  the probability to reject a true  $H_0$  is  $1 - CL$  (falsification).  
see **upper and lower limits** estimates.

### WRONG quotations

- CL is the degree of belief that the true value is in  $[\theta_1, \theta_2]$
- $P\{\theta \in [\theta_1, \theta_2]\} = CL$   
( **$\theta$  is not a random variable!**)

# NEYMAN INTEGRALS



true value

measured value

$$\int_x^{\infty} p(x; \theta_1) dx = c_1 \quad \int_{-\infty}^x p(x; \theta_2) dx = c_2$$

where

$$\theta \in [\theta_1, \theta_2], \quad 1 - (c_1 + c_2) = CL$$

MC techniques can be used: grid over  $\theta$  to find the values  $\theta_1$  and  $\theta_2$  satisfying these integrals

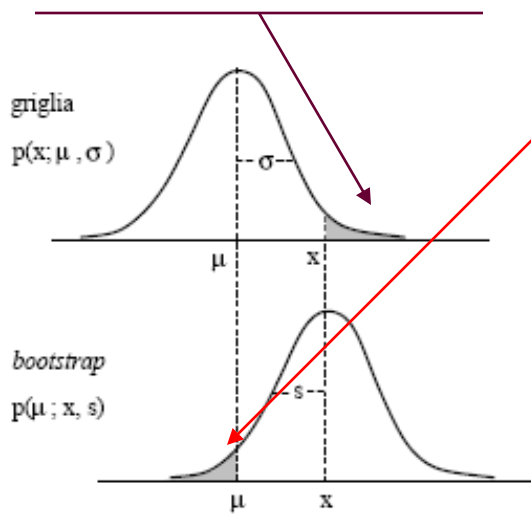
**Important:**

$$\int_{\theta_1}^{\theta_2} p(\theta; x) d\theta = CL$$

**WRONG!!!!**

# When the following property holds

$$1 - \int_{-\infty}^x p(x; \theta) dx = \int_{-\infty}^{\theta} p(\theta; x) d\theta$$



$$1 - F(x; \theta) = F(\theta; x)$$

**Bootstrap property**

$$\int_x^{\infty} p(x; \theta_1) dx = c_1 \quad \int_{-\infty}^x p(x; \theta_2) dx = c_2$$

$$c_1 = \int_x^{\infty} \dots = 1 - \int_{\theta_1}^{\infty} \dots = \int_{-\infty}^{\theta_1} p(\theta; x) d\theta$$

$$c_2 = \int_{-\infty}^x \dots = 1 - \int_{-\infty}^{\theta_2} \dots = \int_{\theta_2}^{\infty} p(\theta; x) d\theta$$

**One can integrate along  $\theta$  in a "bayesian" way**  
(see any elementary textbook)

$$CL = 1 - c_1 - c_2 = \int_{\theta_1}^{\theta_2} p(\theta; x) d\theta$$

## Pivot quantities

Avoid the calculation of the integrals

$$\int_A p(x; \theta) dx = c_i$$

If  $Q(x; \theta)$  is pivotal,  $P\{Q \in A\}$  is independent of  $\theta$ . Example:

$$Q = (X - \theta) \sim N(0, \sigma^2)$$

**Method:**

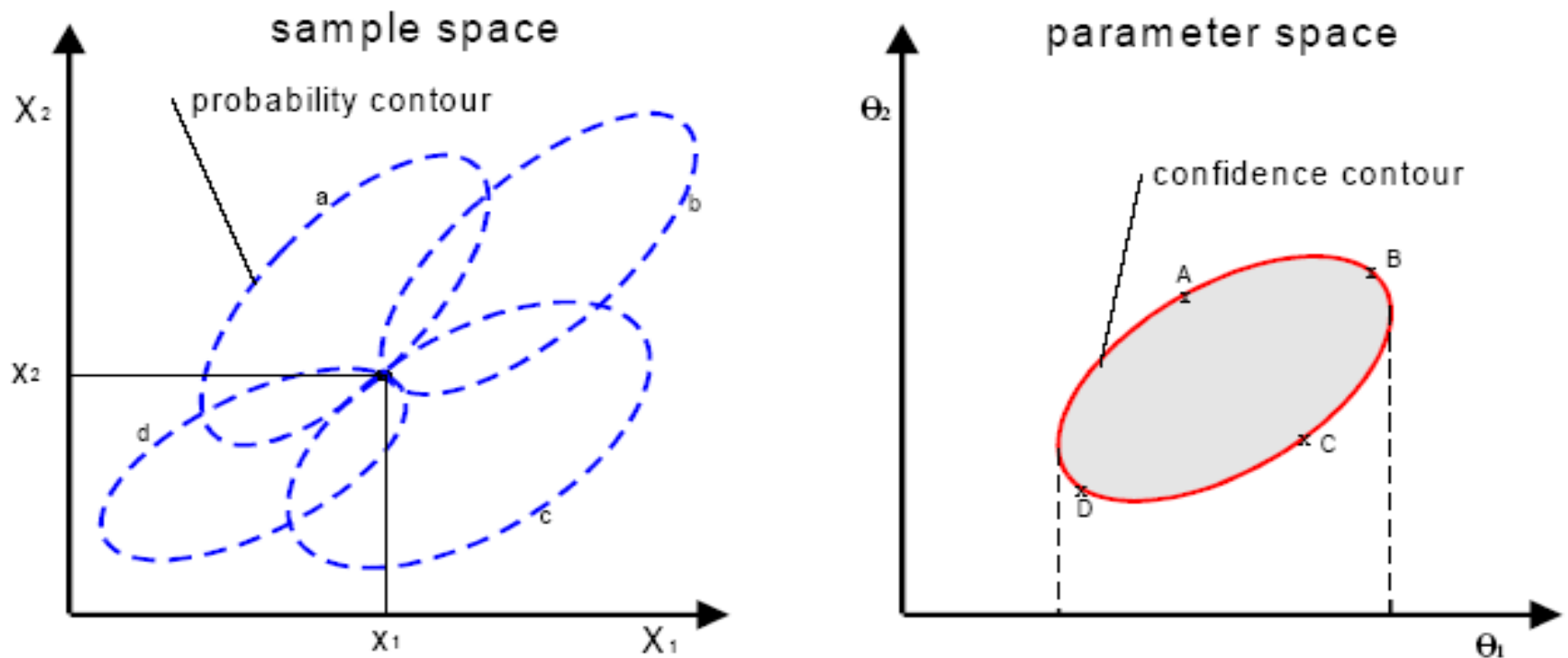
- find  $P\{q_1 \leq Q \leq q_2\} = CL$  ;
- invert the equation:

$$Q(x; \theta) = q \rightarrow \theta = T(x; q)$$

- Then:

$$P\{q_1 \leq Q \leq q_2\} = P\{T_1 \leq \theta \leq T_2\} = CL$$

$$\begin{aligned} P\{\mu - \sigma \leq X \leq \mu + \sigma\} &= P\{-\sigma \leq X - \mu \leq \sigma\} \\ &= P\{X - \sigma \leq \mu \leq X + \sigma\} \end{aligned}$$



**Fig. 2.** Two parameter classical confidence limit for an observation  $x_1, x_2$ . The dashed contours labeled with small letters in the sample space correspond to probability contours of the parameter pairs labeled with capital letters in the parameter space

## Probability estimate big samples

$$\langle F \rangle = \frac{\langle X \rangle}{N} = \frac{Np}{N} = p$$

$$\text{Var}[F] = \frac{\text{Var}[X]}{N^2} = \frac{Np(1-p)}{N^2} = \frac{p(1-p)}{N}$$

**pivot quantity for  $N \gg 1$ :**

$$T = \frac{F - p}{\sigma[F]} \sim N(0, 1) ,$$

**which can be inverted:**

$$P \left\{ \left| \frac{F - p}{\sigma[F]} \right| < 1 \right\} = P \{ F - \sigma[F] \leq p \leq F + \sigma[F] \}$$

$$\sigma[F] = \sqrt{\frac{p(1-p)}{N}} \approx \sqrt{\frac{f(1-f)}{N}}$$

**If  $N \gg 1$  then:**

$$p = f \pm \sqrt{\frac{f(1-f)}{N}} \quad \text{CL} \approx 68\%$$

## small samples

... first difficulties ....

there are no pivot quantities:

$$\sum_{k=x}^n \binom{n}{k} p_1^k (1 - p_1)^{n-k} = c_1 ,$$

$$\sum_{k=0}^x \binom{n}{k} p_2^k (1 - p_2)^{n-k} = c_2 .$$

**Symmetric case:**  $c_1 = c_2 = (1 - CL)/2 = \alpha/2$ .

**When  $x = 0$ ,  $x = n$ ,**  $c_1 = c_2 = 1 - CL$ :

$$x = n \implies p_1^n = 1 - CL ,$$

$$x = 0 \implies (1 - p_2)^n = 1 - CL .$$

**all the attempts had success:**

$$p_1 = \sqrt[n]{1 - CL} \quad p \in [p_1, 1]$$

**no success:**

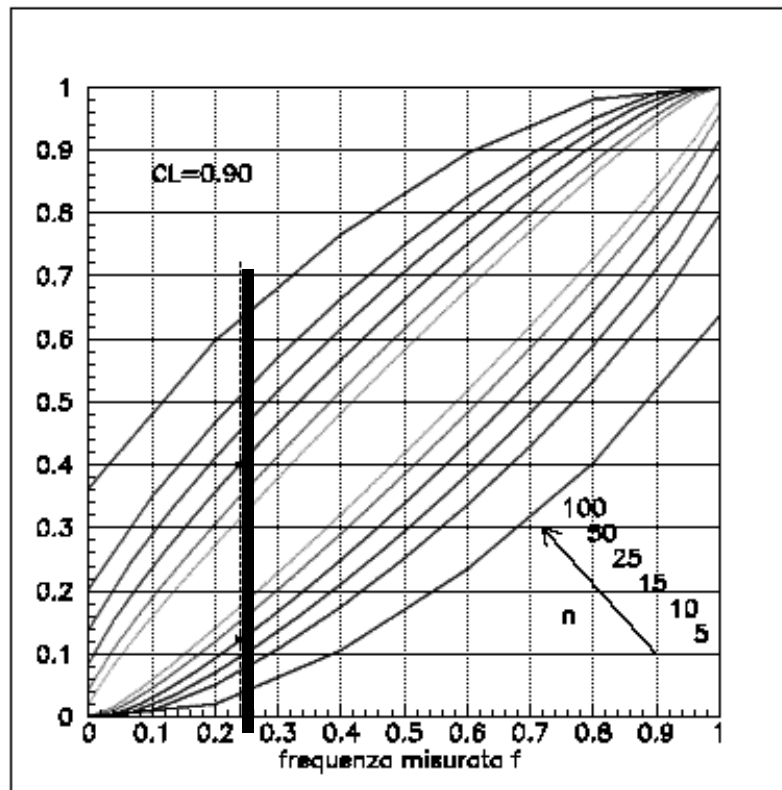
$$p_2 = 1 - \sqrt[n]{1 - CL} \quad p \in [0, p_2]$$

# small samples

$$\sum_{k=x}^n \binom{n}{k} p_1^k (1 - p_1)^{n-k} = c_1 ,$$

$$\sum_{k=0}^x \binom{n}{k} p_2^k (1 - p_2)^{n-k} = c_2 .$$

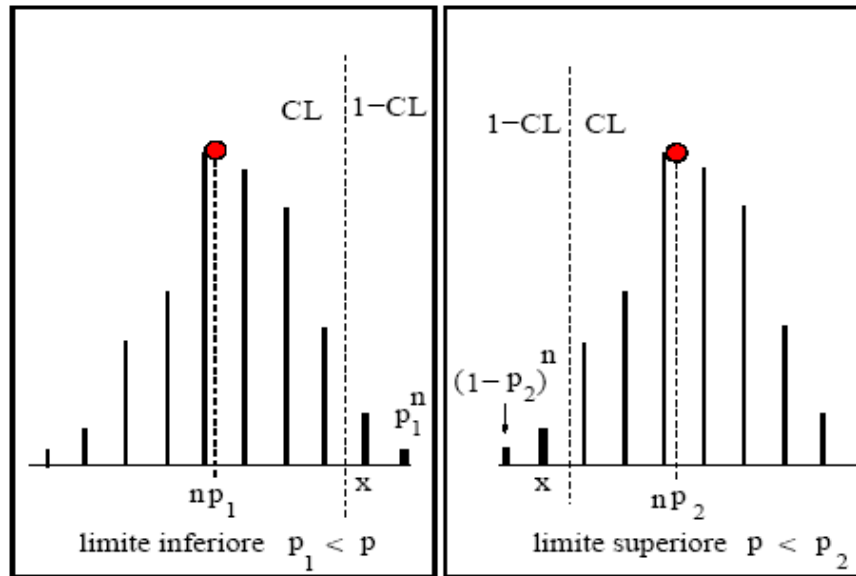
## Neyman curves $CL = 90\%$





# Upper and lower limits

$x$  events are observed:



- **lower limit**  $p \in [p_1, 1]$ : if  $p < p_1$ , one can observe **at least**  $x$  events, but in a fraction of experiments  $< 1 - CL$ .  
If  $x = n$ ,  $p_1^n = 1 - CL$ ;
- **upper limit**  $p \in [0, p_2]$ : if  $p > p_2$ , one can observe **up to**  $x$  events, but in a fraction of experiments  $< 1 - CL$ .  
if  $x = 0$ ,  $(1 - p_2)^n = 1 - CL$ .

# Poisson Limits

$$\sum_{k=x}^{\infty} \frac{\mu_1^k}{k!} \exp(-\mu_1) = c_1, \quad \sum_{k=0}^x \frac{\mu_2^k}{k!} \exp(-\mu_2) = c_2,$$

symmetric case:  $c_1 = c_2 = (1 - CL)/2$ .

**Upper Limits** to the mean number of events having obtained  $x$  events:

$$\sum_{k=0}^x \frac{\mu_2^k}{k!} \exp(-\mu_2) = 1 - CL.$$

For  $x = 0, 1, 2$ , where  $\mu_2 \equiv \mu$

$$e^{-\mu} = 1 - CL,$$

$$e^{-\mu} + \mu e^{-\mu} = 1 - CL,$$

$$e^{-\mu} + \mu e^{-\mu} + \frac{\mu^2}{2} e^{-\mu} = 1 - CL$$

$x$	90%	95%	$x$	90%	95%
0	2.30	3.00	6	10.53	11.84
1	3.89	4.74	7	11.77	13.15
2	5.32	6.30	8	13.00	14.44
3	6.68	7.75	9	14.21	15.71
4	7.99	9.15	10	15.41	16.96
5	9.27	10.51	11	16.61	18.21

When  $\mu > 2.3$ , one can observe no events but in a number of experiments  $< 10\%$ .

# Estimation of the sample mean

$$\text{Var}[M] = \text{Var} \left[ \frac{1}{N} \sum_{i=1}^N X_i \right] = \frac{1}{N^2} \sum_{i=1}^N \text{Var}[X_i] .$$

since  $\text{Var}[X_i] = \sigma^2 \quad \forall i$ ,

$$\text{Var}[M] = \frac{1}{N^2} \sum_{i=1}^N \sigma^2 = \frac{1}{N^2} N \sigma^2 = \frac{\sigma^2}{N} .$$

Due to the **Central Limit theorem** we have a pivot quantity when  $N \gg 1$

$$\frac{\mu - M}{\sigma/\sqrt{N}} \sim N(0, 1)$$

Hence:

$$P \left\{ \left| \frac{\mu - M}{\sigma/\sqrt{N}} \right| \leq 1 \right\} = P \left\{ M - \frac{\sigma}{\sqrt{N}} \leq \mu \leq M + \frac{\sigma}{\sqrt{N}} \right\}$$

( $N > 20 - 30$ ) :

$$\mu = m \pm \frac{\sigma}{\sqrt{N}} \simeq \mu = m \pm \frac{s}{\sqrt{N}} \quad CL \simeq 68\%$$

## The Bayes formula

$$P(B_k|A)P(A) = P(A|B_k)P(B_k)$$

if  $B_k$  are disjoint and cover the set  $S$ ,

$$P(A) = \sum_{i=1}^n P(A|B_i)P(B_i)$$

then  $P(B_k|A)$  can be written as:

$$P(B_k|A) = \frac{P(A|B_k)P(B_k)}{\sum_{i=1}^n P(A|B_i)P(B_i)}, \quad P(A) > 0.$$

**Example** trigger problem

A  $\mu$ - $\pi$  trigger has  $\varepsilon(\pi) = 0.05$  e  $\varepsilon(\mu) = 0.95$ . If the beam is 90%  $\pi$  and 10%  $\mu$  find efficiency and enrichment factor

$$\begin{aligned} P(\mu|T) &= \frac{P(T|\mu)P(\mu)}{P(T|\mu)P(\mu) + P(T|\pi)P(\pi)} \\ &= \frac{0.95 \cdot 0.10}{0.95 \cdot 0.10 + 0.05 \cdot 0.90} = \frac{0.095}{0.14} = 0.678 \end{aligned}$$

efficiency = 14%, enrichment  $\approx 6.8$

## Bayesian use of Bayes formula

An attempt to solve the trigger problem without knowing  
the beam percentages ...!!

The Bayes formula is employed starting from  
subjective probabilities

$$P(H_k|\text{data}) = \frac{P(\text{data}|H_k)P(H_k)}{\sum_{i=1}^n P(\text{data}|H_i)P(H_i)} .$$

an important step,

$$P(H_k|\text{data}) \rightarrow P_{n-1}(H_k)$$

**iteration:**

$$P_n(H_k|E) = \frac{P(E_n|H_k)P_{n-1}(H_k)}{\sum_{i=1}^n P(E_n|H_i)P_{n-1}(H_i)} ,$$

- frequentist approach:

subjective probabilities  
for Hypotheses

**never**  
are assumed.

$P(H|\text{data})$  NO!!!!

# The gambler problem

## Bayesian approach

$$P(\text{Win}|C) = 1 \quad P(\text{Win}|H) = 0.5$$

**Problem:** to find the probability that the gambler is cheat, as a function of the number of consecutive wins  $\{W_n\}$

$$P(H) \equiv P(H|W_0), \quad P(C) \equiv P(C|W_0) \quad P(H) = 1 - P(C)$$

**Iteration:**

$$P(C|W_n) = \frac{P(W_n|C) P(C|W_{n-1})}{P(W_n|C) P(C|W_{n-1}) + P(W_n|H) [1 - P(C|W_{n-1})]}$$

that is

$$P(C|W_n) = \frac{P(C|W_{n-1})}{P(C|W_{n-1}) + 0.5 [1 - P(C|W_{n-1})]}$$

	$P(C)/n$	5	10	15	20
<b>Bayes:</b>	1%	24	91	99.7	99.99
	5%	63	98	99.94	99.998
	50%	97	99.9	99.997	99.999

# The gambler problem

## Frequentist approach

Let us suppose 15 cosecutive wins

### Hypothesis testing:

The null hypothesis  $H_0$  (honest player) gives a significance level (p-value in this case)

$$0.5^{15} = 3.05 \cdot 10^{-5}$$

The probability to be wrong discarding the hypothesis is less then 0.003 %.

The player is cheat.

### Cheat probability estimation:

with  $n = 15$  and  $CL = 90\%$  the probability is

$$p = (0.1)^{1/15} \approx 0.86 .$$

With a “cheat probability”  $p < 0.86$  it is possible to win for 15/15 times, but in a percentage of plays  $< 10\%$

$$0.86 < p < 1 \quad CL = 90\%$$



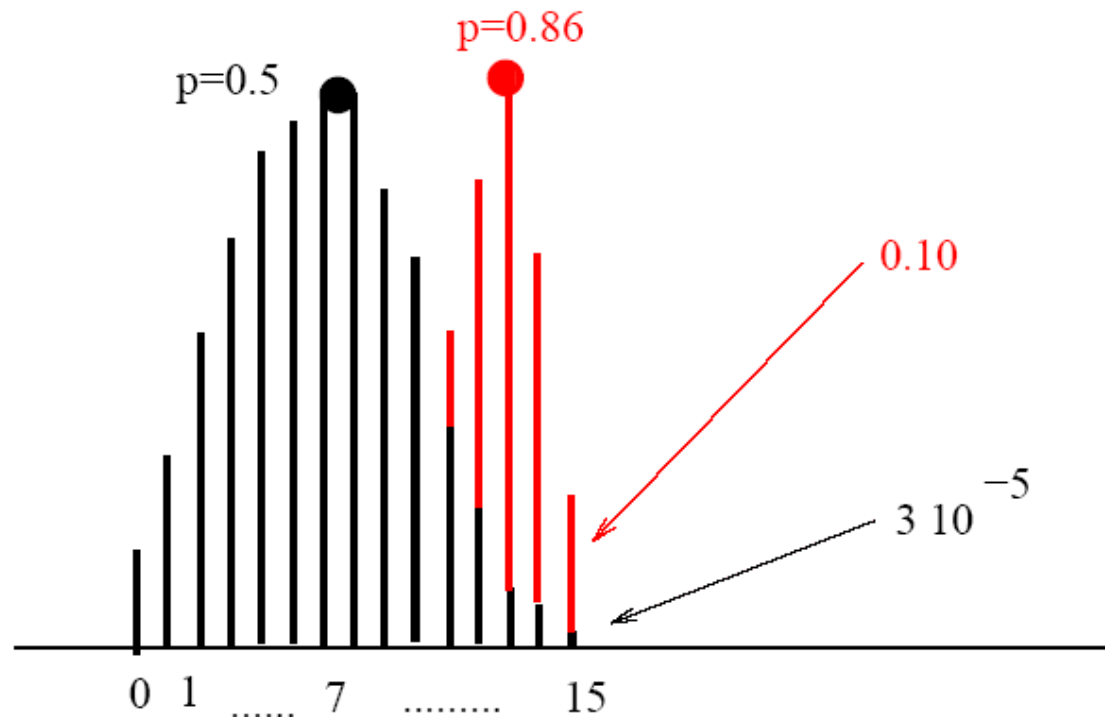
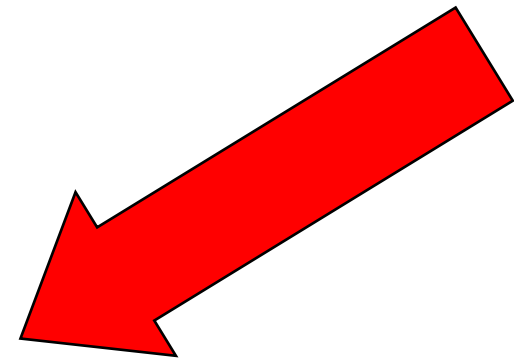
# The gambler problem

## Frequentist approach

Black: hypothesis testing

Red: probability estimation

These conclusions are independent of any a priori hypothesis!



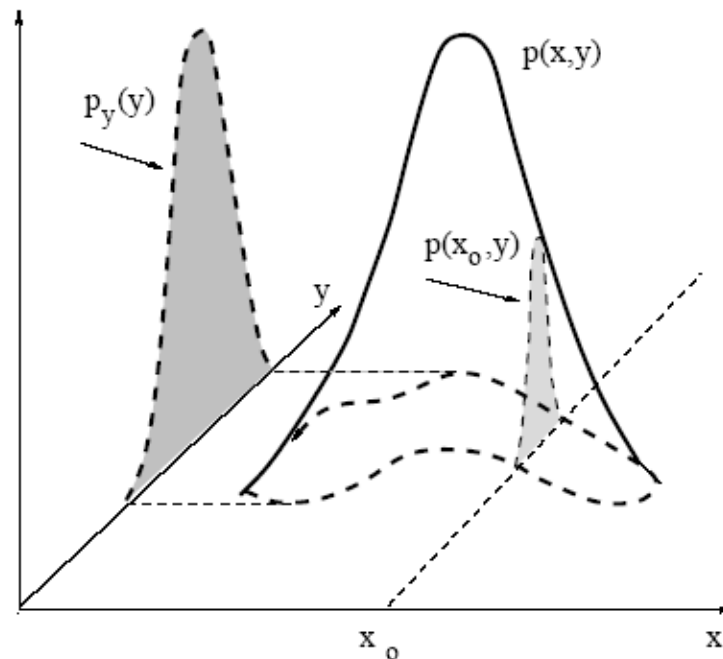
# Marginal and conditional densities

probability product:

$$p(x, y) = p_Y(y) p(x|y) = p_X(x) p(y|x)$$

for independent variables:

$$p(x|y) = p_X(x) , \quad p(y|x) = p_Y(y) ,$$



# Bayes for the continuum

$$p(x, y) = p_Y(y) p(x|y) = p_X(x) p(y|x)$$

hence

$$p(x|y) = \frac{p(y|x) p_X(x)}{p_Y(y)}$$

that is

$$p(x|y) = \frac{p(y|x) p_X(x)}{\int p(y|x) p_X(x) dx}$$

**Bayesian step:**

$$p(\mu; x) = \frac{p(x; \mu) p_\mu(\mu)}{\int p(x; \mu) p_\mu(\mu) d\mu}$$

that is

$$p(\mu; x) = \frac{\text{likelihood} \times \text{prior}}{\text{normalization}}$$



The prior

$p_\mu(\mu)$

that is the subjective probability assigned to  $\mu$ , is **NEVER** used by frequentists

## Bayesian Interval estimate

Degree of belief on  $\mu$  for a **measured**  $x$ :

$$p(\mu; x) = \frac{L(x, \mu) p_{\mu}(\mu)}{\int L(x, \mu) p_{\mu}(\mu) d\mu}$$

Estimate:

$$\mu \in [\mu_1, \mu_2]$$

with **degree of belief**

$$\int_{\mu_1}^{\mu_2} p(\mu; x) d\mu = \text{degree of belief}$$

- one integrates over  $\mu$  considered as a random variable
- this coincides with the frequentist result if the prior  $p_{\mu}(\mu)$  is uniform and the property

$$1 - F(\mu; x) = F(x; \mu)$$

holds

- **but the interpretation is different!**

## Bayesian coin tossing

$$p(p; n, x) = \frac{p^x (1 - p)^{n-x} p_p(p)}{\int p^x (1 - p)^{n-x} p_p(p) dp}$$

With uniform prior,

$$p_p(p) = \text{const} \quad 0 < p < 1$$

Recalling the  $\beta$  function:

$$\int_0^1 p^x (1 - p)^{n-x} dp = \frac{x!(n - x)!}{(n + 1)!}$$

one obtains the **degree of belief of  $p$**

$$p(p; n, x) = \frac{(n + 1)!}{x!(n - x)!} p^x (1 - p)^{n-x}$$

$$\langle p \rangle = \frac{x + 1}{n + 1}$$

$$\text{Var}[p] = \frac{(x + 1)(n - x + 1)}{(n + 3)(n + 2)^2}$$

# Bayesian Interval estimate

$$p \in [p_1, p_2]$$

with **degree of belief**

$$\int_{p_1}^{p_2} \frac{(n+1)!}{x!(n-x)!} p^x (1-p)^{n-x} dp$$

$x = n$ :

$$p(p; x = n) = (n+1)p^n, \quad F(p) = \int_0^p (n+1)p^n dp = p^{n+1}$$

**The 90% bayesian lower bound**

$$0.10 = p^{n+1} \rightarrow p = (0.10)^{1/(n+1)}$$

$x = 0$ :

$$p(p; x = 0, n) = (n+1)(1-p)^n, \\ F(p) = \int_0^p (n+1)(1-p)^n dp = 1 - (1-p)^{n+1}$$

**The 90% bayesian upper bound**

$$0.10 = p^{n+1} \rightarrow p = 1 - (0.10)^{1/(n+1)}$$

**Frequentist  $\rightarrow$  Bayesian**

$$n \rightarrow n + 1$$

**but with a different meaning !!!**

# Elementary example I


In 20 drawings 5 successes have been obtained  
Which is the estimation of the probability with CL=90%?

Frequentist result:  $x=5, n=20, CL=90\%$

$$\sum_{k=n}^n \binom{n}{k} p_1^k (1-p_1)^{n-k} = 0.05$$

$$\sum_{k=0}^x \binom{n}{k} p_2^k (1-p_2)^{n-k} = 0.05$$

$p_1, p_2$




$p=[0.117, 0.434]$

Bayesian result:

What meaning??

$$\frac{\int_{p_1}^{p_2} p^x (1-p)^{n-x} dp}{\int_0^1 p^x (1-p)^{n-x} dp} = 0.90$$

$p_1, p_2$



$p=[0.133, 0.437]$

## Elementary example II

There is a large number of marbles, which are either white or black, and you wish information on the white fraction,  $\mu$ .

You draw a single marble, and it is white. What is the fraction  $\mu$  with 90% of confidence?

Classical:

$$p_1 = 1 - CL = 0.1 \quad \rightarrow \quad \mu \geq 0.1$$

Bayesian:

flat prior  $p_1^2 = 1 - CL = 0.1 \quad \rightarrow \quad \mu \geq 0.316$

$1/\mu$  prior  $p_1 = 1 - CL = 0.1 \quad \rightarrow \quad \mu \geq 0.100$

$\mu$  prior  $p_1^3 = 1 - CL = 0.1 \quad \rightarrow \quad \mu \geq 0.464$



# Bayesian coin tossing

Bayes Theorem:

$$P(\theta | D, I) \propto P(D | \theta, I) \cdot P(\theta | I)$$

$D$  is the *data*,  $I$  summarizes all the relevant information.

Assume a flat prior  $P(\theta | I)$  in a Binomial experiment: cast a coin ( $p$ ).

Bayes formula will update the information on  $p$  at each experiment:

$$P(\theta | noData, I) = P_0(\theta | I) = 1$$

$$P(\theta | H, I) \propto \theta$$

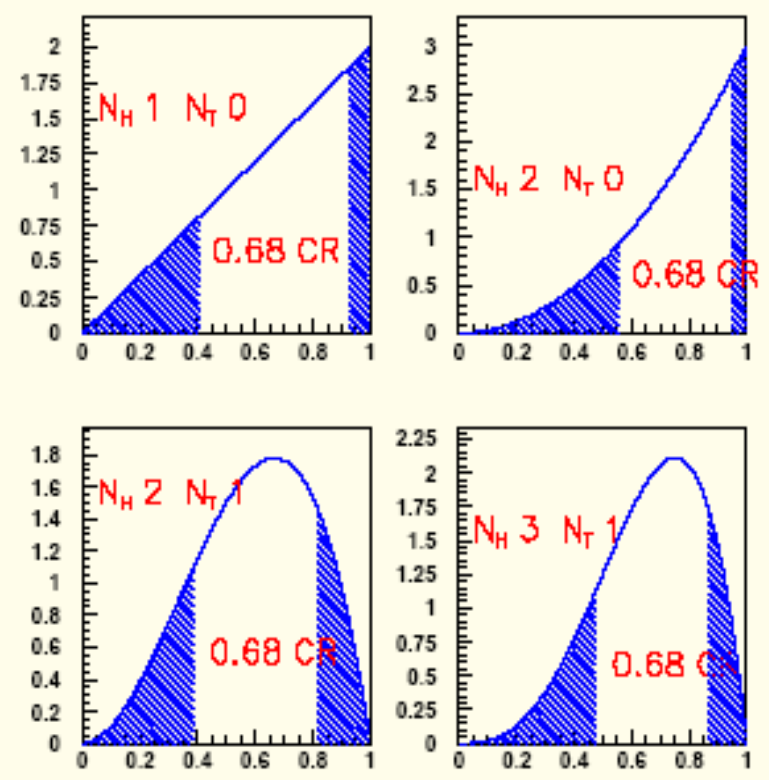
$$P(\theta | H, H, I) \propto \theta^2$$

$$P(\theta | H, H, T, I) \propto \theta^2(1 - \theta)$$

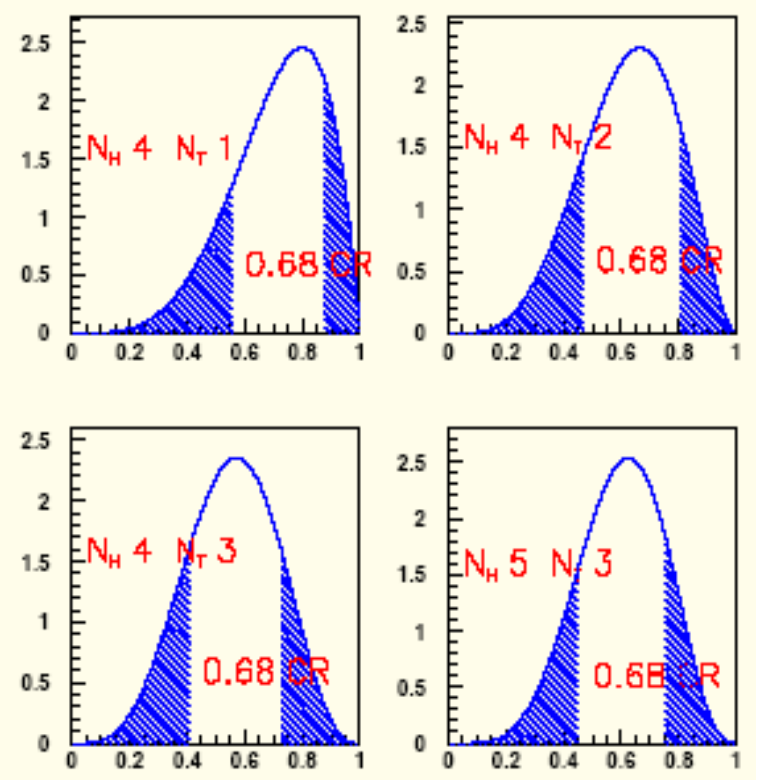
...

$$P(\theta | nN, mT, I) \propto \theta^n(1 - \theta)^m$$

### Bayesian Binomial Inference



### Bayesian Binomial Inference



The plots are the posterior density after each measurement. Also shown the 68% Credible Intervals.



# The 3 event experiment I

A counting experiment registered **3 events**

Find the estimate of  $\mu$ :

$$p(x; \mu) = \frac{\mu^x}{x!} e^{-\mu}$$

~~1. "naïf" physicist~~

$$\mu = 3 \pm \sqrt{3} = [1.27, 4.73] , \quad CL \simeq 68\%$$

wrong

2. standard (frequentist) physicist:

solves the equations

$$\sum_{x=3}^{\infty} \frac{\mu_1^x}{x!} e^{-\mu_1} = 0.16 , \quad \sum_{x=0}^3 \frac{\mu_2^x}{x!} e^{-\mu_2} = 0.16$$

Numerically one obtains the interval:

$$\mu = [1.37, 5.92] , \quad CL = 68\%$$

3. Bayesian physicist:

solves the Bayes formula

$$\int_{\mu_1}^{\mu_2} \frac{\mu^3}{3!} e^{-\mu} p_{\mu}(\mu) d\mu = 0.68 , \quad \text{with}$$

$$p_{\mu}(\mu) = 1 , \quad \int_0^{\mu_1} = \int_{\mu_2}^{\infty} = 0.16$$

The equal tail Bayesian interval:

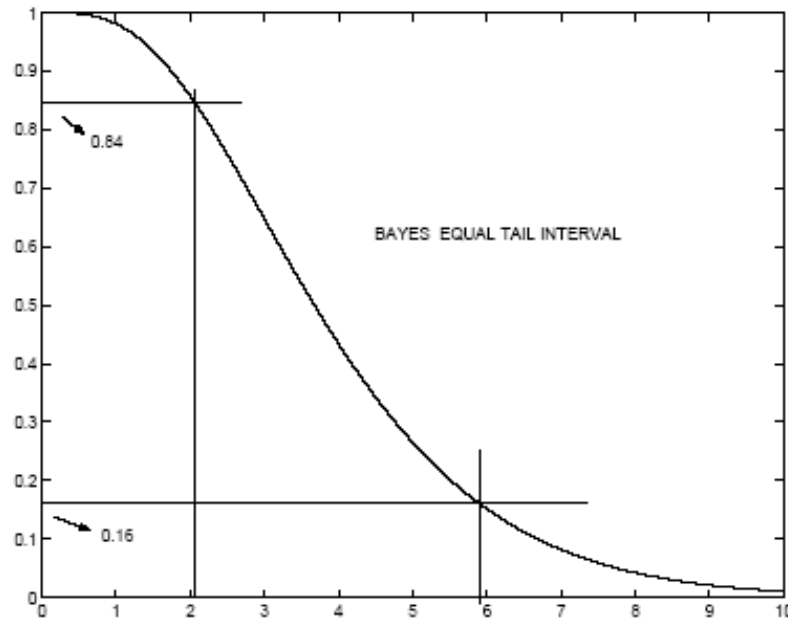
$$\mu = [2.09, 5.92]$$

Last Informative  
Prior (LIP)

The important identity holds:

$$P(\mu) = \int_{\mu}^{\infty} \frac{\mu^x}{x!} e^{-\mu} d\mu = e^{-\mu} \sum_{k=0}^x \frac{\mu^k}{k!}$$

$P(\mu)$  plot for  $x = 3$ :



$$\int_0^{\mu_1} P(\mu) d\mu = \int_{\mu_2}^{\infty} P(\mu) d\mu = 0.16$$

$$\mu = [2.09, 5.92]$$

# Bayesian Interval estimate

## 3. Bayesian physicist:

solves the Bayes formula

$$\int_{\mu_1}^{\mu_2} \frac{\mu^3}{3!} e^{-\mu} p_{\mu}(\mu) d\mu = 0.68, \quad \text{with}$$
$$p_{\mu}(\mu) = 1, \quad \int_{\mu_1}^{\mu} = \int_{\mu}^{\mu_2}$$

The central Bayesian interval is:

$$\mu = [1.55, 5, 15]$$

## 4. Bayesian physicist:

Bayes formula with  $p_{\mu}(\mu) = 1/\mu$ , hence:

$$d(1/\mu) = d\mu/\mu^2, \quad \int_0^{\mu_1} = \int_{\mu_2}^{\infty} = 0.16$$

Uniform  
Jeffreys'  
Prior

$$p(\mu; x) = \int L(\mu; x) p_{\mu}(1/\mu) d\mu$$
$$= \int_{\mu_1}^{\mu_2} \frac{\mu^3}{3!} e^{-\mu} \frac{1}{\mu^2} d\mu = 0.68$$

The central Bayesian interval is:

$$\mu = [1.37, 4.64]$$

# The 3 event experiment

## Summary

method	interval	coverage
naif	[1.27, 4.73]	NO
Neyman	[1.37, 5.92]	68%
Bayes, uniform $p_\mu(\mu)$	[2.09, 5.92]	? < 68%
Bayes, uniform $p_\mu(1/\mu)$	[1.37, 4.64]	? < 68%

- Bayes with uniform  $p_\mu(\mu)$  gives the same frequentist upper limit (5.92);
- Bayes with uniform  $p_\mu(1/\mu)$  gives the same frequentist lower limit (1.37);

# The neutrino mass ...here Bayes helps!

An experiment with a Gaussian resolution of

$$\sigma = 3.3 \text{ eV}/c^2$$

measures the  $\nu_e$  mass as:

$$m = -5.41 \text{ eV}/c^2$$

make the Bayesian estimate of  $m_\nu$ .

Bayes formula

$$p(m_\nu; m, \sigma) = \frac{p(m; m_\nu, \sigma) p_\nu(m_\nu)}{\int p(m; m_\nu, \sigma) p_\nu(m_\nu) dm_\nu}$$

Choosing the prior:

- define  $0 \leq m_\nu \leq 20 - 30 \text{ eV}/c^2$  ;
- define  $\sigma_\nu = 10 \text{ eV}/c^2$
- test three functional forms:
  1. uniform:  $p_\nu = p_u(m_\nu) = 1/30$  ,  $0 \leq m_\nu \leq 30$

2. Gaussian:

$$p_\nu = p_g(m_\nu) = \frac{2}{2\pi\sigma_\nu} \exp[-m_\nu^2/(2\sigma_\nu^2)]$$

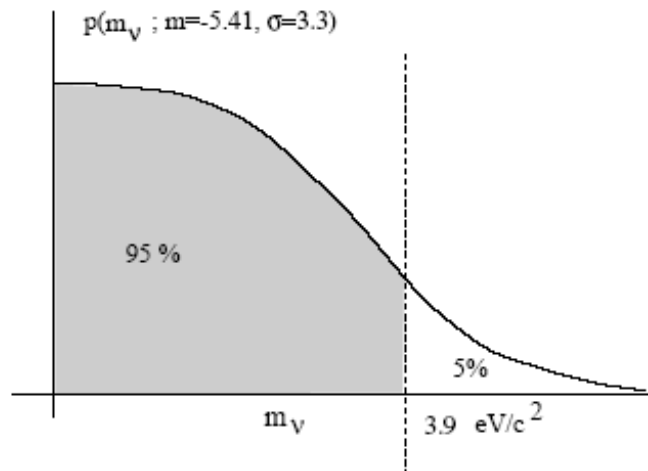
3. triangular:  $p_\nu = p_t(m_\nu) = \frac{1}{450} (30 - m_\nu)$ ,  
 $0 \leq m_\nu \leq 30 \text{ eV}/c^2$

## The neutrino mass II

For example, using the uniform  $p_u(m_\nu)$   
and  $\sigma = 3.3$ ,  $m = -5.41 \text{ eV}/c^2$ :

$$p(m_\nu; m, \sigma) = \frac{\exp\left[-\frac{(m - m_\nu)^2}{2\sigma^2}\right] \frac{1}{30}}{\int_0^{30} \exp\left[-\frac{(m - m_\nu)^2}{2\sigma^2}\right] \frac{1}{30} dm_\nu}$$

one obtains, at 95% probability:



- uniform:  $0 \leq m_\nu \leq 3.9 \text{ eV}/c^2$ ;
- Gaussian:  $0 \leq m_\nu \leq 3.7 \text{ eV}/c^2$ ;
- triangular:  $0 \leq m_\nu \leq 3.7 \text{ eV}/c^2$ .

result “independent” of the prior!

Here the prior represent the **knowledge**, not  
the **ignorance!!!**



# The Gaussian Case

That is... Put in your analysis your **KNOWLEDGE**

Assume that we have made a measurement of the mean of a Gaussian variable and we have obtained:  $x_1 \pm \sigma_1$ . The posterior density, in the case of a flat prior is:

$$f(\mu | x_1, \sigma_1, I_b) = \frac{1}{\sqrt{2\pi}\sigma_1} e^{-(x_1 - \mu)^2 / 2\sigma_1^2}$$

If now we make another measurement yielding:  $x_2 \pm \sigma_2$  the posterior becomes:

$$f(\mu | x_1, \sigma_1, x_2, \sigma_2, I_b) = \frac{N(\mu; x_1, \sigma_1^2) \cdot N(\mu; x_2, \sigma_2^2)}{\int_{-\infty}^{\infty} N(\mu; x_1, \sigma_1^2) \cdot N(\mu; x_2, \sigma_2^2) d\mu}$$

# The Gaussian Case

A boring calculation leads to the following result:

$$f(\mu | x_1, \sigma_1, x_2, \sigma_2, I_b) = \frac{1}{\sqrt{2\pi}\sigma_a} e^{-(x_a - \mu)/2\sigma_a^2}$$
$$x_a = \frac{\frac{x_1}{\sigma_1^2} + \frac{x_2}{\sigma_2^2}}{\frac{1}{\sigma_1^2} + \frac{1}{\sigma_2^2}}$$
$$\sigma_a^2 = \frac{1}{\frac{1}{\sigma_1^2} + \frac{1}{\sigma_2^2}}$$

The most probable value of  $\mu$  is just the weighted mean.

## Conclusions

- don't be **dogmatic**
- use Bayes to parametrize the **a priori knowledge** if any, not the **ignorance**
- in the case of **poor** a priori knowledge, use the **frequentist methods**

Quantum Mechanics:  
frequentist or bayesian?  
Born or Bhor?

$$\int |\psi|^2 dx$$

The standard interpretation is  
frequentist

# Use of the likelihood principle in physics

# Maximum Likelihood

Likelihood function:

$$L(\boldsymbol{\theta}; \underline{\mathbf{x}}) = p(x_{11}, x_{21}, \dots, x_{m1}; \boldsymbol{\theta}) p(x_{12}, x_{22}, \dots, x_{m2}; \boldsymbol{\theta}) \cdot \\ \times p(x_{1n}, x_{2n}, \dots, x_{mn}; \boldsymbol{\theta}) = \prod_{i=1}^n p(\mathbf{x}_i; \boldsymbol{\theta}) ,$$

the product covers

all the  $n$  values of the  $m$  variables  $\mathbf{X}$ .

Log-likelihood:

$$\mathcal{L} = -\ln(L(\boldsymbol{\theta}; \underline{\mathbf{x}})) = -\sum_{i=1}^n \ln(p(\mathbf{x}_i; \boldsymbol{\theta})) ,$$

Max  $L$  corresponds to Min  $\mathcal{L}$ .

For a given set of

$$\underline{\mathbf{x}} = \mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n$$

observed values, from a

$$\mathbf{X} = (\mathbf{X}_1, \mathbf{X}_2, \dots, \mathbf{X}_n)$$

sample with density  $p(\mathbf{x}; \boldsymbol{\theta})$ , the ML estimate  $\hat{\boldsymbol{\theta}}$  of  $\boldsymbol{\theta}$  is the maximum (if any) of the function

$$\max_{\boldsymbol{\theta}} [L(\boldsymbol{\theta}; \underline{\mathbf{x}})] = \max_{\boldsymbol{\theta}} \left[ \prod_{i=1}^n p(\mathbf{x}_i; \boldsymbol{\theta}) \right] = L(\hat{\boldsymbol{\theta}}; \underline{\mathbf{x}})$$

## Maximum likelihood

$$\frac{\partial L}{\partial \theta_k} = \frac{\partial \left[ \prod_{i=1}^n p(\mathbf{x}_i; \boldsymbol{\theta}) \right]}{\partial \theta_k} = 0$$

or

$$\frac{\partial \mathcal{L}}{\partial \theta_k} = \sum_{i=1}^n \left[ \frac{1}{p(\mathbf{x}_i; \boldsymbol{\theta})} \frac{\partial p(\mathbf{x}_i; \boldsymbol{\theta})}{\partial \theta_k} \right] = 0, \quad (k = 1, 2, \dots, p).$$

- *before the trial*, the likelihood function  $L(\boldsymbol{\theta}; \underline{\mathbf{x}})$  is  $\propto$  to the pdf of  $(\mathbf{X}_1, \mathbf{X}_2, \dots, \mathbf{X}_n)$ ;
- *before the trial*, the likelihood function  $L(\boldsymbol{\theta}; \underline{\mathbf{X}})$  is a random function of  $X$ ;

- **frequentist view:** maximize **the function**

$$L(\boldsymbol{\theta}; \underline{\mathbf{x}}) = \prod_{i=1}^n p(\mathbf{x}_i; \boldsymbol{\theta}), \quad \text{or} \quad \ln(L(\boldsymbol{\theta}; \underline{\mathbf{x}})) = \sum_{i=1}^n \ln(p(\mathbf{x}_i; \boldsymbol{\theta})),$$

or minimize

$$-2 \ln(L(\boldsymbol{\theta}; \underline{\mathbf{x}})) = -2 \sum_{i=1}^n \ln(p(\mathbf{x}_i; \boldsymbol{\theta}))$$

w.r.t the parameters  $\boldsymbol{\theta}$ .

- **Bayesian view:**  
maximize the **posterior probability**

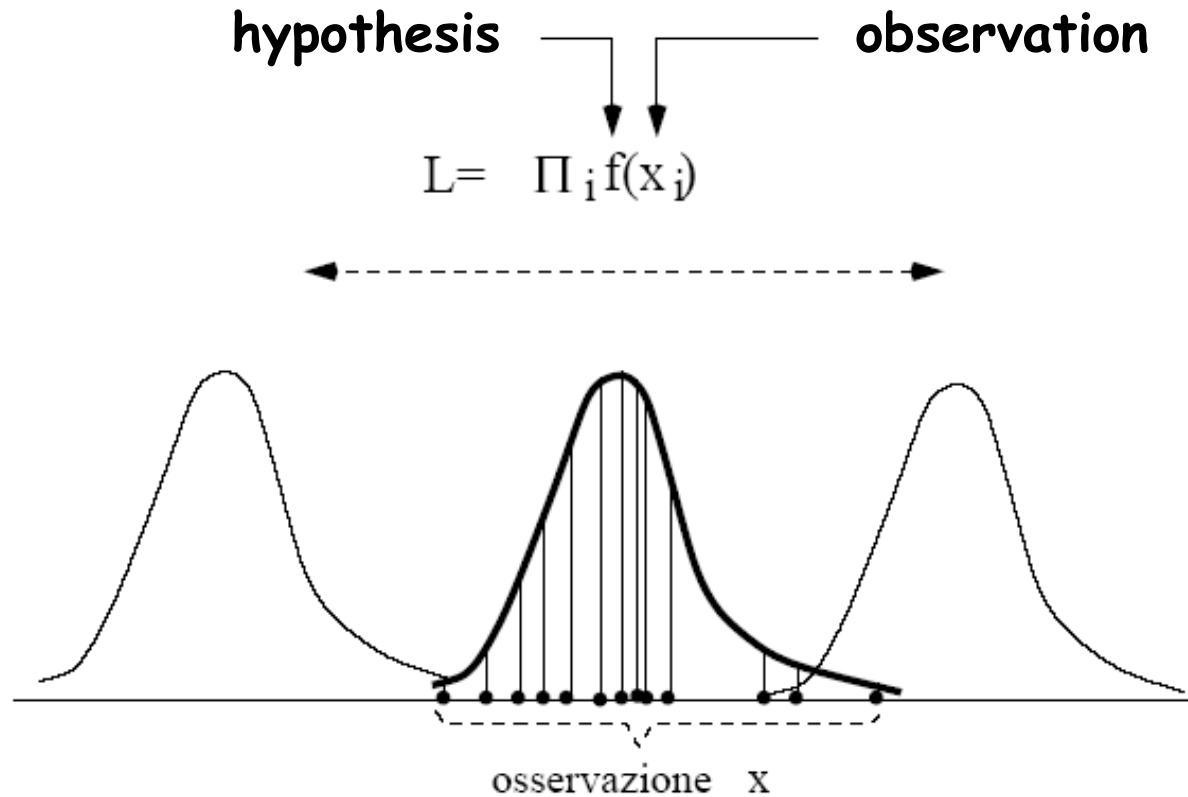
$$p(\boldsymbol{\theta}|\mathbf{x}) = \frac{L(\mathbf{x}|\boldsymbol{\theta}) p(\boldsymbol{\theta})}{\int L(\mathbf{x}|\boldsymbol{\theta}') p(\boldsymbol{\theta}') d\boldsymbol{\theta}'} \propto L(\mathbf{x}|\boldsymbol{\theta}) p(\boldsymbol{\theta})$$

- Bayes maximization updates the **prior**  $p(\boldsymbol{\theta})$
- when the prior  $p(\boldsymbol{\theta})$  is uniform (constant) **technically** the frequentist and the Bayesian approaches coincide because both maximize  $L(\boldsymbol{\theta}; \underline{\mathbf{x}})$  (**but the meaning is different**)
- Bayesian estimators **are not independent of the transformation of the parameters**, the frequentist ones **are independent of them!**

**Bayesians  
vs  
Frequentists**



# Why ML does work?



The  $p(x; \theta)$  form  
is fitted to data  
by maximizing  
the ordinates of the observed data

## Example

An urn with three marbles

$$\begin{array}{cc} \bullet \bullet \circ & \circ \circ \bullet \\ p = 1/3 & p = 2/3 \end{array}$$

An experiment with 4 drawings:

$$p(x; n = 4, p) = \frac{4!}{x!(4-x)!} p^x (1-p)^{4-x}$$

	x=0	x=1	x=2	x=3	x=4
$p(x; 4, p = 1/3)$	16/81	32/81	24/81	8/81	1/81
$p(x; 4, p = 2/3)$	1/81	8/81	24/81	32/81	16/81

The likelihood estimate:

$$\hat{p} = 1/3 \text{ if } 0 \leq x \leq 1$$

$$\hat{p} = 2/3 \text{ if } 3 \leq x \leq 4$$

no maximum if  $x = 2$

## Example

In  $n$  trial  $x$  successes have been obtained. Make the ML estimate of  $p$ .

**Binomial density**

$$\mathcal{L} = -x \ln(p) - (n - x) \ln(1 - p) .$$

**Minimum w.r.t.  $p$ :**

$$\frac{d\mathcal{L}}{dp} = -\frac{x}{p} + \frac{n - x}{1 - p} = 0 \implies \hat{p} = \frac{x}{n} = f$$

**Make the ML estimate of  $p$  when  $x_1$  successes on  $n_1$  trials and  $x_2$  successes on  $n_2$  trials have been obtained.**

**Two binomials with the same  $p$ :**

$$L = p^{x_1} p^{x_2} (1 - p)^{n_1 - x_1} (1 - p)^{n_2 - x_2} .$$

**With logarithms:**

$$\mathcal{L} = -(x_1 + x_2) \ln(p) - (n_1 - x_1 + n_2 - x_2) \ln(1 - p) ,$$

$$\frac{d\mathcal{L}}{dp} = -\frac{x_1 + x_2}{p} + \frac{(n_1 + n_2) - x_1 - x_2}{1 - p} = 0$$

$$\implies \hat{p} = \frac{x_1 + x_2}{n_1 + n_2}$$

# Estimators

- Estimator of  $\theta$

If  $\underline{X}$  is a data sample with dimension  $n$  of a  $m$ -dimensional random variable  $\mathbf{X}$  having  $p(\mathbf{X}; \theta)$  as a pdf, an estimator is a statistics

$$T_n(\underline{X}) \equiv t_n(\underline{X})$$

for which  $T : S \rightarrow \theta$ .

- Consistent estimator of  $\theta$

$$\lim_{n \rightarrow \infty} P \{ |T_n - \theta| < \epsilon \} = 1, \quad \forall \epsilon > 0 .$$

- Correct or unbiased estimator

$$\langle T_n \rangle = \theta, \quad \forall n$$

- The most efficient estimator

$T_n$  is more efficient than  $Q_n$  if

$$\text{Var}[T_n] < \text{Var}[Q_n], \quad \forall \theta \in \Theta .$$

## Theorems on $L(\theta; X)$

The mean value of the **Score Function** is zero:

$$\left\langle \frac{\partial}{\partial \theta} \ln p(\mathbf{X}; \theta) \right\rangle = 0 .$$

The variance of the **Score Function** is the Fisher information:

$$\begin{aligned} \text{Var} \left[ \frac{\partial}{\partial \theta} \ln p(\mathbf{X}; \theta) \right] &= \left\langle \left( \frac{\partial}{\partial \theta} \ln p(\mathbf{X}; \theta) - \left\langle \frac{\partial}{\partial \theta} \ln p(\mathbf{X}; \theta) \right\rangle \right)^2 \right\rangle \\ &= \left\langle \left( \frac{\partial}{\partial \theta} \ln p(\mathbf{X}; \theta) \right)^2 \right\rangle \equiv I(\theta) \end{aligned}$$

These remarkable relations hold:

$$I(\theta) = \left\langle \left( \frac{\partial}{\partial \theta} \ln p(\mathbf{X}; \theta) \right)^2 \right\rangle = - \left\langle \frac{\partial^2}{\partial \theta^2} \ln p(\mathbf{X}; \theta) \right\rangle .$$

$$\left\langle \left( \frac{\partial}{\partial \theta} \ln L \right)^2 \right\rangle = \left\langle \left( \frac{\partial}{\partial \theta} \sum_i \ln p(\mathbf{X}_i; \theta) \right)^2 \right\rangle = n \left\langle \left( \frac{\partial}{\partial \theta} \ln p \right)^2 \right\rangle = nI(\theta) ,$$

The **Cramér Rao theorem**:

If  $T_n$  is an unbiased estimator

$$\text{Var}[T_n] \geq \frac{1}{n \left\langle \left( \frac{\partial}{\partial \theta} \ln p(\mathbf{X}; \theta) \right)^2 \right\rangle} = \frac{1}{nI(\theta)}$$

# Binomial, Poisson, Gauss

$$\ln b(X; p) = \ln n! - \ln(n - X)! - \ln X! + X \ln p + (n - X) \ln(1 - p)$$

$$\ln p(X; \mu) = X \ln \mu - \ln X! - \mu$$

$$\ln g(X; \mu, \sigma) = \ln \left( \frac{1}{\sqrt{2\pi}\sigma} \right) - \frac{1}{2} \left( \frac{X - \mu}{\sigma} \right)^2$$

These are **random functions**.

$$\frac{\partial}{\partial p} \ln b(X; p) = \frac{X}{p} - \frac{n - X}{1 - p} = \frac{X - np}{p(1 - p)}$$

$$\frac{\partial}{\partial \mu} \ln p(X; \mu) = \frac{X}{\mu} - 1 = \frac{X - \mu}{\mu},$$

$$\frac{\partial}{\partial \mu} \ln g(X; \mu, \sigma) = -\frac{X - \mu}{\sigma} \left( -\frac{1}{\sigma} \right) = \frac{X - \mu}{\sigma^2}$$

according to  $\left\langle \frac{\partial}{\partial \theta} \ln p(\mathbf{X}; \theta) \right\rangle = 0$

**Information:**

$$I(p) = \frac{1}{p^2(1 - p)^2} \langle (X - np)^2 \rangle = \frac{np(1 - p)}{p^2(1 - p)^2} = \frac{n}{p(1 - p)},$$

$$I(\mu) = \frac{1}{\mu^2} \langle (X - \mu)^2 \rangle = \frac{\sigma^2}{\mu^2} = \frac{1}{\mu} = \frac{1}{\sigma^2},$$

$$I(\mu) = \frac{1}{\sigma^4} \langle (X - \mu)^2 \rangle = \frac{\sigma^2}{\sigma^4} = \frac{1}{\sigma^2},$$

## Golden results

1. If  $T_n$  is the **best** estimator of  $\tau(\theta)$ , it coincides with the ML estimator (if any)

$$T_n = \tau(\hat{\theta}) .$$

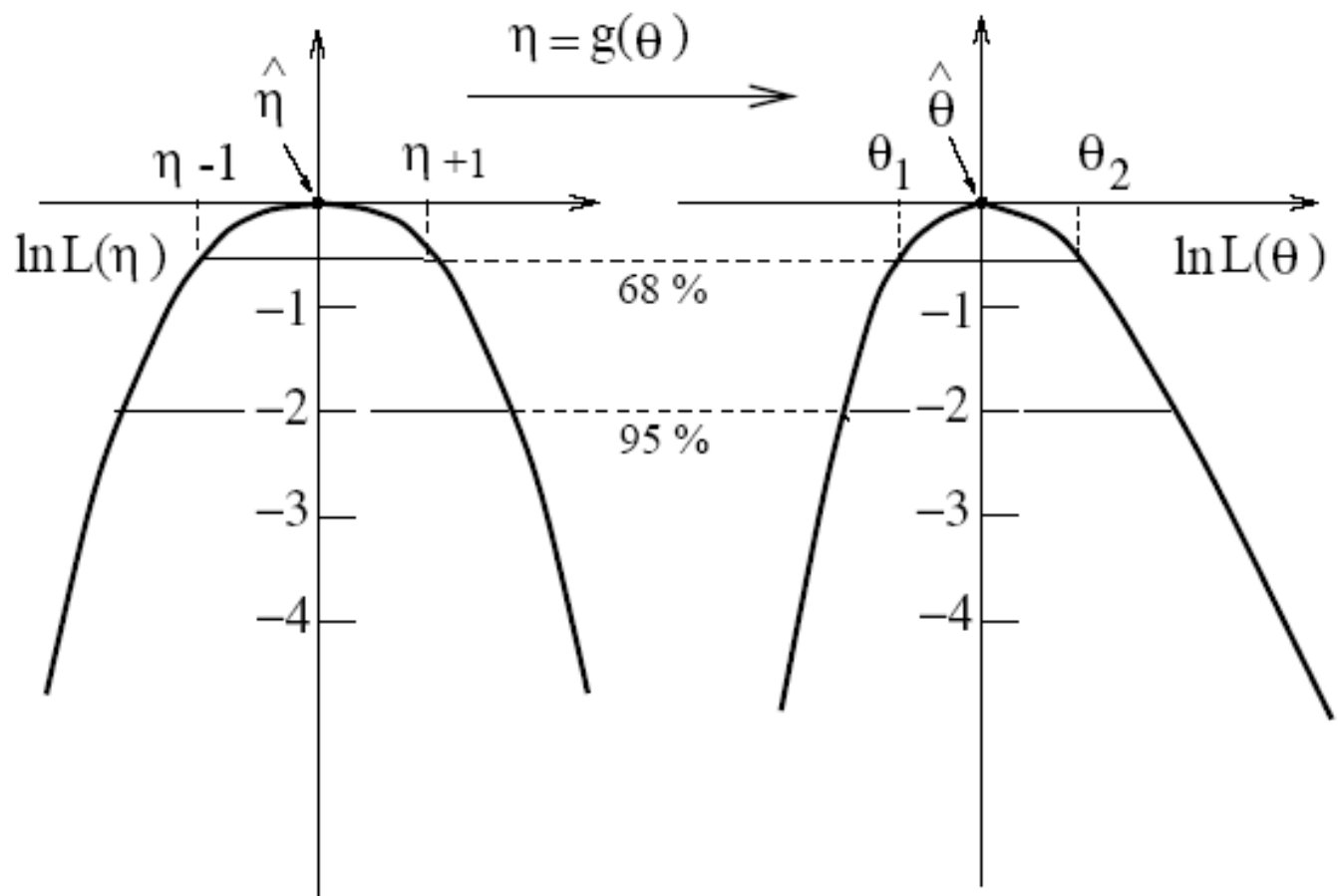
2. the ML estimator is **consistent**
3. under broad conditions, the ML estimators are asymptotically normal. That is  $(\theta - \hat{\theta})$  is **asymptotically normal** with variance

$$\frac{1}{nI(\theta)}$$

4. the **score function**  $\partial \ln L / \partial \theta$  has zero mean,  $nI(\theta)$  variance and is asymptotically normal
5. the variable

$$2[\ln L(\hat{\theta}) - \ln L(\theta)]$$

**tends asymptotically to  $\chi^2(p)$** , where  $p$  is the dimension of  $\theta$





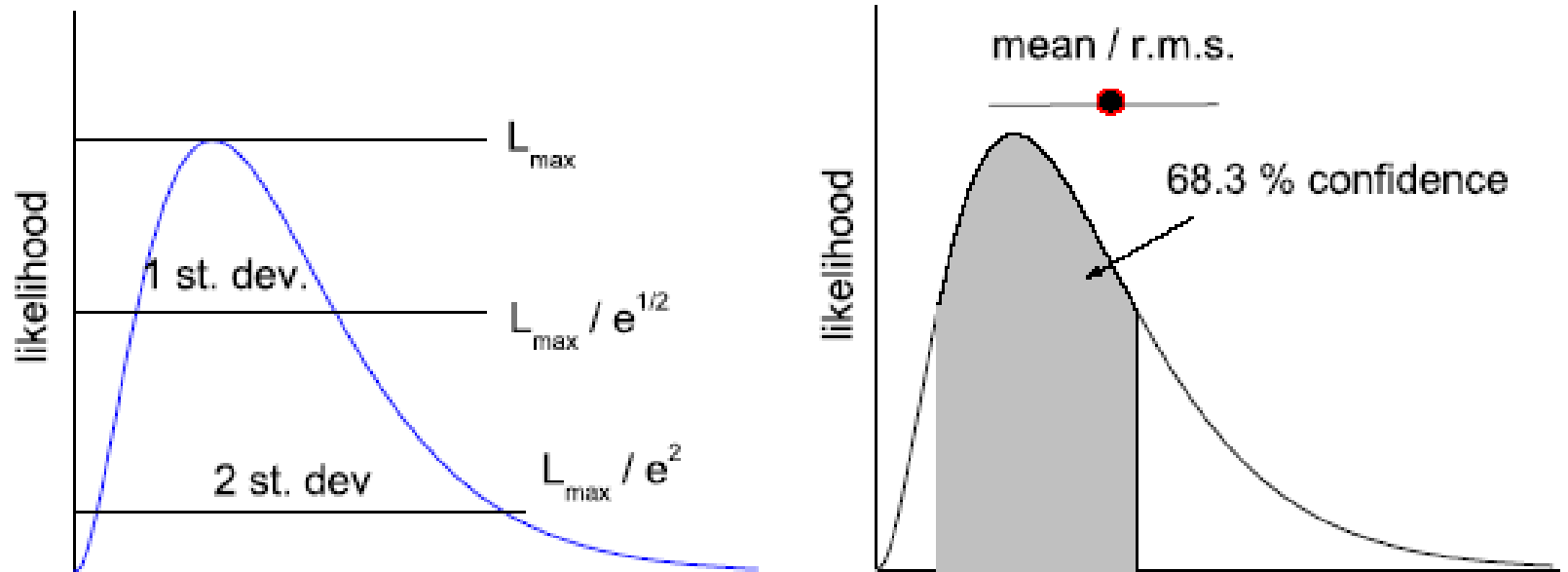
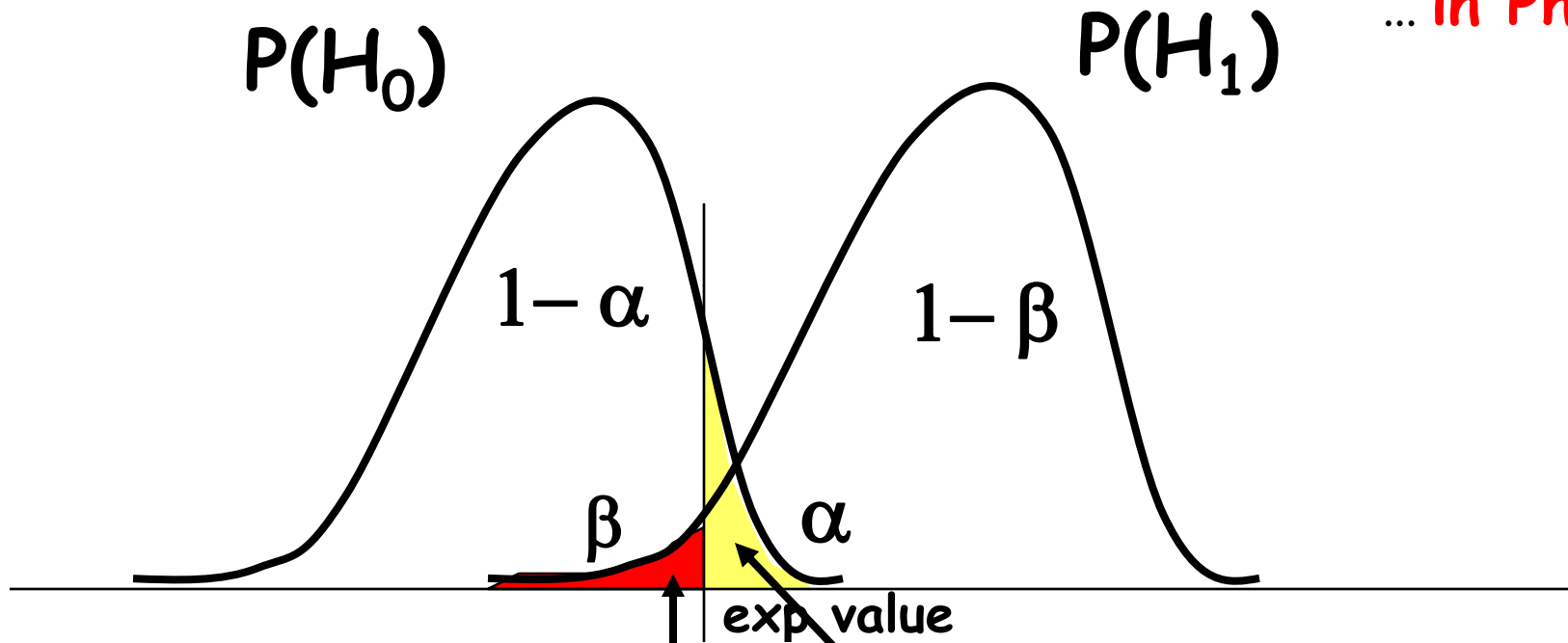


Fig. 18. Likelihood ratio limits (left) and Bayesian limits (right)

# The other branch of Statistics: Hypothesis Testing



true hypothesis	Decision	
	$H_0$	$H_1$
$H_0$ no effect	correct decision $1 - \alpha$ good rejection	type I error $\alpha$ contamination
$H_1$ effect	type II error $\beta$ event loss	correct decision $1 - \beta$ good acceptance

**power** ←

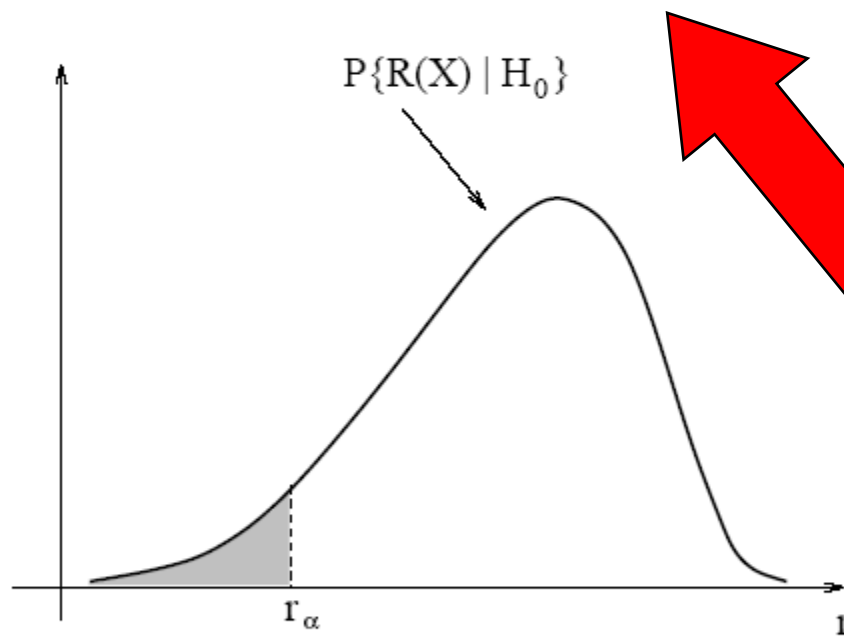
If  $H_1$  is the discovery, the maximum power test maximizes the discovery probability, that is the **good acceptance**

When two **simple** hypotheses are given

$$H_0 : \theta = \theta_0 , \quad H_1 : \theta = \theta_1 .$$

the most powerful test, for  $\alpha$  given, is

reject  $H_0$  if  $\left\{ R(X) = \frac{L(\theta_0; X)}{L(\theta_1; X)} \leq r_\alpha \right\}$  ,



**A Milestone:  
the Neyman-Pearson  
theorem**

**Likelihood Ratio  
Test**

That is:

**the best test statistics is  $R$   
or any random variable  $T : R = \psi(T)$ .**

## A Milestone: the Neyman-Pearson theorem: limitations

- it holds for **simple** hypotheses
- for **composite hypotheses** like

$$H_0 : \theta_1 = a , \quad \theta_2 = b$$

$$H_1 : \theta_1 \neq a , \quad \theta_2 \neq b$$

or

$$H_0 : \theta = a ,$$

$$H_1 : \theta \geq a$$

the NP ratio

$$R = \frac{L(\theta|H_0)}{\max_{[\theta \in \Theta_1]} L(\theta|H_1)}$$

is optimal, **but only asymptotically**

(theory is complicated!!)

- if  $H_1$  has  $r$  free parameters more than  $H_0$ , **then**

$$-2 \ln R \sim \chi^2(r)$$

The powerful LR test is used usually on histograms with  $N_c$  channels:

$$Q = \frac{\prod_{i=1}^{N_c} (s_i + b_i)^{n_i} e^{-(s_i+b_i)} / n_i!}{\prod_{i=1}^{N_c} b_i^{n_i} e^{-b_i} / n_i!}, \quad S_{\text{tot}} = \sum_{i=1}^{N_c} s_i .$$

where  $n_i$  is the number of observed events  $s_i$  and  $b_i$  are the expected signal and background events,  $b_i$  and  $s_i$  are obtained via MC

One obtains easily:

$$\ln Q = -S_{\text{tot}} + \sum_{i=1}^{N_c} n_i \ln \left( 1 + \frac{s_i}{b_i} \right)$$

Usually one compare the quantity

$$-2 \ln Q \sim \chi^2 \quad (\text{asymptotically})$$

obtained experimentally ( $n_i =$  contents of the experimental bins) with the background ( $n_i = b_i$ ) and the signal plus background ( $n_i = s_i + b_i$ ) hypotheses. In this way, for an established signal to noise ratio, one performs the most powerful test, maximizing the signal discovery probability, *taking into account not only the global number of the events, but also the shape of the distributions (see LEP data).*



$n_i$  from MC samples!

## Steps of the likelihood ratio test

$$\ln Q = -S_{\text{tot}} + \sum_{i=1}^{N_c} n_i \ln \left( 1 + \frac{s_i}{b_i} \right)$$

Determine the ratio  $s_i/b_i$  for each bin  
(model + MC simulation)

$n_i$

# The Higgs at LEP in 2000

On 3 November 2000 in a seminar at CERN the LEP Higgs working group presented preliminary results of an analysis indicating a possible  $2.9\sigma$  observation of a 115 GeV Higgs boson [1]. Based on this analysis the four LEP collaborations requested the continuation of LEP to collect more data at  $\sqrt{s} = 208$  GeV. However, the arguments presented by the LEP collaborations did not convince the LEP management and in retrospect, it turned out that the LEP accelerator turn-off date of 2 November 2000 ended its eleven years of forefront research.

enough. However, the statistical arguments presented by the LEP Higgs working group were not based on these distributions, but rather on a sophisticated, though beautiful statistical analysis of the data. Two years after the event, when the last analysis of the LEP data indicated that the significance of a Higgs observation in the vicinity of 115 GeV went down to less than  $2\sigma$  [2], it becomes apparent that the LEP Standard Model (SM) Higgs heritage will in fact be a lower bound on the mass of the Higgs boson. However, the LEP Higgs working group has taught us powerful and instructive lessons of statistical methods for deriving limits and confidence levels in the presence of mass dependent backgrounds from various channels and experiments. These lessons will remain with us long after the lower bound becomes outdated.



## Search for the Standard Model Higgs boson at LEP

ALEPH Collaboration<sup>1</sup>  
DELPHI Collaboration<sup>2</sup>  
L3 Collaboration<sup>3</sup>  
OPAL Collaboration<sup>4</sup>

The LEP Working Group for Higgs Boson Searches<sup>5</sup>

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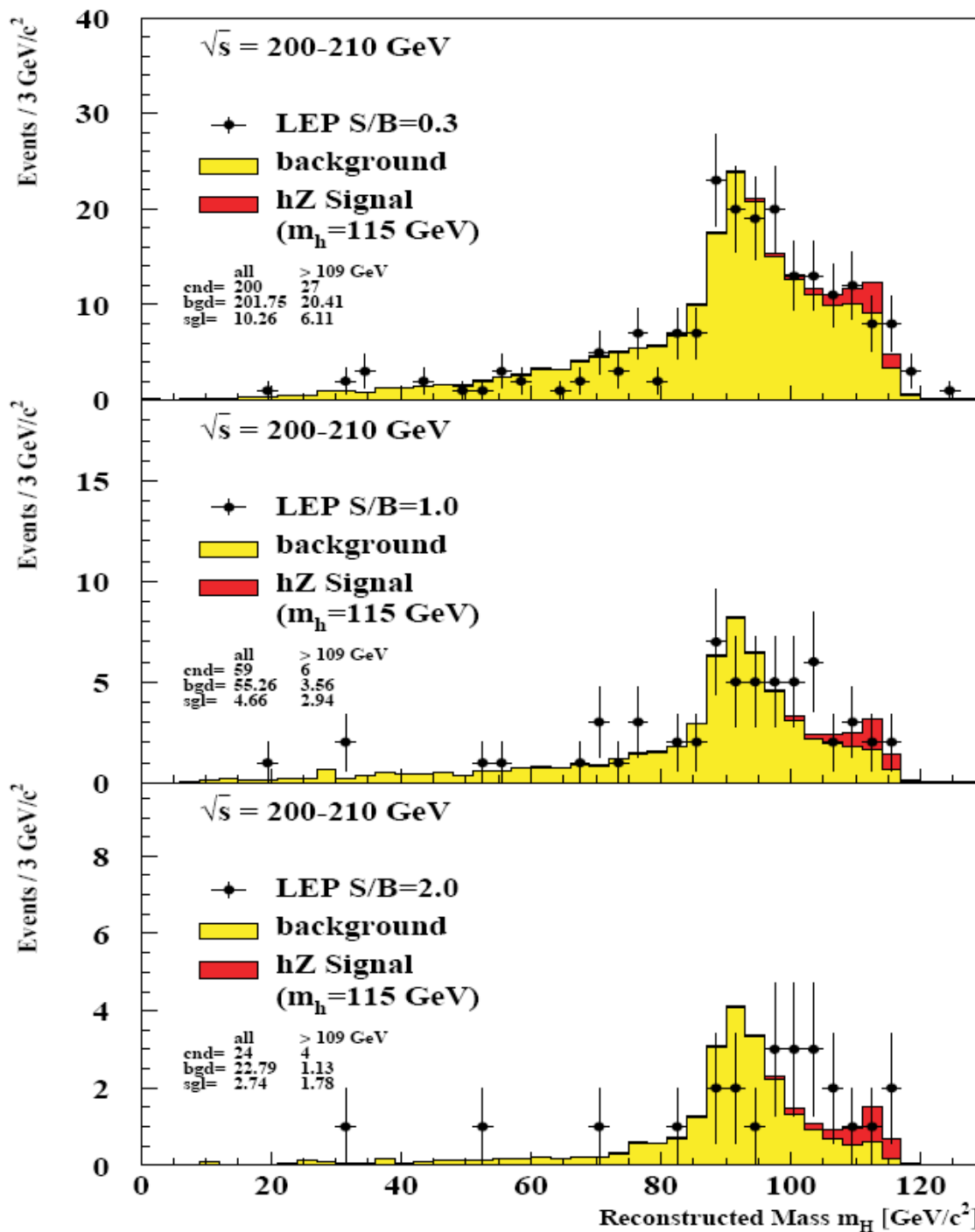
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### Abstract

The four LEP Collaborations, ALEPH, DELPHI, L3 and OPAL, have collected a total of  $2461 \text{ pb}^{-1}$  of  $e^+e^-$  collision data at centre-of-mass energies between 189 and 209 GeV. The data are used to search for the Standard Model Higgs boson. The search results of the four Collaborations are combined and examined in a likelihood test for their consistency with two hypotheses: the background hypothesis and the signal plus background hypothesis. The corresponding confidences have been computed as functions of the hypothetical Higgs boson mass. A lower bound of  $114.4 \text{ GeV}/c^2$  is established, at the 95% confidence level, on the mass of the Standard Model Higgs boson. The LEP data are also used to set upper bounds on the HZZ coupling for various assumptions concerning the decay of the Higgs boson.

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# LEP real data



Three selections of the reconstructed Higgs mass of 115 GeV to obtain 0.5/1/2/ times as many expected signal as Background above 109 GeV

	Expt	$E_{cm}$	Decay channel	$m_{rec}$ (GeV)	$\ln(1 + s/b)$ at 115 GeV
1	ALEPH	206.6	4-jet	114.1	1.76
2	ALEPH	206.6	4-jet	114.4	1.44
3	ALEPH	206.4	4-jet	109.9	0.59
4	L3	206.4	E-miss	115.0	0.53
5	ALEPH	205.1	Lept	117.3	0.49
6	ALEPH	206.5	Taus	115.2	0.45
7	OPAL	206.4	4-jet	111.2	0.43
8	ALEPH	206.4	4-jet	114.4	0.41
9	L3	206.4	4-jet	108.3	0.30
10	DELPHI	206.6	4-jet	110.7	0.28
11	ALEPH	207.4	4-jet	102.8	0.27
12	DELPHI	206.6	4-jet	97.4	0.23
13	OPAL	201.5	E-miss	108.2	0.22
14	L3	206.4	E-miss	110.1	0.21
15	ALEPH	206.5	4-jet	114.2	0.19
16	DELPHI	206.6	4-jet	108.2	0.19
17	L3	206.6	4-jet	109.6	0.18

Table 1: Properties of the candidates with the highest weight at  $m_H = 115$  GeV. Table is taken from [2].

## Steps of the likelihood ratio test

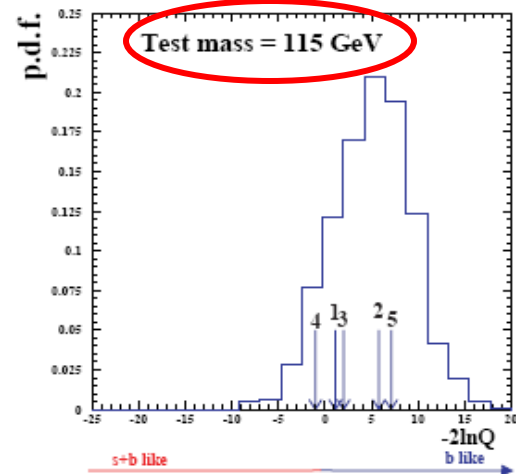
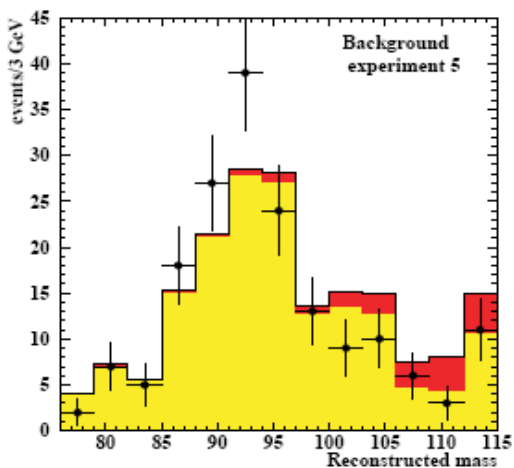
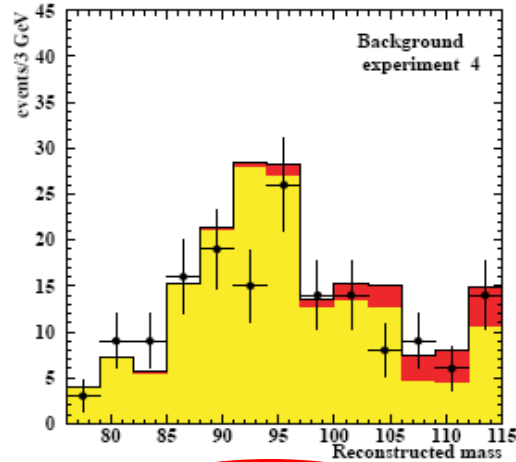
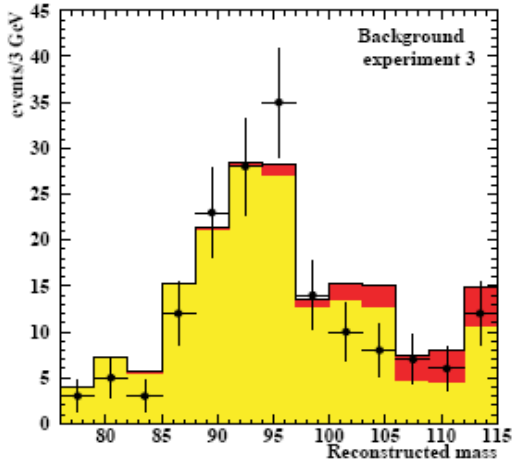
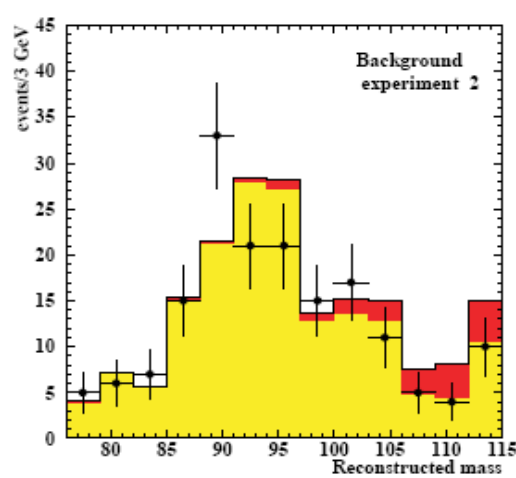
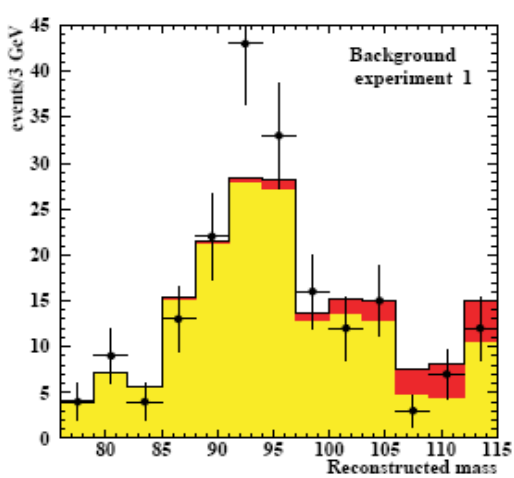
$$\ln Q = -S_{\text{tot}} + \sum_{i=1}^{N_c} n_i \ln \left( 1 + \frac{s_i}{b_i} \right)$$

Determine the ratio  $s_i/b_i$  for each bin  
(model + MC simulation)

# MC toy model

$s_i$  red  
 $b_i$  yellow

Crosses: MC data,  
Background only



$\ln(1+s/b)$  plot

1,2,3,4,5,...n

# MC toy model

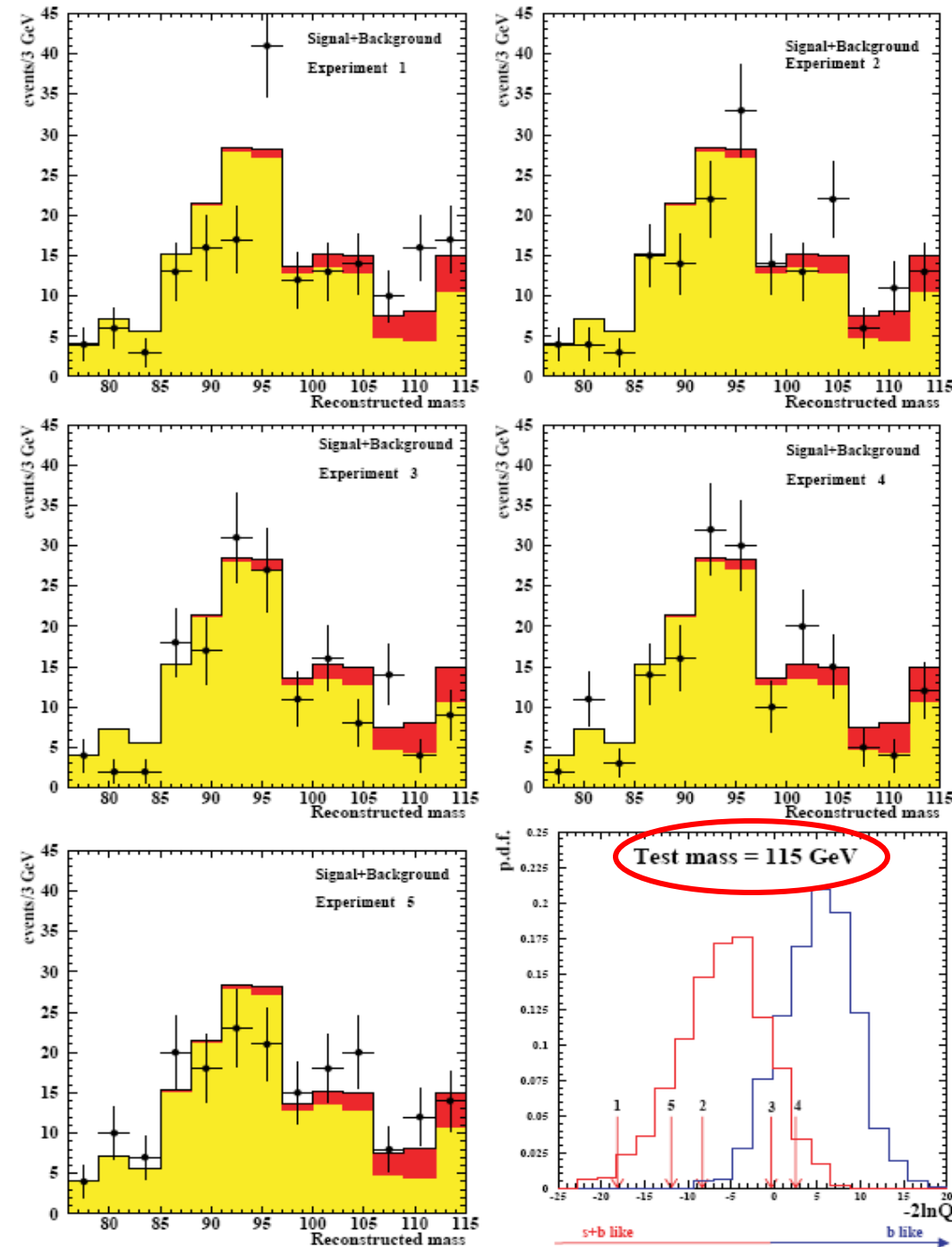
$s_i$  red  
 $b_i$  yellow

Crosses: MC data,  
Background + Signal  
 $m_H = 115 \text{ GeV}$

$\ln(1+s/b)$  plot

1,2,3,4,5,...n

(in blue is the previous one  
with background only)



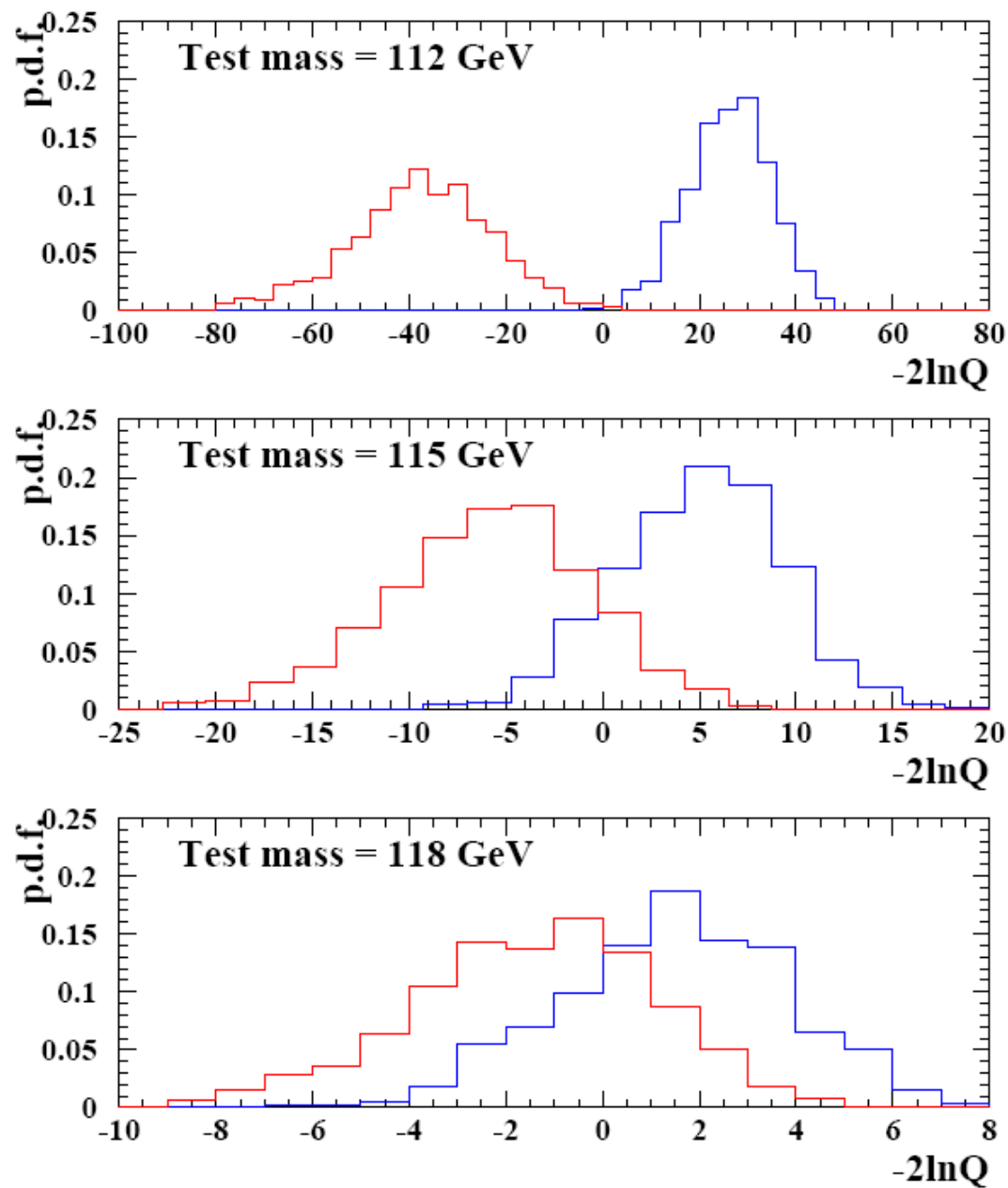


Figure 6: The separation between the Signal and the Background for various Higgs masses is shown by their likelihood p.d.f.'s.

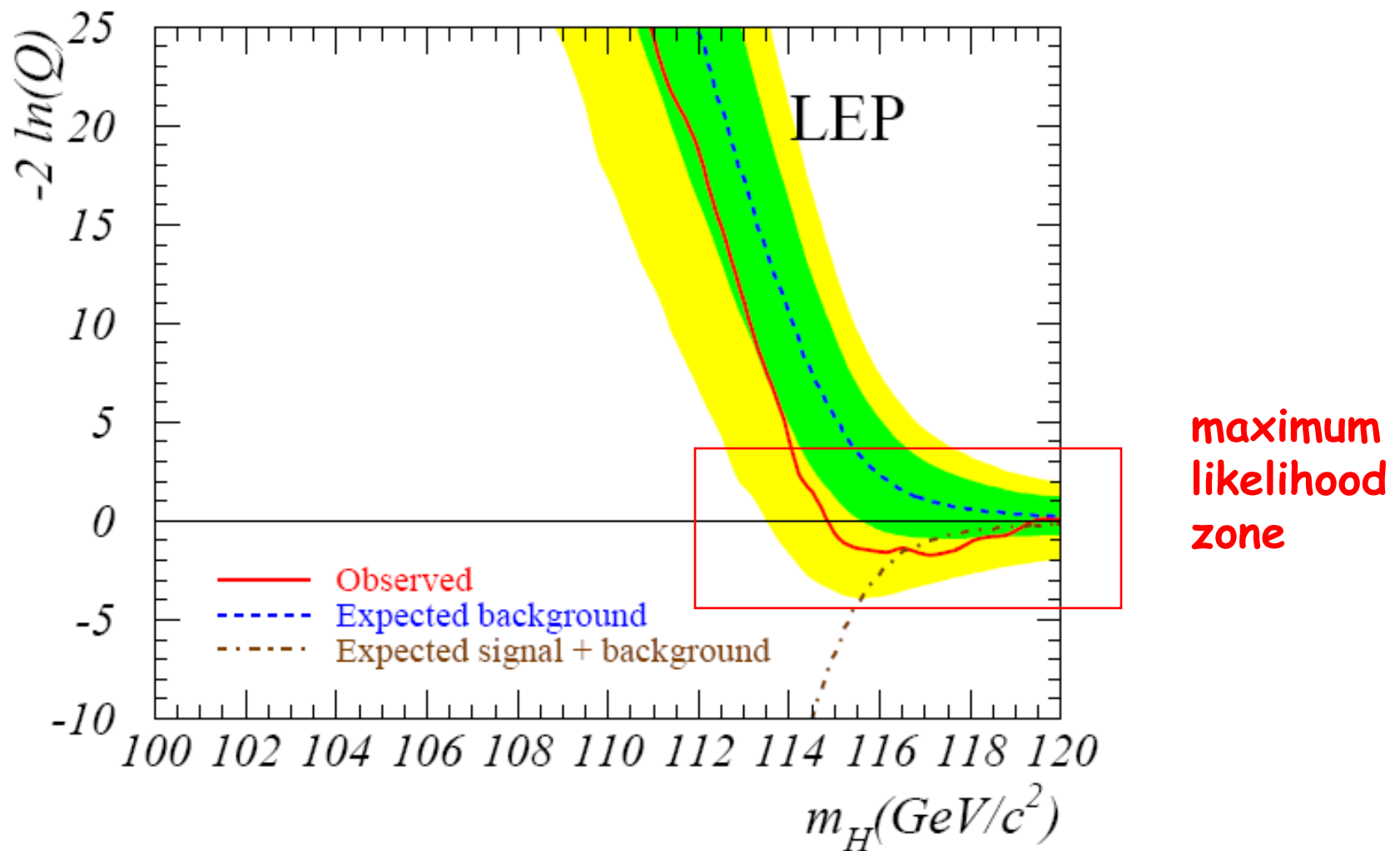


Figure 8: Observed and expected behavior of the likelihood  $-2\ln Q$  as a function of the test-mass  $m_H$  for combined LEP experiments. The solid/red line represents the observation; the dashed/dash-dotted lines show the median background/signal+background expectations. The dark/green and light/yellow shaded bands represent the  $1$  and  $2\sigma$  probability bands about the median background expectation [2].



3 $\sigma$  effect!

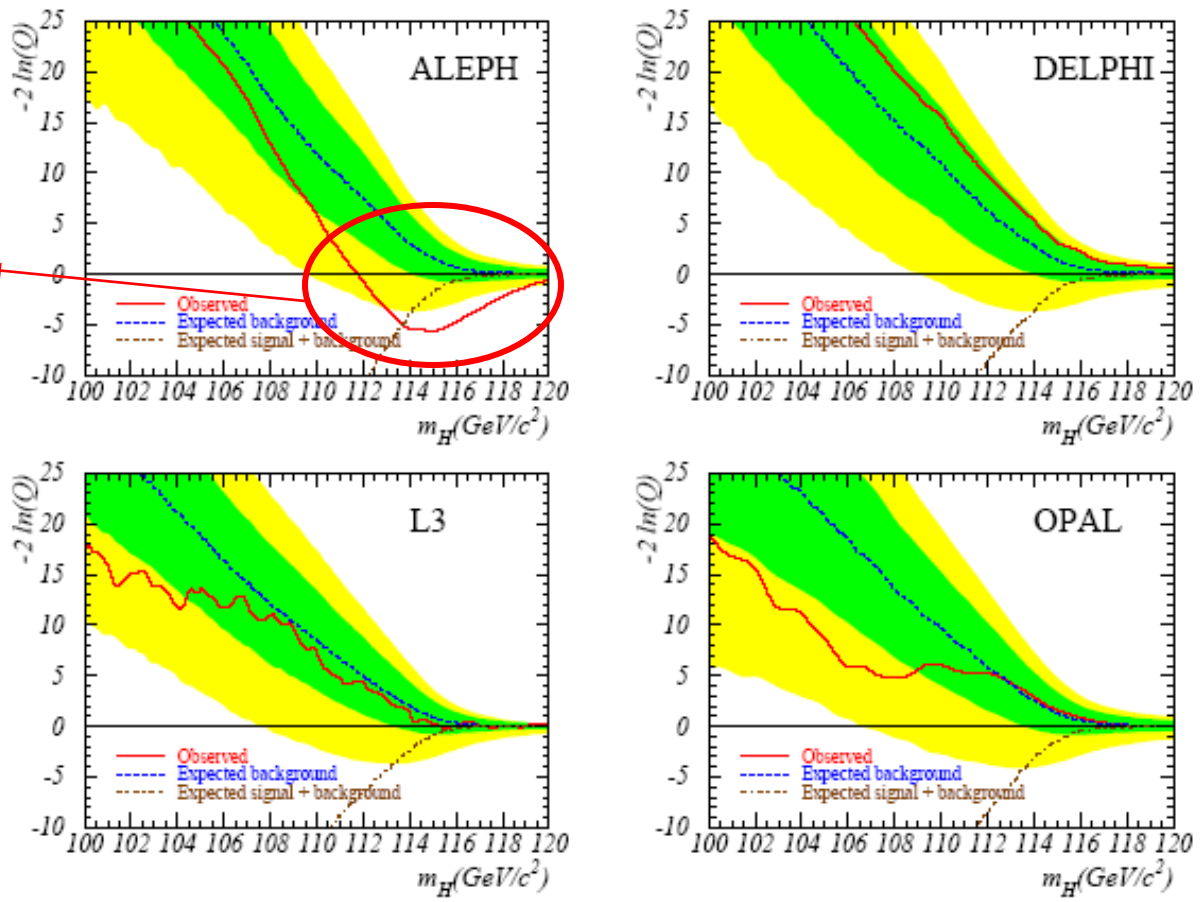
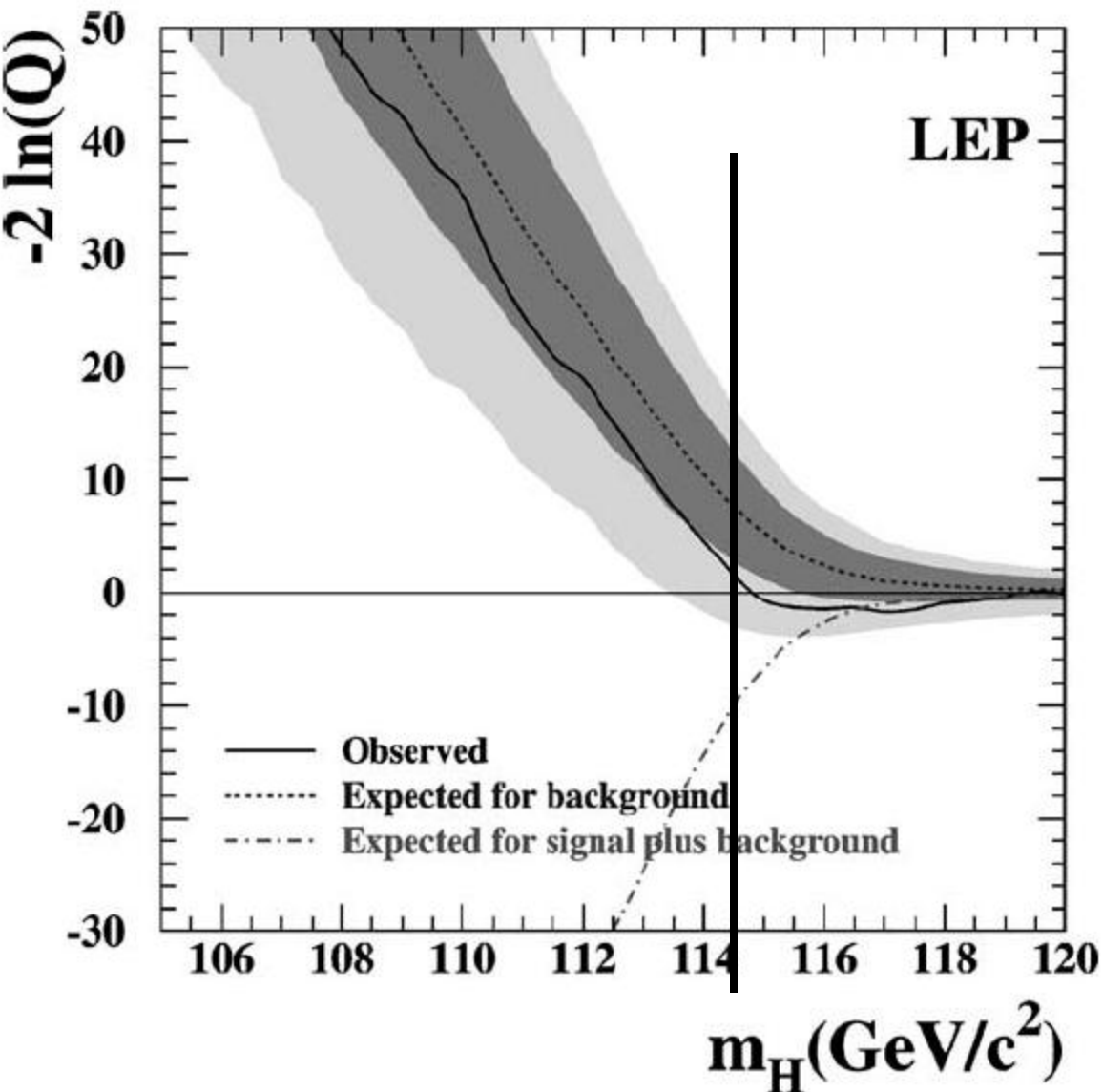


Figure 9: Observed and expected behavior of the likelihood  $-2 \ln Q$  as a function of the test-mass  $m_H$  for the various experiments. The solid/red line represents the observation; the dashed/dash-dotted lines show the median background/signal+background expectations. The dark/green and light/yellow shaded bands represent the 1 and 2  $\sigma$  probability bands about the median background expectation [2].

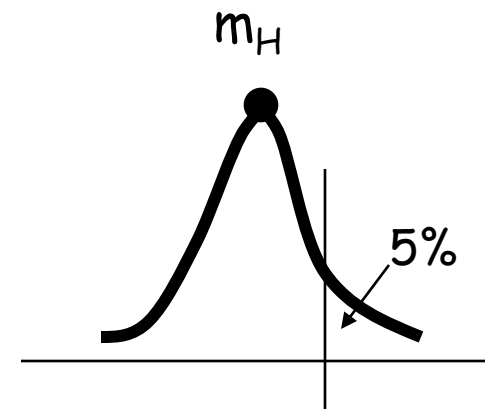
# Conclusions

The broad minimum of the combined LEP likelihood from  $m_H \sim 115 - 118$  GeV which crosses the expectation for  $s+b$  around  $m_H \sim 116$  GeV can be interpreted as a preference for a Standard Model Higgs boson at this mass range, however, at less than the  $2\sigma$  level. When the LEP Higgs working group presented these results for the first time the significance was  $2.9\sigma$  [1], and this relatively high significance generated a storm which unfortunately turned out to be in a tea cup...

The ALEPH observed likelihood has a  $3\sigma$  signal-like behavior around  $m_H \sim 114$  GeV, which led the collaboration to claim a possible observation of a SM Higgs boson [3]. This behavior originated mainly from the 4-jet channel and its significance is reduced when all experiments are combined. No other experiment or channel indicated a signal-like behavior.



**ALEPH  
DELPHI  
L3  
OPAL  
2003**



**$m_H \geq 114.4 \text{ GeV}/c^2$  CL=95%**

1. the Bayesian **refuses** the concept of an ideal ensemble of repeated, identical experiments;
2. the probabilities of the errors of I and II kind are then replaced by the **probabilities of the hypotheses**

	test statistics	parameters
Bayesian	certain	random
frequentist	random	certain

A **BIG** problem:

$$P(H_0|\text{data}) = \frac{P(\text{data}|H_0)P(H_0)}{\underbrace{\sum_i P(\text{data}|H_i) P(H_i)}_{\text{unknown!}}}$$

A solution: **the Relative belief updating ratio:**

$$R = \frac{P(H_0|\text{data})}{P(H_1|\text{data})} = \frac{P(\text{data}|H_0)P(H_0)}{P(\text{data}|H_1)P(H_1)}$$

- the  $R$  values **help** the model choice, but the choice is subjective!!
- the  $P(H_0)$ ,  $P(H_1)$  priors are necessary
- $\alpha$ ,  $\beta$ ,  $1 - \beta$  are not calculated

# Bayesian Hypothesis test

# Gravitational Bursts

(P.Astone, G.Pizzella,workshop (2000))

$n_c$  counts are observed in a time  $T$

$r_b$  and  $r_s$  are the background and signal frequencies:

$$n_s = r_s T \text{ unknown} , \quad n_b = r_b T \text{ measured}$$

Relative belief updating ratio

with  $P(H_0) = P(H_1)$ :

$$R(r_s; n_c, r_b, T) = \frac{e^{-(r_s+r_b)T} [(r_s + r_b)t]^{n_c}}{e^{-r_b T} [r_b T]^{n_c}} = e^{-r_s T} \left(1 + \frac{r_s}{r_b}\right)^{n_c}$$

If  $n_c = 0$

$$R = e^{-r_s T}$$

depends on the signal frequency only.

**Arbitrary Standard Sensitivity Bound:**

$$R = e^{-r_s T} = 0.05 \longrightarrow r_s = 2.99 \approx 3$$

**Rule: this is the sensitivity of the experiment**

# Gravitational bursts

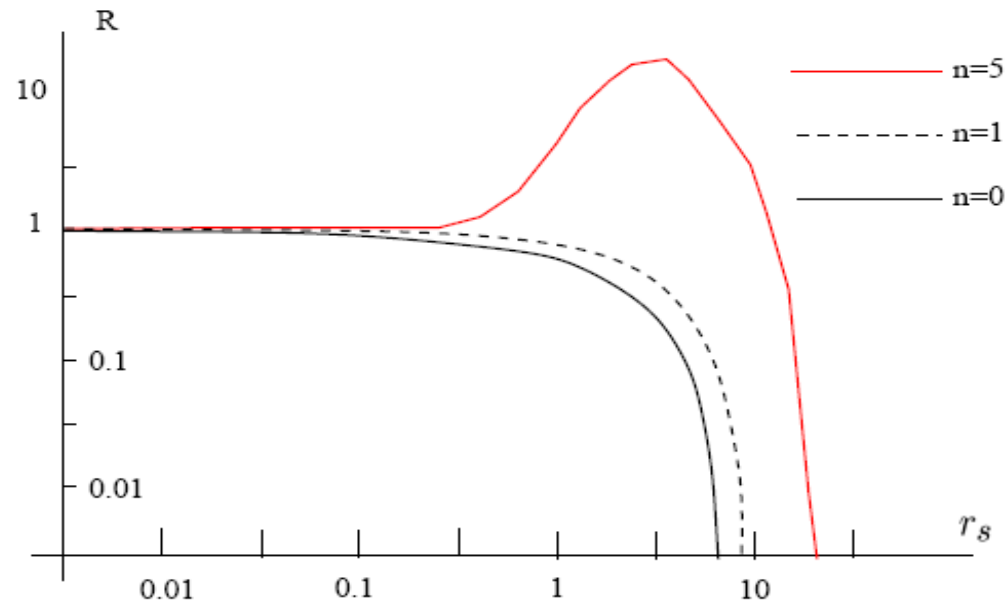


Figure 1: ratio  $R$  for the poisson intensity parameter  $r$  in units of events per month for an expected background rate  $r_b = 1$  event/month and for  $n = 0, 1, 5$  observed events

$$e^{-r_s T} \left(1 + \frac{r_s}{r_b}\right)^{n_c}, \quad r_b = 1$$

## Bayesian Conclusions:

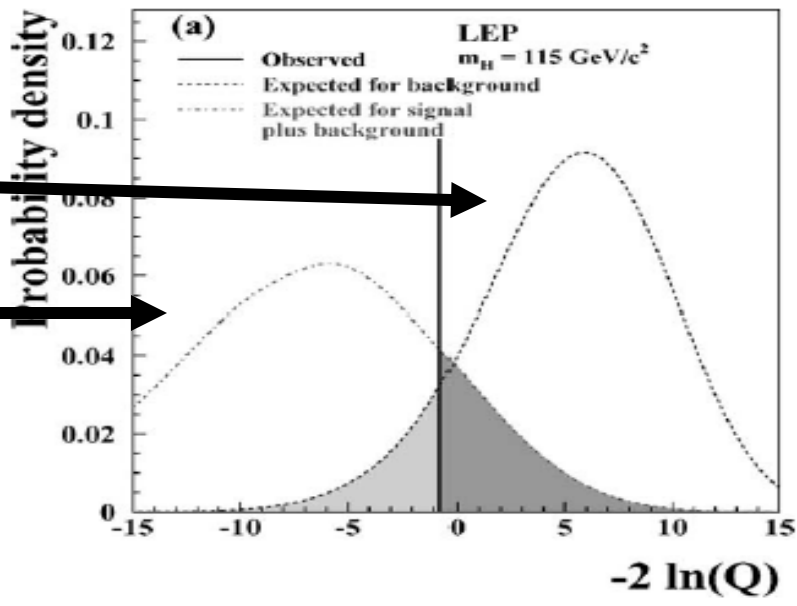
- If  $r_s < 0.1$  the data are not relevant;
- $r_s > 20$  is excluded by the experiment;
- if  $n=5$  the most probable hypothesis is  $r_s = 4$

# Conclusions

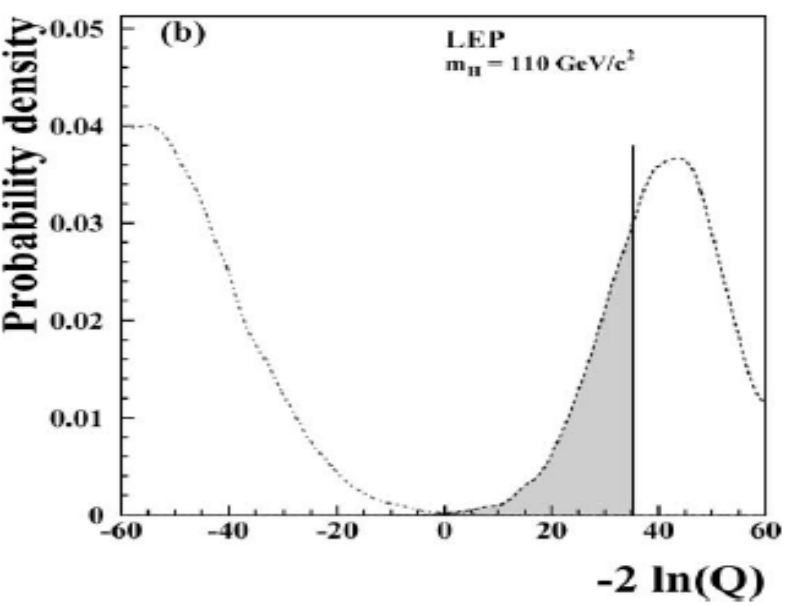
- The maximum likelihood (ML) is the best estimator in the case of parametric statistics problems
- The likelihood ratio is the maximum power test, that maximize the discovery potential
- The likelihood ratio permits to match together different experiments and to realize the Neyman frequentist scheme

**MC samples**

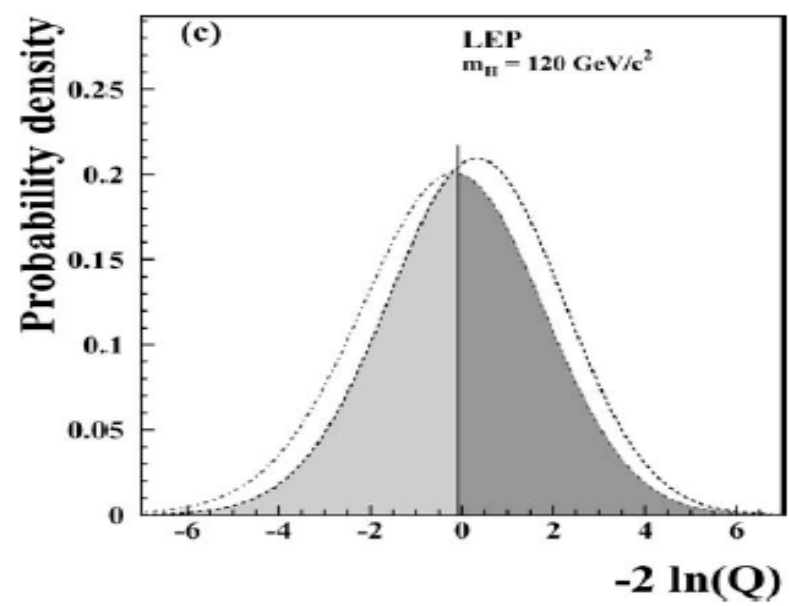
background  
signal



With a mass of 116 GeV  
 10% of the background  
 only experiments give  
 the observed signal



With a Higgs mass of 110 GeV the data are  
 consistent with the background only hypothesis



With a Higgs  
 mass of  
 120 GeV the  
 data are not  
 able to  
 discriminate  
 between the  
 hypotheses



From the  $n$  values  $x_i$  of a Gaussian variable, find the ML estimate of mean and variance

**Likelihood function:**

$$L(\mu, \sigma) = \frac{1}{(\sqrt{2\pi} \sigma)^n} e^{-\frac{1}{2\sigma^2} \sum_i (x_i - \mu)^2} .$$

**The log-likelihood:**

$$\mathcal{L}(\mu, \sigma) = +\frac{n}{2} \ln(2\pi\sigma^2) + \frac{1}{2\sigma^2} \sum_{i=1}^n (x_i - \mu)^2 ,$$

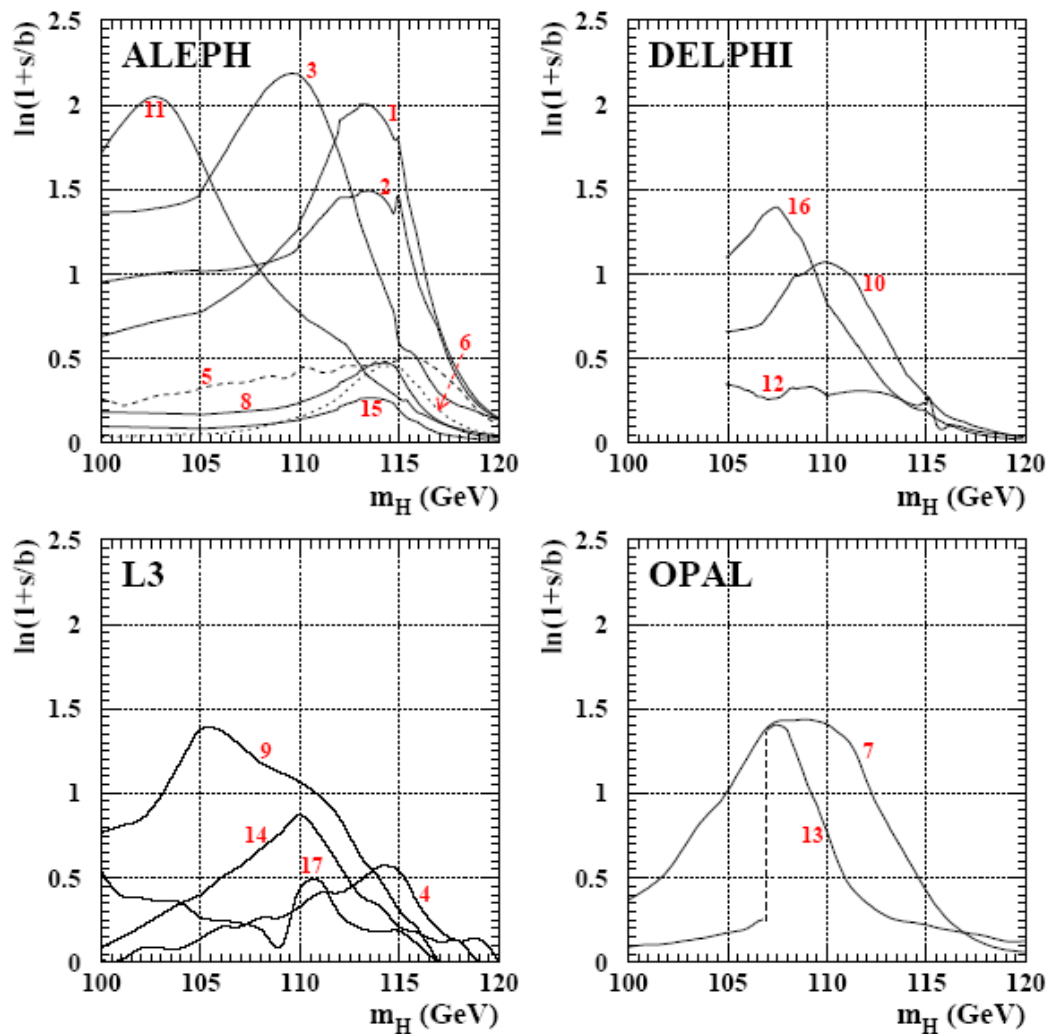
**Put the derivative =0:**

$$\frac{\partial \mathcal{L}}{\partial \mu} = \frac{1}{\sigma^2} \sum_{i=1}^n (x_i - \mu) = 0$$

$$\implies \hat{\mu} = \sum_{i=1}^n \frac{x_i}{n} \equiv m$$

$$\frac{\partial \mathcal{L}}{\partial \sigma^2} = -\frac{n}{2\sigma^2} + \frac{1}{2\sigma^4} \sum_{i=1}^n (x_i - \mu)^2 = 0$$

$$\implies \hat{\sigma}^2 = \sum_{i=1}^n \frac{(x_i - m)^2}{n}$$



LEP real data

Figure 3: Evolution of the event weight  $\ln(1 + s/b)$  with test-mass  $m_H$  for the events with the largest weight at  $m_H = 115$  GeV. The labels correspond to the candidate numbers in the first column of Table 1. The sudden increase in the weight of the OPAL missing-energy candidate labeled “13” at  $m_H = 107$  GeV is due to the switching from the low-mass to high-mass optimization of the search at that mass. A similar increase is observed in the case of the L3 four-jet candidate labeled “17” which is due to a test-mass dependent attribution of the jet-pairs to the Z and Higgs bosons. The Figure is taken from [2].

# Signal over Background in Physics

How to count

Some case studies

# The case of Pentaquark

The **pentaquark** is a baryon with **five** valence quarks.  
The clearest signature is that of a

$$u u d d \bar{s} , \quad S = +1$$

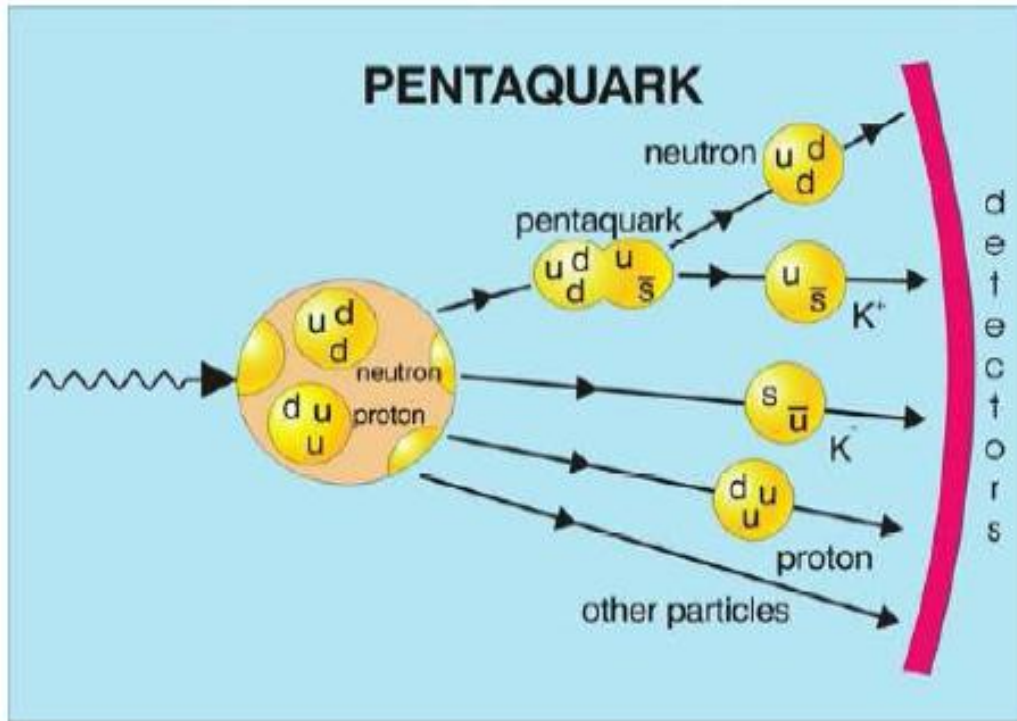
pentaquark, the **unique** baryon with positive strangeness.

The  $\bar{s}$  antiquark cannot annihilate with the  $u$  or  $d$  quark by the strong interaction.

Some models predict a mass around 1.5 GeV and a very small width ( $\simeq 0.015$  GeV)

The recent pentaquark saga began at 2002 PANIC conference when **Nakano** measured the following reaction on a Carbon nucleus

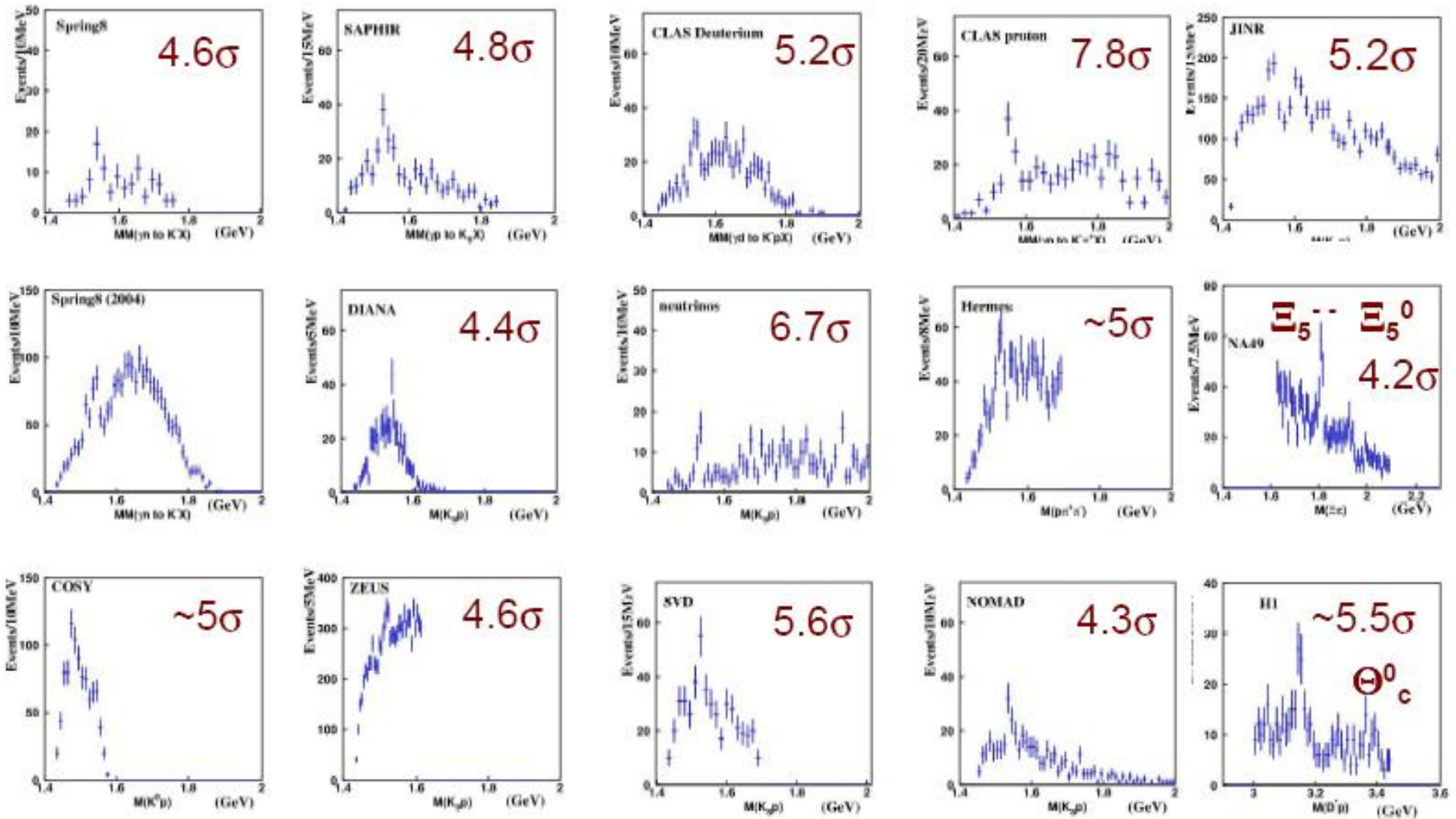
$$\gamma n \rightarrow \Theta^+ K^- \rightarrow K^+ K^- n$$



**Before 2003** .... searches for flavor exotic baryons showed no evidence for such states.

1997: Diakonov, Petrov and Polykov use a chiral soliton model to predict a decuplet of pentaquark baryons. The lightest has  $S=+1$  and a mass of **1530 MeV** and expected to be narrow. Zeit. Phys. A359, 305 (1997).

# .. From the Curtis Meyer review (Miami 2004)



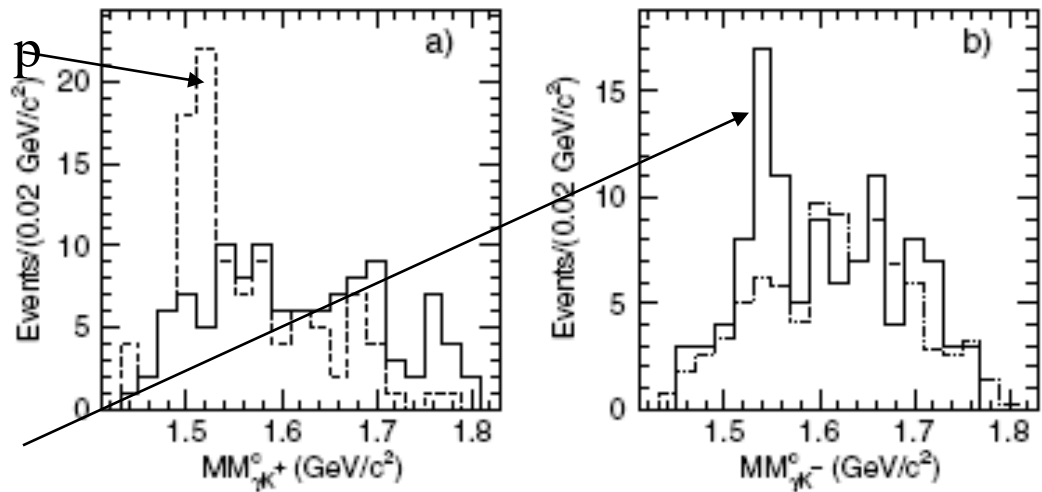
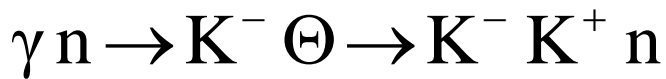
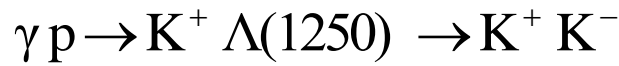


FIG. 3. (a) The  $MM_{\gamma K^+}^c$  spectrum [Eq. (2)] for  $K^+K^-$  productions for the signal sample (solid histogram) and for events from the SC with a proton hit in the SSD (dashed histogram). (b) The  $MM_{\gamma K^-}^c$  spectrum for the signal sample (solid histogram) and for events from the  $LH_2$  (dotted histogram) normalized by a fit in the region above  $1.59 \text{ GeV}/c^2$ .

## The first result

PRL 91(2003)012002

$$\left( \sum_{in} E_{in} - \sum_{fin} E_{fin} \right)^2 - \left( \sum_{in} \vec{p}_{in} - \sum_{fin} \vec{p}_{fin} \right)^2$$

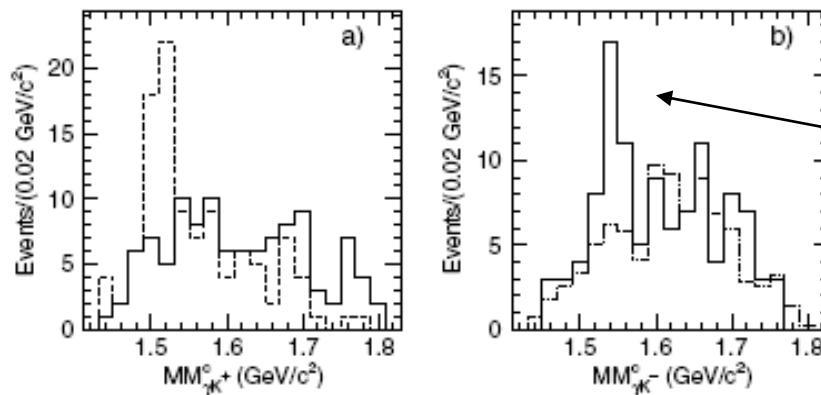
The neutron presence was detected by the  $MM_{\gamma K^+ K^-}$  **missing mass**

The  $\gamma p \rightarrow K^+ K^- p$  reaction was eliminated by direct proton detection.

The neutron was reconstructed from the missing momentum and energy of  $K^+$  and  $K^-$ .

The background was measured from a  $LH_2$  target.





4.6 sigma!

Is it convincing???

FIG. 3. (a) The  $MM_{\gamma K^+}^c$  spectrum [Eq. (2)] for  $K^+K^-$  productions for the signal sample (solid histogram) and for events from the SC with a proton hit in the SSD (dashed histogram). (b) The  $MM_{\gamma K^-}^c$  spectrum for the signal sample (solid histogram) and for events from the  $LH_2$  (dotted histogram) normalized by a fit in the region above  $1.59 \text{ GeV}/c^2$ .

012002-3

The background level in the peak region is estimated to be  $17.0 \pm 2.2 \pm 1.8$ , where the first uncertainty is the error in the fitting in the region above  $1.59 \text{ GeV}/c^2$  and the second is a statistical uncertainty in the peak region. The combined uncertainty of the background level is  $\pm 2.8$ . The estimated number of the events above the background level is  $19.0 \pm 2.8$ , which corresponds to a Gaussian significance of  $4.6_{-1.0}^{+1.2} \sigma$  ( $19.0/\sqrt{17.0} = 4.6$ ).



# The signal over background

There are two way to count in Physics experiments

- **Poissonian counting**

The samples are collected in runs of fixed time. The background is evaluated with MC methods, with *blank* runs, with *sideband counting*, etc

- **Binomial counting** The runs collect a *total number*  $N_t$  of events and  $N_y$  of them pass the selection cuts (tagging) or the triggers.

Signal and background have different probabilities to pass these cuts

To avoid mistakes the notation is very important

- $N$  counts considered as a **random variable**
- $n$  counts considered as the result of an experiment
- $\mu$  expected value of the counting distribution (Binomial or Poissonian).

## Poissonian counting Fundamental theorem

Let's count a Poisson variable  $N$  with mean  $\lambda$  with a detector of efficiency  $\varepsilon$ . The registered number of counts  $n$  follows the distribution

$$P(n|N)P(N) = \frac{e^{-\lambda}\lambda^N}{N!} \frac{N!}{n!(N-n)!} \varepsilon^n (1-\varepsilon)^{N-n}$$

By using the new variables

$$e^{-\lambda} = e^{-\lambda\varepsilon} e^{-\lambda(1-\varepsilon)}$$

$$m = N - n$$

$$\lambda^N = \lambda^{N-n} \lambda^n \equiv \lambda^m \lambda^n$$

one has

$$P(n|N)P(N) = \frac{e^{-\lambda\varepsilon} (\lambda\varepsilon)^n}{n!} \frac{e^{-\lambda(1-\varepsilon)} \lambda^m (1-\varepsilon)^m}{m!}$$

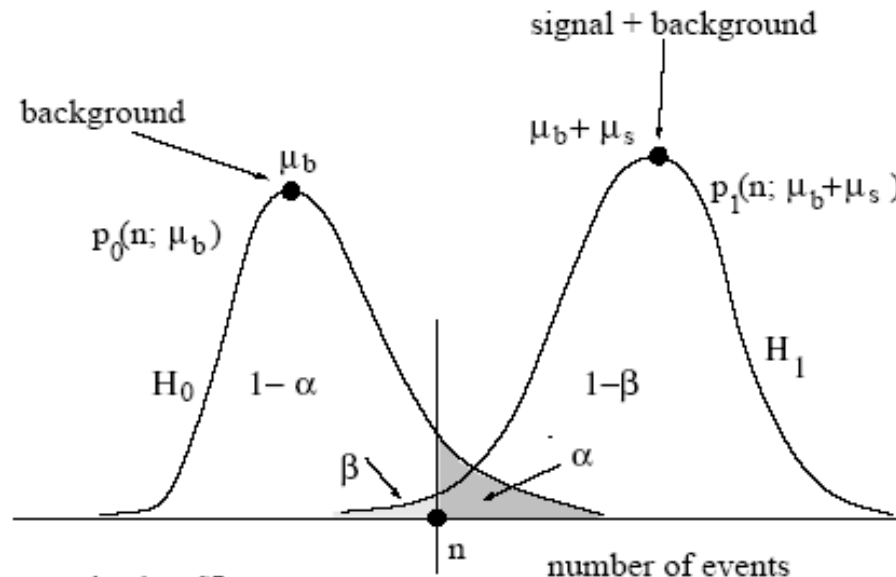
The number of counts  $n$  is still an independent Poisson variable with mean  $\lambda\varepsilon$ !

(also the lost counts  $m$  with mean  $\lambda(1-\varepsilon)$ )

$\{N = n\}$  events are observed, that are supposed to come from a distribution with expected value  $\mu_b + \mu_s$ , where the expected amount of signal  $\mu_s$  is unknown.

$$p(n, \mu_b) = \frac{\mu_b^n e^{-\mu_b}}{n!} \quad (1)$$

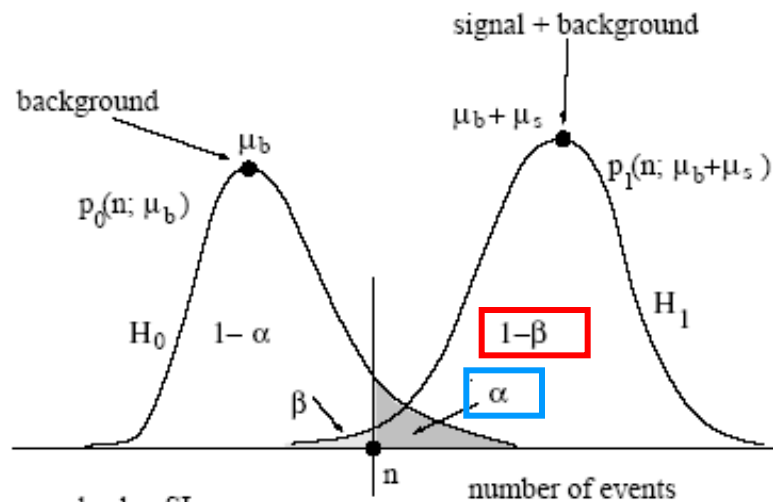
$$p(n, \mu_b + \mu_s) = \frac{(\mu_b + \mu_s)^n e^{-\mu_b + \mu_s}}{n!} \quad (2)$$



$\alpha$  = backg. SL

$\beta$  = signal 1- CL

$1 - \beta$  = signal CL or power of the test



- $\alpha \leq 2.8 \cdot 10^{-7}$   $5\sigma$  discovery
- $\alpha \leq 1.3 \cdot 10^{-3}$   $3\sigma$  strong evidence
- $\alpha \leq 2.3 \cdot 10^{-2}$   $2\sigma$  weak evidence

$\alpha$  = backg. SL  
 $\beta$  = signal 1- CL  
 $1-\beta$  =signal CL or power of the test

true Hypothesis	Decision	
	$H_0$	$H_1$
$H_0$	correct decision $1 - \alpha$	Type I error $\alpha$
<b>background</b>	<b>good rejection</b>	<b>false acceptance</b>
$H_1$	Type II error $\beta$	Correct decision $1 - \beta$
<b>signal + background</b>	<b>false exclusion</b>	<b>good acceptance</b>

**Discovery Probability or Discovery Potential (DP):**  
 the **power**  $1 - \beta$  when the critical value  $n$  is decided **before** the measurement and when  $p(n; \mu_b + \mu_s)$  is **true**.

# Poissonian Signal detection

There are many formulas used for detecting a signal over the background ( $3\sigma$ ,  $5\sigma$ ,  $6\sigma$ , and so on)

$N = N_s + N_b$  are the registered counts

$$S_0 = \frac{N - N_b}{\sqrt{N + N_b}} = \frac{N_b + N_s - N_b}{\sqrt{N + N_b}} = \frac{N_s}{\sqrt{N + N_b}}$$

$$\frac{x - \mu}{\sigma} = \frac{N - N_b - 0}{\sqrt{N + N_b}}$$

$$S_b = \frac{N - \mu_b}{\sqrt{\mu_b}} = \frac{N_b + N_s - \mu_b}{\sqrt{\mu_b}} \simeq \frac{N_s}{\sqrt{\mu_b}}$$

$$S_s = \frac{N - \mu_s}{\sqrt{\mu_s}} = \frac{N_b + N_s - \mu_s}{\sqrt{\mu_s}} \simeq \frac{N_s}{\sqrt{\mu_s}}$$

$$S_{sb} = \sqrt{N} - \sqrt{\mu_b} = \sqrt{N_s + N_b} - \sqrt{\mu_b}$$



This is the most common

Unclear (to me)

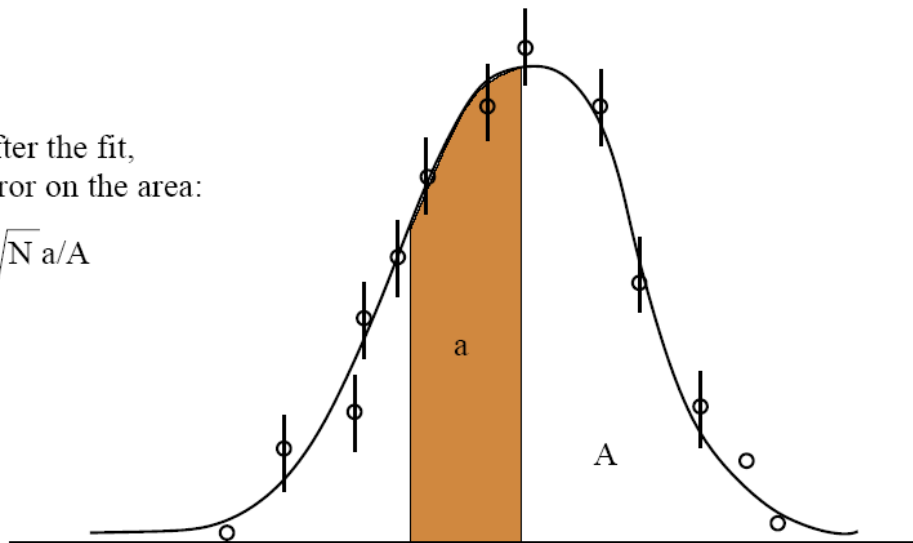
Recently Proposed (hypothesis test)

Please take care of the notation: often  $\mu$  is exchanged with  $N_b$  and so on, the formulae are obscure and used improperly!!

The background level in the peak region is estimated to be  $17.0 \pm 2.2 \pm 1.8$ , where the first uncertainty is the error in the fitting in the region above  $1.59 \text{ GeV}/c^2$  and the second is a statistical uncertainty in the peak region. The combined uncertainty of the background level is  $\pm 2.8$ . The estimated number of the events above the background level is  $19.0 \pm 2.8$ , which corresponds to a Gaussian significance of  $4.6^{+1.2}_{-1.0} \sigma$  ( $19.0/\sqrt{17.0} = 4.6$ ).

after the fit,  
error on the area:

$$\sqrt{N} a/A$$



$$\frac{19}{\sqrt{19 + 17 + 17}} = 2.6$$

$$\frac{19}{\sqrt{19 + 17 + 2.8^2}} = 2.9$$

## Observation of an Exotic Baryon with $S = +1$ in Photoproduction from the Proton

V. Kubarovsky,<sup>1,3</sup> L. Guo,<sup>2</sup> D. P. Weygand,<sup>3</sup> P. Stoler,<sup>1</sup> M. Battaglieri,<sup>18</sup> R. DeVita,<sup>18</sup> G. Adams,<sup>1</sup> Ji Li,<sup>1</sup> M. Nozar,<sup>3</sup> C. Salgado,<sup>26</sup> P. Ambrozewicz,<sup>13</sup> E. Anciant,<sup>5</sup> M. Anghinolfi,<sup>18</sup> B. Asavapibhop,<sup>24</sup> G. Audit,<sup>5</sup> T. Auger,<sup>5</sup> H. Avakian,<sup>3</sup> H. Bagdasarvan,<sup>28</sup> J. P. Ball,<sup>4</sup> S. Barrow,<sup>14</sup> K. Beard,<sup>21</sup> M. Bektasoglu,<sup>27</sup> M. Bellis,<sup>1</sup> N. Benmouna,<sup>15</sup> B. L. Berman,<sup>15</sup> C. S. Whisnant,<sup>32</sup> E. Wolin,<sup>3</sup> M. H. Wood,<sup>32</sup> A. Yegneswaran,<sup>3</sup> and J. Yun<sup>28</sup>

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PHYSICAL REVIEW

(CLAS Collaboration)

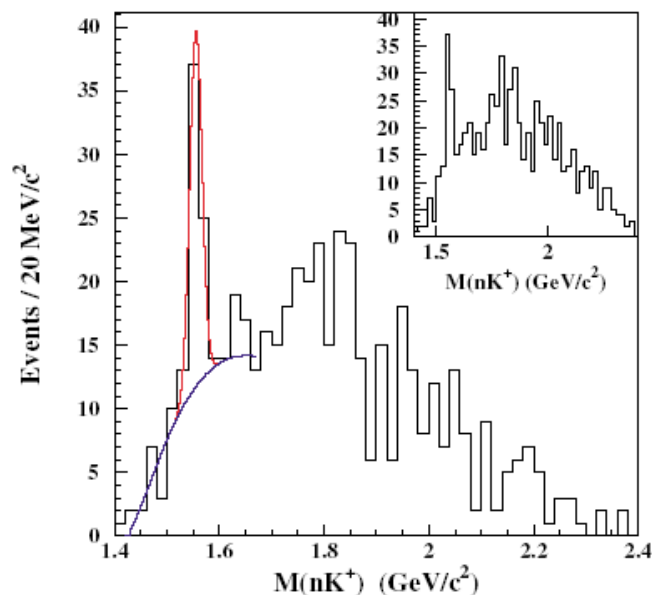
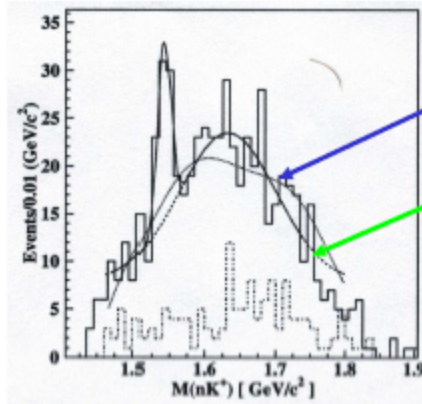


FIG. 4 (color online). The  $nK^+$  invariant mass spectrum in the reaction  $\gamma p \rightarrow \pi^+ K^- K^+(n)$  with the cut  $\cos\theta_{\pi^+}^* > 0.8$  and  $\cos\theta_{K^+}^* < 0.6$ .  $\theta_{\pi^+}^*$  and  $\theta_{K^+}^*$  are the angles between the  $\pi^+$  and  $K^+$  mesons and photon beam in the center-of-mass system. The background function we used in the fit was obtained from the simulation. The inset shows the  $nK^+$  invariant mass spectrum with only the  $\cos\theta_{\pi^+}^* > 0.8$  cut.

The final  $nK^+$  effective mass distribution (Fig. 4) was fitted by the sum of a Gaussian function and a background function obtained from the simulation. The fit parameters are  $N_{\Theta+} = 41 \pm 10$ ,  $M = 1555 \pm 1 \text{ MeV}/c^2$ , and  $\Gamma = 26 \pm 7 \text{ MeV}/c^2$  (FWHM), where the errors are statistical. The systematic mass scale uncertainty is estimated to be  $\pm 10 \text{ MeV}/c^2$ . This uncertainty is larger than our previously reported uncertainty [6] because of the different energy range and running conditions and is mainly due to the momentum calibration of the CLAS detector and the photon beam energy calibration. The statistical significance for the fit in Fig. 4 over a  $40 \text{ MeV}/c^2$  mass window is calculated as  $N_P/\sqrt{N_B}$ , where  $N_B$  is the number of counts in the background fit under the peak and  $N_P$  is the number of counts in the peak. We estimate the significance to be  $7.8 \pm 1.0\sigma$ . The uncertainty of  $1.0\sigma$  is due to

# Statistical Fluctuation

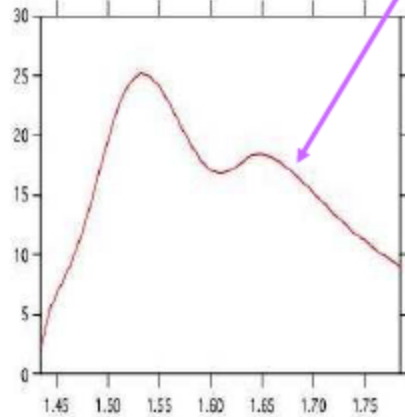
CLAS Published



Simple Physics Background

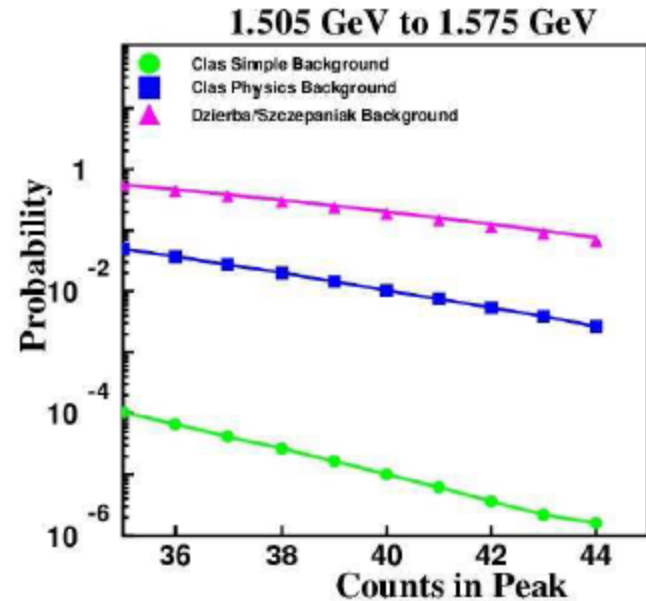
Naïve Background

Dzierba Background

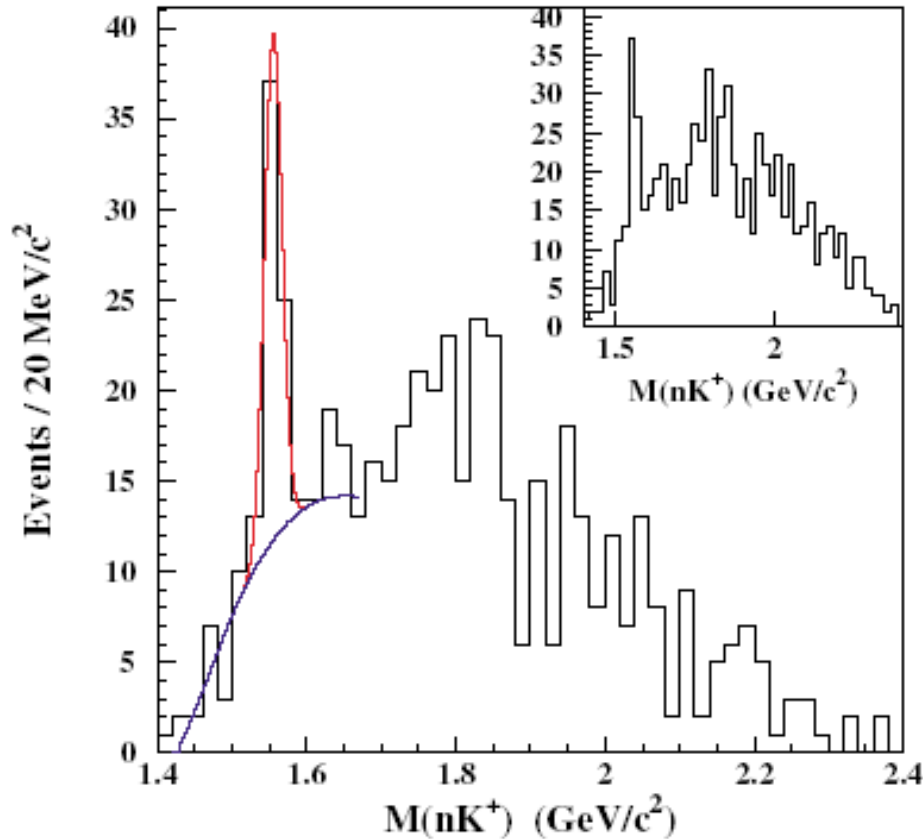


You need to understand your background to claim a new discovery!

Chance of the Background Fluctuating into the observed signal







$$\frac{41}{\sqrt{27}} = 7.8 \quad ???$$

$$\frac{41}{\sqrt{41 + 27}} = 5$$

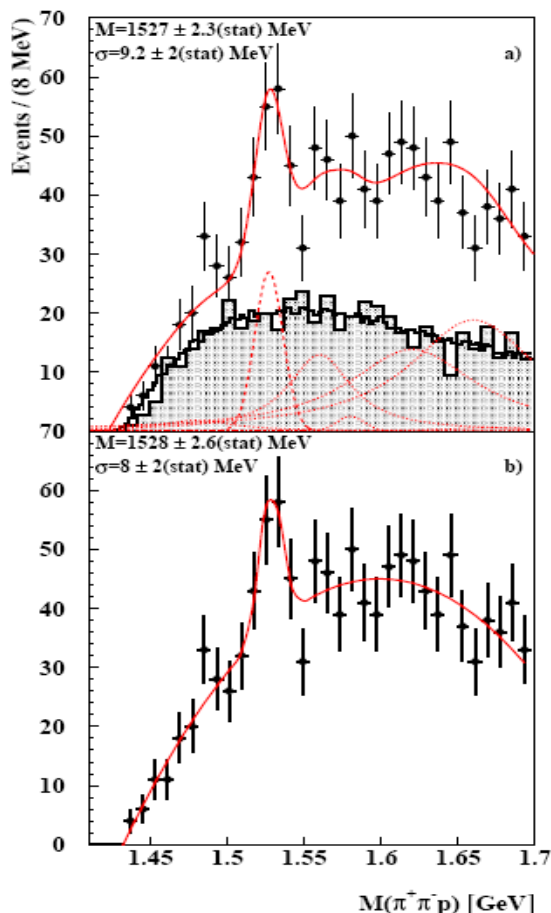
FIG. 4 (color online). The  $nK^+$  invariant mass spectrum in the reaction  $\gamma p \rightarrow \pi^+ K^- K^+ (n)$  with the cut  $\cos\theta_{\pi^+}^* > 0.8$  and  $\cos\theta_{K^+}^* < 0.6$ .  $\theta_{\pi^+}^*$  and  $\theta_{K^+}^*$  are the angles between the  $\pi^+$  and  $K^+$  mesons and photon beam in the center-of-mass system. The background function we used in the fit was obtained from the simulation. The inset shows the  $nK^+$  invariant mass spectrum with only the  $\cos\theta_{\pi^+}^* > 0.8$  cut.

# Evidence for a narrow $|S| = 1$ baryon state at a mass of 1528 MeV in quasi-real photoproduction

A. Airapetian,<sup>31</sup> N. Akopov,<sup>31</sup> Z. Akopov,<sup>31</sup> M. Amarian,<sup>8,31</sup> V.V. Ammosov,<sup>23</sup> A. Andrus,<sup>16</sup> E.C. Aschenauer,<sup>8</sup> W. Augustyniak,<sup>30</sup> R. Avakian,<sup>31</sup> A. Avetissian,<sup>31</sup> E. Avetissian,<sup>12</sup> P. Bailey,<sup>16</sup> D. Balin,<sup>22</sup> V. Baturin,<sup>22</sup> M. Beckmann,<sup>7</sup> S. Belostotski,<sup>22</sup> S. Bernreuther,<sup>10</sup> N. Bianchi,<sup>12</sup> H.P. Blok,<sup>21,29</sup> H. Böttcher,<sup>8</sup> A. Borissov,<sup>18</sup> A. Bratschkov,<sup>12</sup> M. Bratschkov,<sup>16</sup> J. Brath,<sup>6</sup> A. Bratskii,<sup>17</sup> V. Bratskii,<sup>23</sup> C.D. Calvert,<sup>12</sup> T. Chou,<sup>4</sup> V. Chou,<sup>4</sup> I. V. Khrifov,<sup>1</sup> M.G. Vincer,<sup>1</sup> C. Vogel,<sup>1</sup> M. Vogt,<sup>1</sup> J. Vomer,<sup>1</sup> C. Weiskopf,<sup>1</sup> J. Weidhard,<sup>1</sup> J. Wiedert,<sup>1</sup> G. Ybeles Smit,<sup>29</sup> Y. Ye,<sup>5</sup> Z. Ye,<sup>5</sup> S. Yen,<sup>27</sup> W. Yu,<sup>4</sup> B. Zihlmann,<sup>21</sup> H. Zohrabian,<sup>31</sup> and P. Zupranski<sup>30</sup>

(The HERMES Collaboration)

<sup>1</sup> Department of Physics, University of Alberta, Edmonton, Alberta T6G 2J1, Canada



## Photoproduction on a deuterium target

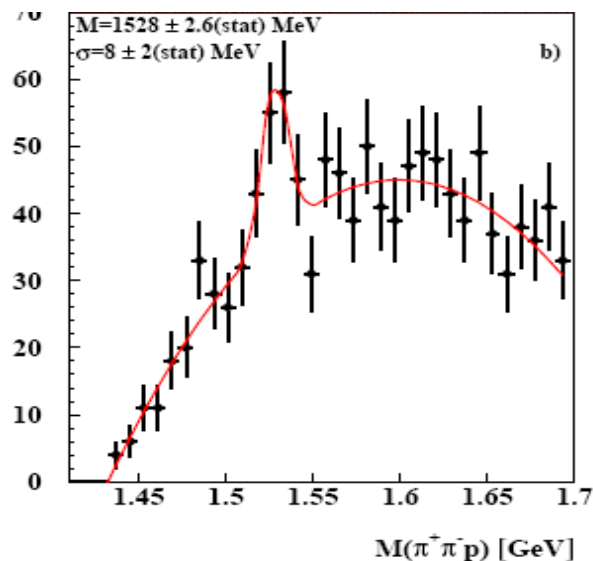


FIG. 2: Distribution in invariant mass of the  $p\pi^+\pi^-$  system subject to various constraints described in the text. The experimental data are represented by the filled circles with statistical error bars, while the fitted smooth curves result in the indicated position and  $\sigma$  width of the peak of interest. In panel a), the PYTHIA6 Monte Carlo simulation is represented by the gray shaded histogram, the mixed-event model normalised to the PYTHIA6 simulation is represented by the fine-binned histogram, and the fitted curve is described in the text. In panel b), a fit to the data of a Gaussian plus a third-order polynomial is shown.

# HERMES : 27.6 positron beam on deuterium

TABLE I: Mass values and experimental widths, with their statistical and systematic uncertainties, for the  $\Theta^+$  from the two fits, labelled by a) and b), shown in the corresponding panels of Fig. 2. Rows a') and b') are based on the same background models as rows a) and b) respectively, but a different mass reconstruction expression that is expected to result in better resolution. Also shown are the number of events in the peak  $N_s$  and the background  $N_b$ , both evaluated from the functions fitted to the mass distribution, and the results for the naïve significance  $N_s^{2\sigma} / \sqrt{N_b^{2\sigma}}$  and realistic significance  $N_s / \delta N_s$ . The systematic uncertainties are common (correlated) between rows of the table.

	$\Theta^+$ mass [MeV]	FWHM [MeV]	$N_s^{2\sigma}$ in $\pm 2\sigma$	$N_b^{2\sigma}$ in $\pm 2\sigma$	naïve signif.	Total $N_s \pm \delta N_s$	signif.
a)	$1527.0 \pm 2.3 \pm 2.1$	$22 \pm 5 \pm 2$	74	145	$6.1 \sigma$	$78 \pm 18$	$4.3 \sigma$
a')	$1527.0 \pm 2.5 \pm 2.1$	$24 \pm 5 \pm 2$	79	158	$6.3 \sigma$	$83 \pm 20$	$4.2 \sigma$
b)	$1528.0 \pm 2.6 \pm 2.1$	$19 \pm 5 \pm 2$	56	144	$4.7 \sigma$	$59 \pm 16$	$3.7 \sigma$
b')	$1527.8 \pm 3.0 \pm 2.1$	$20 \pm 5 \pm 2$	52	155	$4.2 \sigma$	$54 \pm 16$	$3.4 \sigma$



$$S_b = \frac{N - \mu_b}{\sqrt{\mu_b}} = \frac{N_b + N_s - \mu_b}{\sqrt{\mu_b}} \simeq \frac{N_s}{\sqrt{\mu_b}}$$

$$S_0 = \frac{N - N_b}{\sqrt{N + N_b}} = \frac{N_b + N_s - N_b}{\sqrt{N + N_b}} = \frac{N_s}{\sqrt{N + N_b}}$$

$$74 / \sqrt{74 + 145 + 74} = 4.3$$

$$S_0 = \frac{N - N_b}{\sqrt{N + N_b}} = \frac{N_b + N_s - N_b}{\sqrt{N + N_b}} = \frac{N_s}{\sqrt{N + N_b}}$$

Several alternative expressions for the significance of the peak observed in Fig. 2 were considered. The first expression is the naïve estimator  $N_s^{2\sigma} / \sqrt{N_b^{2\sigma}}$  used in Refs. [11, 12, 13, 14, 15, 16]. The corresponding result is listed in Table I. Because this statistic neglects the uncertainty in the background fit, it overestimates the significance of the peak [29]. A second estimator that was used in the analysis presented in Ref. [20],  $N_s^{2\sigma} / \sqrt{N_s^{2\sigma} + N_b^{2\sigma}}$ , gives a somewhat lower value, but may still underestimate the background uncertainty. A third estimate of the significance is given by  $N_s / \delta N_s$ , where  $N_s$  is now the full area of the peak from the fit and  $\delta N_s$  is its fully correlated uncertainty. This ratio measures how far the peak is away from zero in units of its own standard deviation. All correlated uncertainties from the fit, including those of the background parameters, are accounted for in  $\delta N_s$ . The results obtained with this expression are also given in Table I.

# Statistics

$$\xi_1 = \frac{s}{\sqrt{b}}$$

$$\xi_2 = \frac{s}{\sqrt{s+b}}$$

$$\xi_3 = \frac{s}{\sqrt{s+2b}}$$

Experiment	Signal	Background	Publ.	Significance $\xi_1$	$\xi_2$	$\xi_3$
Spring8	19	17	4.6 $\sigma$	4.6	3.2	2.6
Spring8	56	162		4.4	3.8	2.9
SPAHIR	55	56	4.8 $\sigma$	7.3	5.2	4.3
CLAS (d)	43	54	5.2 $\sigma$	5.9	4.4	3.5
CLAS (p)	41	35	7.8 $\sigma$	6.9	4.7	3.9
DIANA	29	44	4.4 $\sigma$	4.4	3.4	2.7
v	18	9	6.7 $\sigma$	6.0	3.5	3.0
HERMES	51	150	4.3-6.2 $\sigma$	4.2	3.6	2.7
COSY	57	95	4-6 $\sigma$	5.9	4.7	3.7
<b>ZEUS</b>	<b>230</b>	<b>1080</b>	<b>4.6<math>\sigma</math></b>	<b>7.0</b>	<b>6.4</b>	<b>4.7</b>
SVD	35	93	5.6 $\sigma$	3.6	3.1	2.4
NOMAD	33	59	4.3 $\sigma$	4.3	3.4	2.7
NA49	38	43	4.2 $\sigma$	5.8	4.2	3.4
NA49	69	75	5.8 $\sigma$	8.0	5.8	4.7
H1	50.6	51.7	5-6 $\sigma$	7.0	5.0	4.1

No 5 $\sigma$  effect!!

## Poissonian Signal detection

When **the background is well known** people use

$$S_b = \frac{N - \mu_b}{\sqrt{\mu_b}}$$

Recently Bityukov and Krasnikov (2000) proposed

$$S_{sb} = \sqrt{N} - \sqrt{\mu_b} = \sqrt{N_s + N_b} - \sqrt{\mu_b}$$

**Proof:** In gaussian approx ( $\mu_b > 10$ ), the abscissa  $n$  satisfies the equation

$$t = \frac{n - N_b}{\sqrt{N_b}} = - \frac{n - N_s - N_b}{\sqrt{N_s + N_b}},$$

which implies

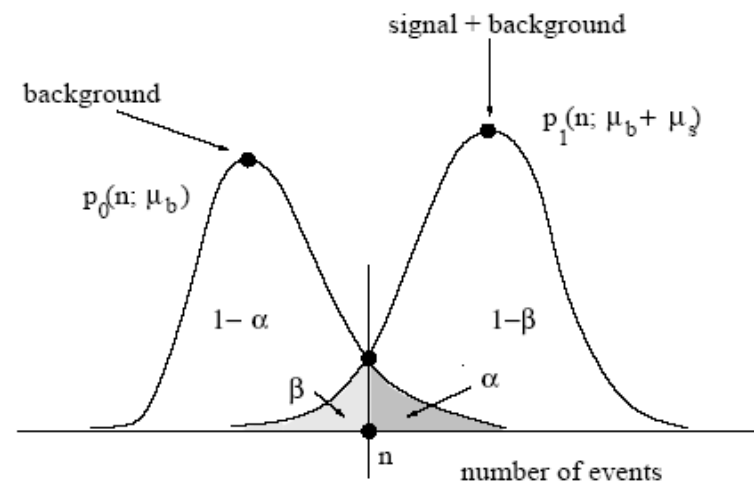
$$n = \sqrt{N_b(N_b + N_s)} \quad \text{and} \quad t = \sqrt{N_b + N_s} - \sqrt{N_b}.$$

Therefore, one can define the statistic

$$S_{bs} = \sqrt{N} - \sqrt{N_b},$$

with expectation value

$$\langle S_{bs} \rangle = \sqrt{\mu_b + \mu_s} - \sqrt{\mu_b},$$



# Poissonian Signal detection

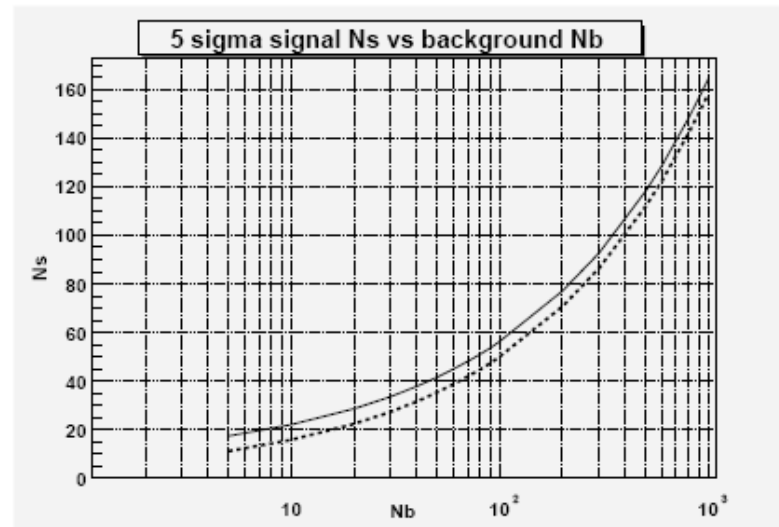
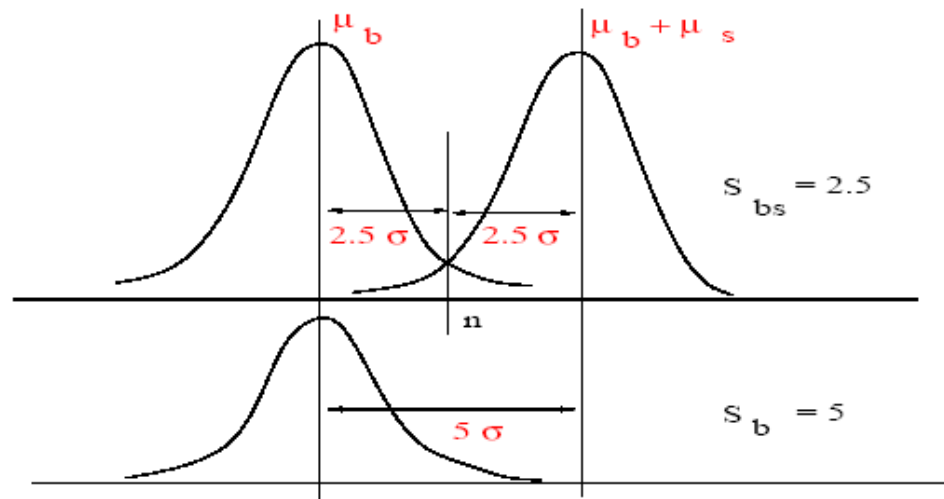
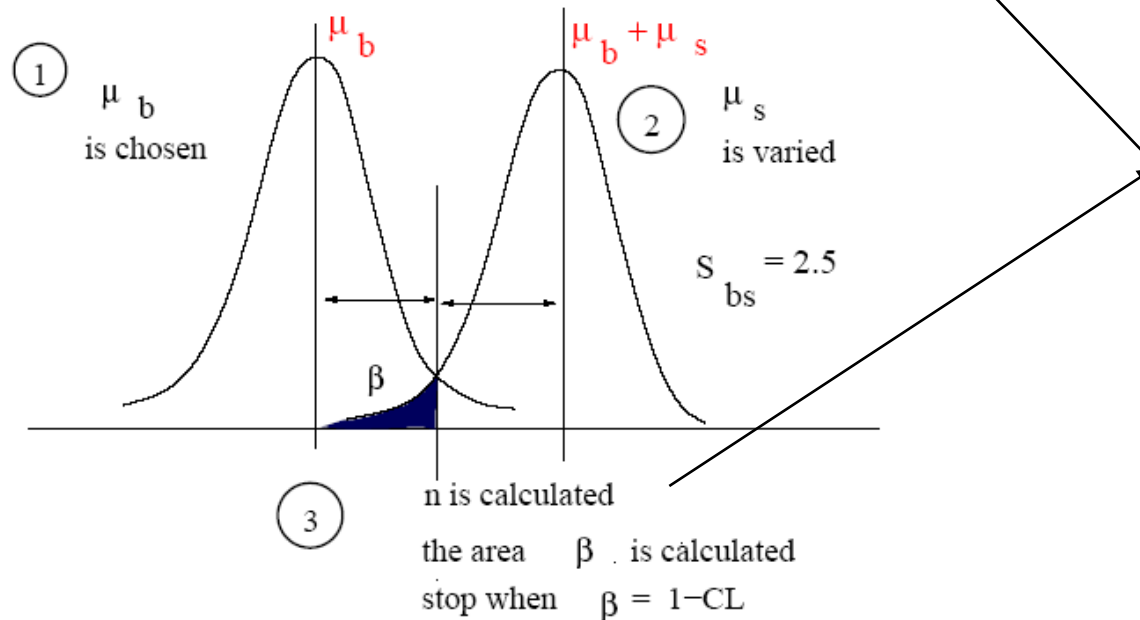


Figure 1: Number  $N_s$  of the signal events for  $S_b = 5$  (dotted line) and  $S_{bs} = 2.5$  (full line) versus the number  $N_b$  of background events.

# Poissonian Signal Detection

$$\frac{N_b^n}{n!} e^{-N_b} = \frac{(N_b + N_s)^n}{n!} e^{-N_b + N_s} \implies n = \frac{N_s}{\ln(1 + N_s/N_b)}$$



$\mu_b$	$n$	$\mu_s$	$\alpha$
10	19	22	0.004
20	32	26	0.005
30	45	33	0.005
60	80	43	0.006
200	234	73	0.008
500	554	111	0.008
$x$	$\mu_b + 2.33\sqrt{x}$	$2 \times 2.33\sqrt{x}$	0.010

Table 1: When the expected background value is  $\mu_b$ , if  $n$  events are observed,  $\mu_s$  is the upper limit of the signal intensity with  $CL = 99\%$ .



# Binomial counting: candidate selection

A sample  $N_t$  can be considered as an ensemble of signal and background events:

$$N_t = N_s + N_b$$

The **measurement is a linear operator  $M$**  that acts on  $N_s + N_b$  and divides this sample into events that pass the selection (the “yes” events  $N_y$ ) and events that do not pass the selection (the “no” events  $N_n$ ).

$$N_t = N_s + N_b = N_y + N_n$$

$$\begin{pmatrix} N_y \\ N_n \end{pmatrix} = \mathbf{M} \begin{pmatrix} N_s \\ N_b \end{pmatrix}$$

$$\begin{pmatrix} N_y \\ N_n \end{pmatrix} = \mathbf{M} \begin{pmatrix} N_s \\ N_b \end{pmatrix}$$

$\varepsilon$  is the efficiency on the signal events and  $b$  that on the background:

$$N_{ys} = \varepsilon N_s, \quad N_{ns} = (1 - \varepsilon) N_s$$

$$N_{yb} = b N_b, \quad N_{nb} = (1 - b) N_b,$$

Since

$$N_y = N_{ys} + N_{yb} = \varepsilon N_s + b N_b,$$

$$N_n = N_{ns} + N_{nb} = (1 - \varepsilon) N_s + (1 - b) N_b,$$

the  $M$  matrix becomes:

$$\mathbf{M} = \begin{pmatrix} \varepsilon & b \\ 1 - \varepsilon & 1 - b \end{pmatrix}.$$

The inverse of the measurement matrix is:

$$\mathbf{M}^{-1} = \frac{1}{\varepsilon - b} \begin{pmatrix} 1 - b & -b \\ \varepsilon - 1 & \varepsilon \end{pmatrix},$$

When the knowledge of the  $\varepsilon$  and  $b$ -efficiencies is achieved, one can solve the general Measurement Problem (MP):

*having measured  $N_y$  and  $N_n$  from a sample  $N_t = N_y + N_n$ , what are  $N_s$  and  $N_b$ ? :*

$$N_s = \frac{(1 - b)N_y - bN_n}{\varepsilon - b} = \frac{N_y - bN_t}{\varepsilon - b}$$

$$N_b = \frac{(\varepsilon - 1)N_y + \varepsilon N_n}{\varepsilon - b} = \frac{N_n - (1 - \varepsilon)N_t}{\varepsilon - b} = \frac{\varepsilon N_t - N_y}{\varepsilon - b}$$

When  $\varepsilon \gg b$  and  $\varepsilon, b \ll 1$ ,

$$N_s = \frac{N_y}{\varepsilon}, \quad N_b = N_t - N_s.$$

The errors come from the binomial formula ( $N_t$  is not random):

$$\sigma[N_s] = \sigma[N_b] = \frac{1}{\varepsilon - b} \sigma[N_y] = \frac{1}{\varepsilon - b} \sqrt{N_y(1 - N_y/N_t)}$$

When there are more background sources

$$b \rightarrow b_{\text{tot}} = \sum_i b_i w_i, \quad w_i = \frac{N_{b_i}}{\sum_i N_{b_i}}.$$

**Problem:** when  $\varepsilon \simeq b$  the system is **ill-conditioned!**

$$t = \frac{N_s}{\sigma[N_b]} = \frac{(\varepsilon - b)N_s}{\sqrt{N_y(1 - N_y/N_t)}}$$

$$= \frac{N_y - bN_t}{\sqrt{N_y(1 - N_y/N_t)}} \left( \begin{array}{l} \geq 5 \text{ for the } 5\sigma \text{ discovery} \\ \text{binomial case} \end{array} \right), (3)$$

If the b-efficiency is deduced from a background sample, it must be considered as a random variable:

$$b = \frac{N_{yb}}{N_t},$$

if the signal and background runs have the same  $N_t$ :

$$t = \frac{N_s}{\sigma[N_b]} = \frac{N_y - N_{yb}}{\sqrt{N_y(1 - N_y/N_t) + N_{yb}(1 - N_{yb}/N_t)}} \simeq \frac{N_y - N_{yb}}{\sqrt{N_y + N_{yb}}},$$

where the last term is the well known  $S_0$  result.

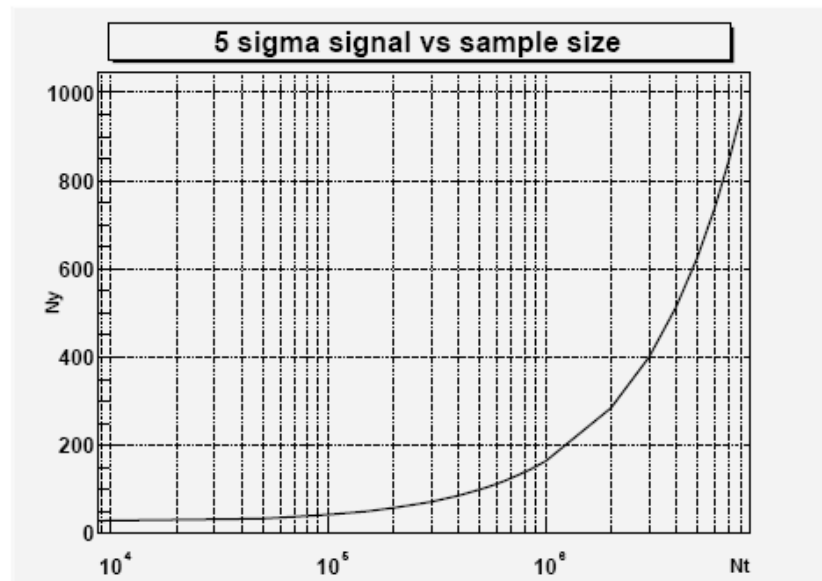


Figure 2: Number  $N_y$  of the events that pass the selection at a  $5\sigma$  level versus the sample size  $N_t$  with a  $b$ -efficiency  $1 \cdot 10^{-4}$ .

Having found  $N_s$  and  $N_b$ , the percentage of signal in the accepted events  $N_y$  can be found with the Bayes formula (used in a frequentist way, because  $P(S)$  is not subjective)

# Bayes formula

$$P(S|T) = \frac{P(T|S) P(S)}{P(T|S) P(S) + P(T|B) P(B)}$$

where:

$P(S)$  =  $N_s/N_t$  = percentage of events in the triggered sample

$P(B)$  =  $N_b/N_t$  = percentage of background in the triggered sample

$P(T|S)$  =  $\varepsilon$  = probability that a signal event passes the selection

$P(T|B)$  =  $b$  = probability that a background event passes the selection

$P(S|T)$  = probability that a selected event is the signal

$$P(S|T) = \varepsilon \frac{N_y - bN_t}{(\varepsilon - b)N_y} = \frac{\varepsilon}{\varepsilon - b} \left( 1 - b \frac{N_t}{N_y} \right) = \frac{\varepsilon N_s}{N_y}$$

$$P(B|T) = 1 - P(S|T) ,$$

$$\sigma[P(\bar{H}|S)] = \frac{\varepsilon b}{\varepsilon - b} \frac{N_t}{N_y^2} \sqrt{N_y(1 - N_y/N_t)} \simeq \frac{\varepsilon b}{\varepsilon - b} N_t N_y^{-3/2} .$$

In summary,

$$P(S|T) \simeq \frac{\varepsilon}{\varepsilon - b} \left( 1 - b \frac{N_t}{N_y} \right) \pm \frac{\varepsilon b}{\varepsilon - b} N_t N_y^{-3/2}$$

# The top quark discovery of CDF

The CDF experiment claimed the top quark discovery (Phys. Rev. Lett.74(1995)2626) with two different selection methods of discriminating the signal

$$t\bar{t} \rightarrow WbW\bar{b}$$

from background:

- **SVX tagging:**  $b$  jets identification by searching for secondary vertices in the Silicon Vertex detector;
- **SLT tagging:** to search for an additional soft lepton from semileptonic  $b$  decay

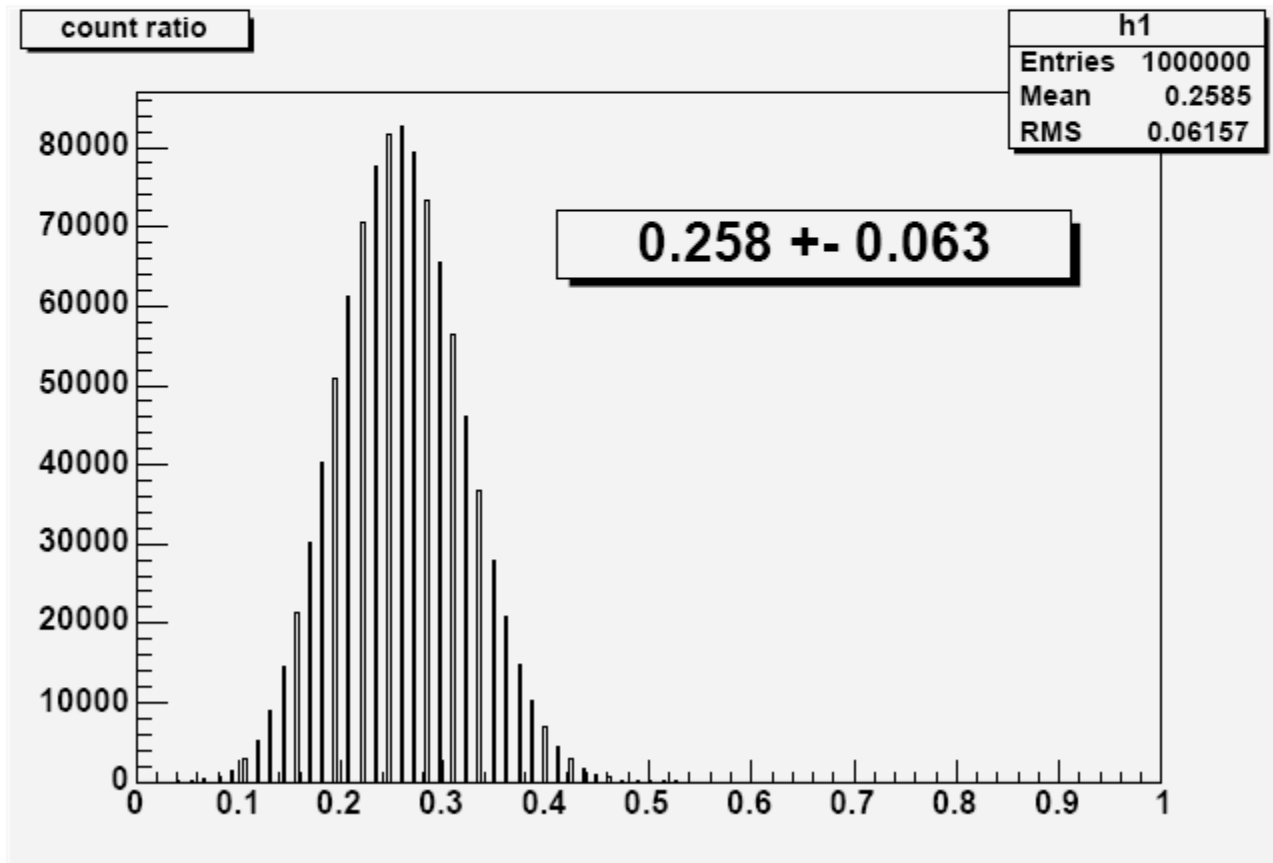
tag	$N_t$	$N_y$	$\epsilon$ %	$b$ %	$N_s/N_t$	$N_t P(S T)$
SVX	203	27	$42 \pm 5$	$3.3 \pm 0.1$	$0.25^{+0.08}_{-0.07}$	$22.5^{+2.3}_{-2.9}$
SLT	203	23	$20 \pm 2$	$7.6 \pm 0.1$	$0.24^{+0.22}_{-0.18}$	$13.2^{+4.6}_{-6.0}$

The error on  $N_s/N_t$  from the standard formula is  $\pm 0.06$  for SVX and  $\pm 0.18$  for SLT, slightly underestimated.

To take into account the uncertainties on the efficiencies (nuisance parameters) a grid MC is necessary

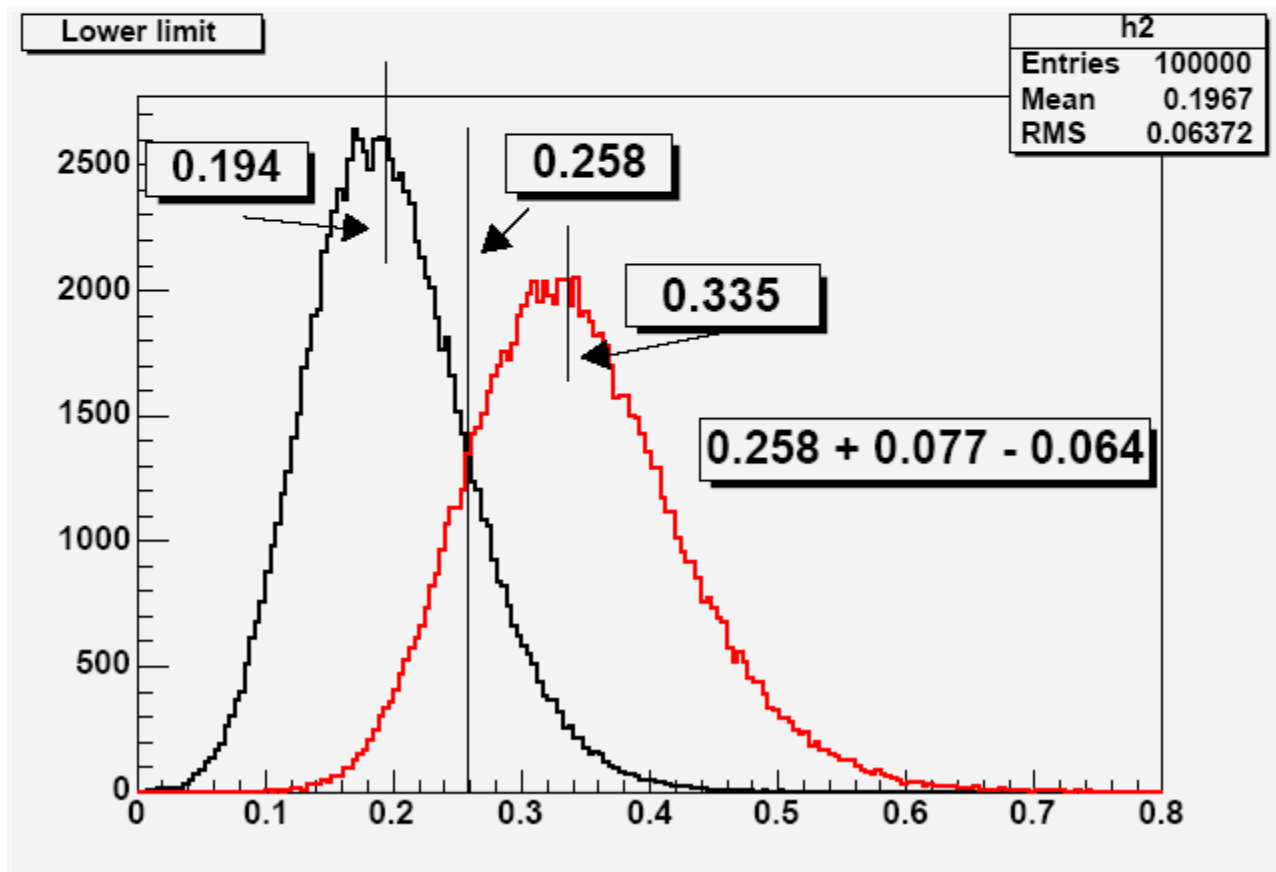
# The bootstrap method for confidence levels

With fixed efficiencies we have the binomial/gaussian distribution



# The grid method for confidence levels

For each value of  $p = N_s/N_t$  a sample of 100 000 events is generated sampling randomly the  $\varepsilon$  and  $b$  efficiencies.

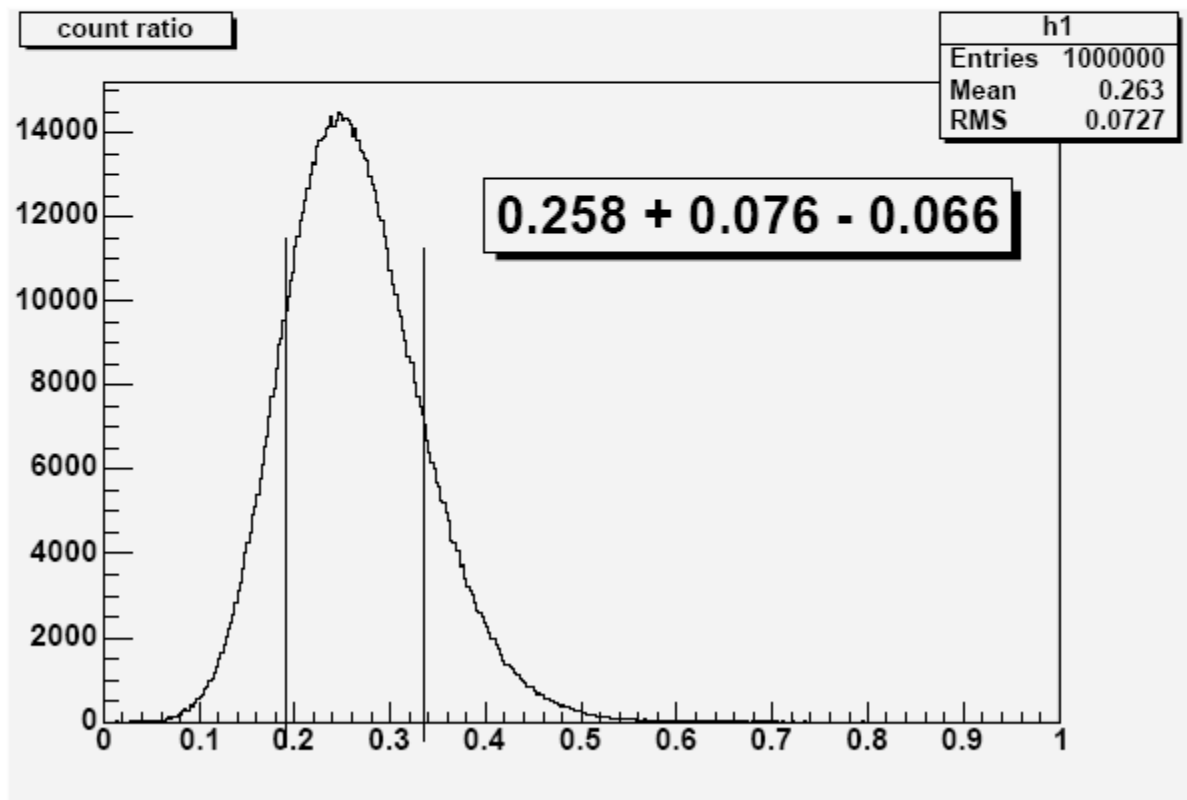




# The bootstrap method for confidence levels

In this case also the approximate **bootstrap** method gives the same result.

This method is called **Parametric Bootstrap**



# The bootstrap method for BR

- **A=15** Reaction **A** events in a **N=200** event sample
- **B=30** Reaction **B** events in a **N=200** event sample

Standard error propagation for 95% CL

$$\sigma(A/B) = 1.96 \times \frac{A}{B} \sqrt{\frac{\sigma^2(A)}{A^2} + \frac{\sigma^2(B)}{B^2}} = 0.15 \rightarrow [0.21, 0.79], \text{ CL} = 95\%$$

$$\sigma(A) = \sqrt{A \left(1 - \frac{A}{N}\right)}$$

Bootstrap methods:

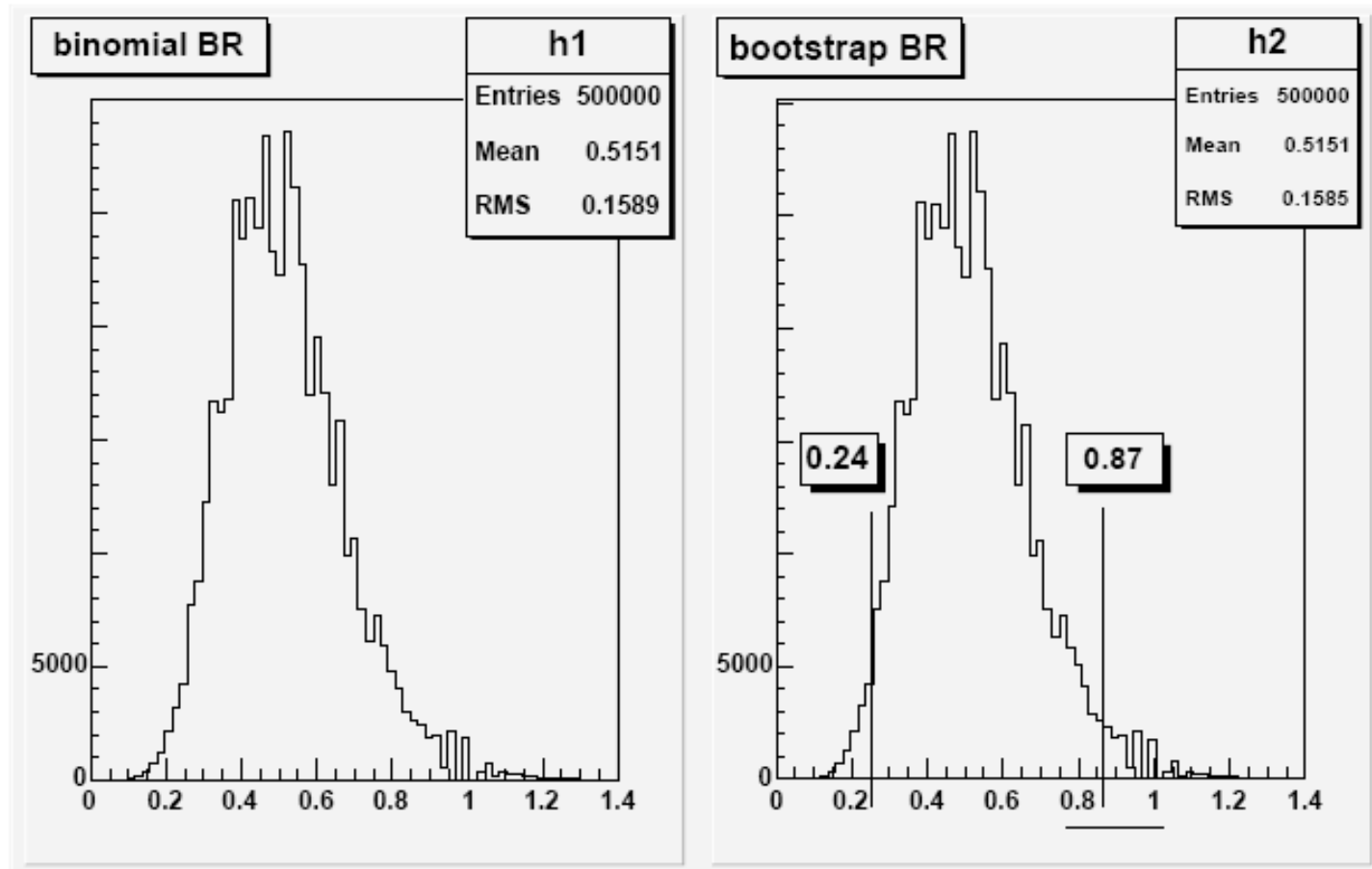
- **parametric** bootstrap: the events  $A$  and  $B$  are MC-sampled from two binomial distributions with  $N = 200$  and  $p_1 = A/N$  and  $p_2 = B/N$ ;
- **non parametric** bootstrap: the events  $A$  and  $B$  are sampled **with replacement** from **two experimental samples** with  $N = 200$  and  $A$  or  $B$  events = 1, the others = 0

Obviously, in this case the two methods give the same result:

$$[A/B] \in [0.24, 0.86], \quad CL = 95\%$$

**Are the published BR really all RELIABLE??**

# The bootstrap method for BR



Consider a sample  $X$  containing  $N$  objects. We need an estimate of  $\theta$  as  $\hat{\theta}(X)$ .

**No model of the  $X$  distribution is known or considered**  
Statisticians have elaborated the following (**non parametric**) methods:

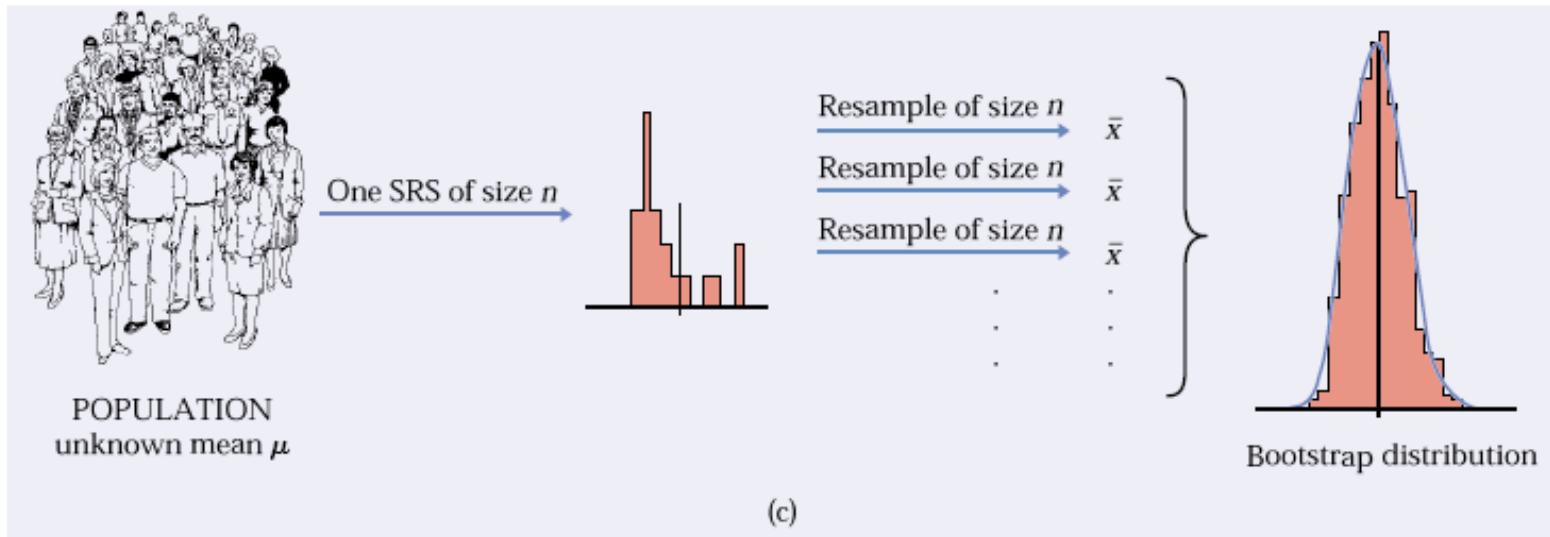
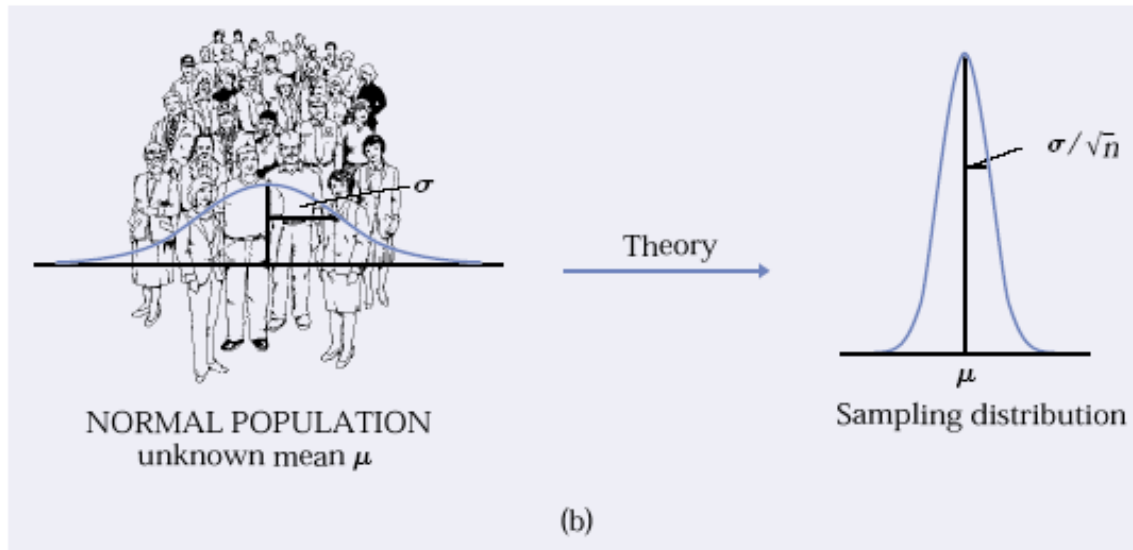
## The non parametric Sampling methods

- **Jackknife** (Quenouille, 1949):  
 $N$  samples are generated leaving out one element at a time;
- **Subsampling**:  
 $S$  resamples of dimension  $N_B$  are created by repeatedly sampling **without replacement** from the experimental sample. Obviously one has  $N_B < N$ .
- **Bootstrap** (Efron 1979):  
 $S$  resamples of dimension  $N_B$  are created by repeatedly sampling **with replacement** from the experimental sample. Usually  $N_B = N$  is set.
- **Permutation**:  
used in the test between two hypotheses, by resampling in a way that moves observations between the two groups, under the assumption that the null hypothesis is true

The best one !!!

These methods, familiar among statisticians, are practically not (yet) used by physicists (**only 3 papers with non parametric Bootstrap!**)

# Non parametric Bootstrap



# The non parametric BOOTSTRAP

Consider a sample  $X$  containing  $N$  objects. We need an estimate of  $\theta$  as

$$\hat{\theta}(X)$$

Using the Bootstrap sample, we obtain the estimator

$$\hat{\theta}^* = \hat{\theta}(X^*)$$

The Bootstrap samples have expectation values  $\hat{\theta}^*$  that differ from the true one  $\theta$  (bias), but ...

the Bootstrap approximates the distribution of

$$\hat{\theta} - \theta$$

with the distribution of

$$\hat{\theta}^* - \hat{\theta}$$

obtained by resampling.

# Limits of non parametric BOOTSTRAP

Drawback: the Bootstrap samples **are correlated**.  
Some important results on this:

- the sharing of the same elements in different samples **reduces** the variance  $s_{\text{res}}$  of the (re)samples:

$$s_{\text{res}}^2 \rightarrow (1 - \rho)\sigma^2$$

where  $\rho = N_B/N$  in subsampling without replacement;

- the sampling with replacement in bootstrap **increases** the variance of the (re)samples:

$$s_{\text{res}}^2 \rightarrow (1 - \rho)\rho_1\sigma^2$$

- in many cases in the bootstrap the positive bias due to the within sample correlation and the negative bias due to the between sample correlation **cancel exactly**

$$\sqrt{1 - \rho}\sqrt{\rho_1} \simeq 1$$

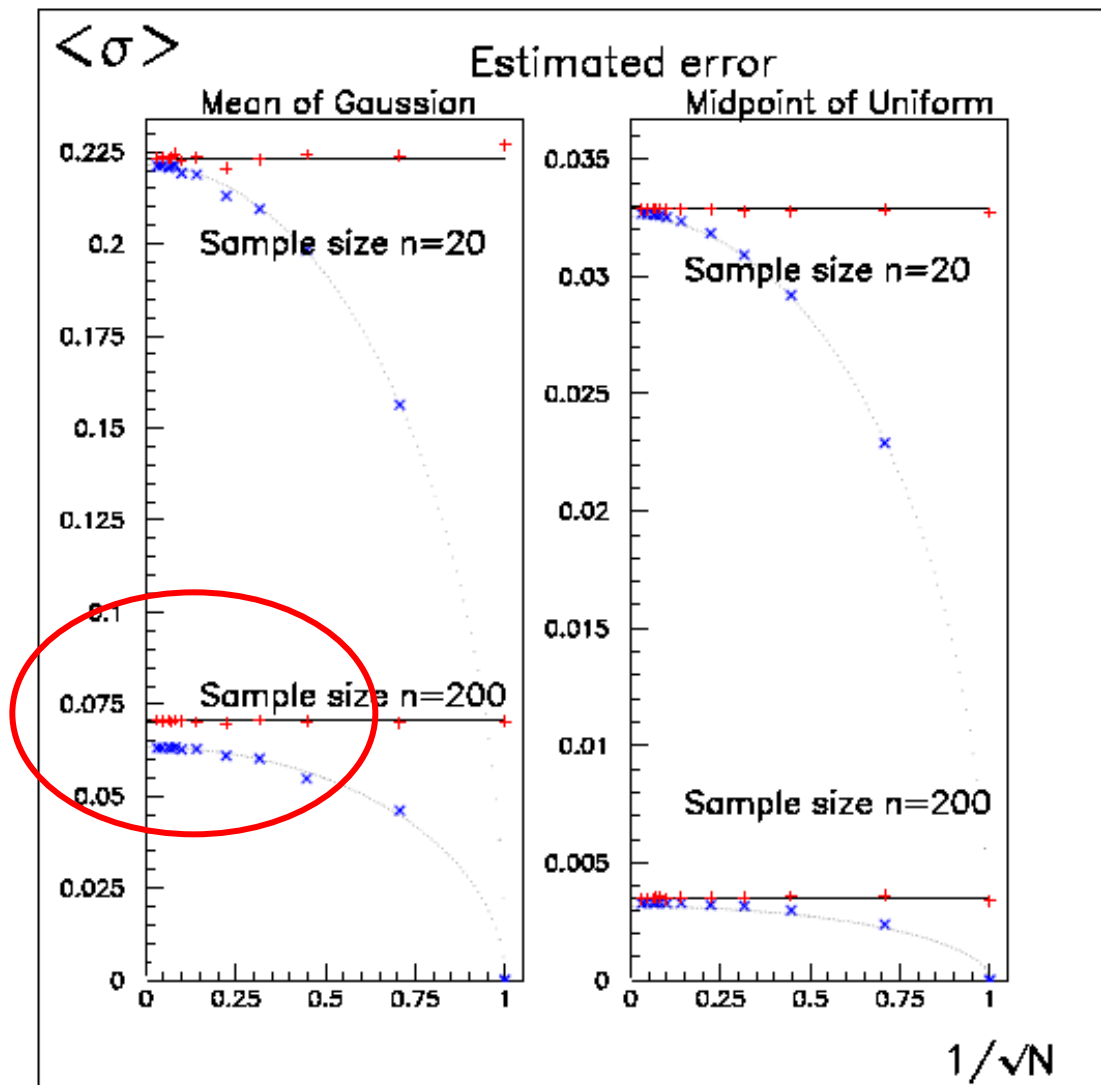


Figure 4: The mean estimated error as a function of the number of samples. Sampling was done **without replacement**



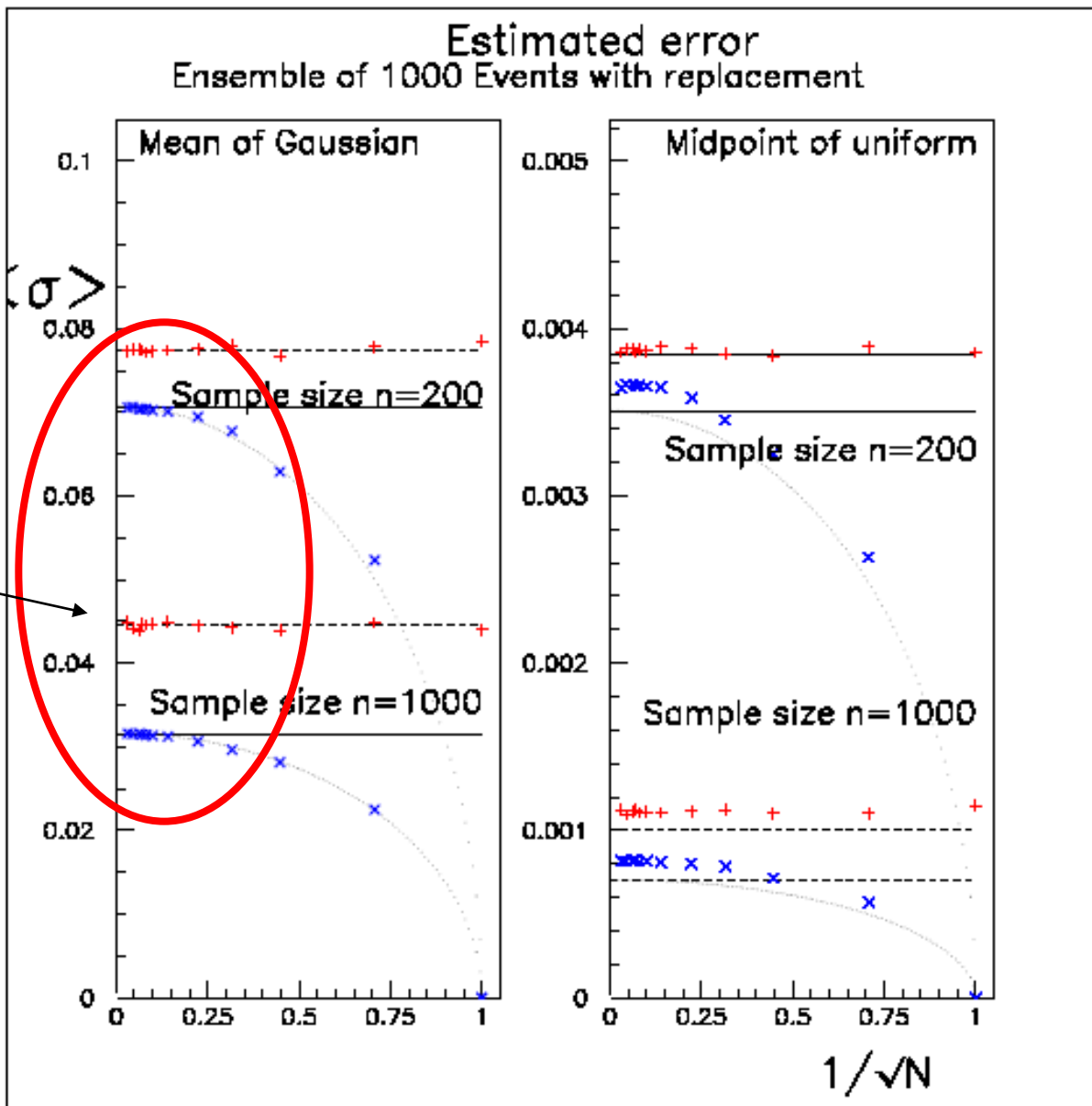


Figure 5: Mean estimated error using 'with replacement' samples

# The non parametric BOOTSTRAP

When does the Bootstrap work?

For the consistency of the method, the reliability must be Bootstrap-checked, through the Bootstrap samples themselves!

The important checks are:

- check the symmetry of the Bootstrap distribution, that assures the **bootstrap property**. Find if necessary a transformation  $h$  such as

$$h(\hat{\theta}) - h(\theta) \quad \text{and} \quad h(\hat{\theta}^*) - h(\hat{\theta})$$

are pivotal, that is follow the same distribution. Then make the estimate of the  $h$  intervals before anti-transforming with  $h^{-1}$

- make different estimates with different bootstrap samples (with replacement)  $N_B \leq N$  and verify that the variances scales as  $1/N_B$ . This verify the condition

$$\sqrt{1 - \rho} \sqrt{\rho_1} \simeq 1$$

There exists a wide statistical literature on the subject....

## Application of the bootstrap statistical method to the tau-decay-mode problem

Kenneth G. Hayes and Martin L. Perl

*Stanford Linear Accelerator Center, Stanford University, Stanford, California 94309*

Bradley Efron

*Department of Statistics, Stanford University, Stanford, California 94309*

(Received 18 July 1988)

The bootstrap statistical method is applied to the discrepancy in the one-charged-particle decay modes of the tau lepton. This eliminates questions about the correctness of the errors ascribed to the branching-fraction measurements and the use of Gaussian error distributions for systematic errors. The discrepancy is still seen when the results of the bootstrap analysis are combined with other measurements and with deductions from theory. But the bootstrap method assigns less statistical significance to the discrepancy compared to a method using Gaussian error distributions.

At present there is a problem<sup>1,2</sup> in fully understanding the decay modes of the tau lepton to one-charged particle. The average directly measured value<sup>1</sup> of the inclusive, one-charged-particle, branching fraction  $B_1$  is  $(86.6 \pm 0.3)\%$ . The same number should be obtained by adding up the branching fractions of the individual one-charged-particle modes. Examples of these individual branching fractions are

$$\begin{aligned}
 B_e, \quad \tau^- &\rightarrow \nu_\tau + e^- + \bar{\nu}_e, \\
 B_\mu, \quad \tau^- &\rightarrow \nu_\tau + \mu^- + \bar{\nu}_\mu, \\
 B_\pi, \quad \tau^- &\rightarrow \nu_\tau + \pi^-, \\
 B_\rho, \quad \tau^- &\rightarrow \nu_\tau + \rho^- \rightarrow \nu_\tau + \pi^- + \pi^0, \\
 B_{\pi 2\pi^0}, \quad \tau^- &\rightarrow \nu_\tau + \pi^- + 2\pi^0, \\
 B_{\pi 3\pi^0}, \quad \tau^- &\rightarrow \nu_\tau + \pi^- + 3\pi^0.
 \end{aligned}$$

As shown in Table I from Ref. 2, this sum is less than  $(80.6 \pm 1.5)\%$ , 6% less than the directly measured value of  $B_1$ . This is the  $\tau$ -decay-mode problem.

# Bootstrap of $B_1$ and $B_i$ data

TABLE II.  $B_1$  topological branching fractions in percent. The statistical error is given first, the systematic error second.

$B_1$	Combined error	Energy (GeV)	Experimental group	Reference
84.0	$\pm 2.0$	32.0–36.8	CELLO	H. J. Behrend <i>et al.</i> , Phys. Lett. <b>114B</b> , 282 (1982)
$85.2 \pm 2.6 \pm 1.3$	$\pm 2.9$	14.0	CELLO	H. J. Behrend <i>et al.</i> , Z. Phys. C <b>23</b> , 103 (1984)
$85.1 \pm 2.8 \pm 1.3$	$\pm 3.1$	22.0	CELLO	H. J. Behrend <i>et al.</i> , Z. Phys. C <b>23</b> , 103 (1984)
$87.8 \pm 1.3 \pm 3.9$	$\pm 4.1$	34.6 average	PLUTO	Ch. Berger <i>et al.</i> , Z. Phys. C <b>28</b> , 1 (1985)
$84.7 \pm 1.1 \pm 1.3$	$^{+1.9}_{-1.7}$	13.9–43.1	TASSO	M. Althoff <i>et al.</i> , Z. Phys. C <b>26</b> , 521 (1985)
$86.7 \pm 0.3 \pm 0.6$	$\pm 0.7$	29.0	MAC	E. Fernandez <i>et al.</i> , Phys. Rev. Lett. <b>54</b> , 1624 (1985)
$86.9 \pm 0.2 \pm 0.3$	$\pm 0.4$	29.0	HRS	C. Akerlof <i>et al.</i> , Phys. Rev. Lett. <b>55</b> , 570 (1985)
$86.1 \pm 0.5 \pm 0.9$	$\pm 1.0$	30.0–46.8	JADE	W. Bartel <i>et al.</i> , Phys. Lett. <b>161B</b> , 188 (1985)
$87.9 \pm 0.5 \pm 1.2$	$\pm 1.3$	29.0	DELCO	W. Ruckstuhl <i>et al.</i> , Phys. Rev. Lett. <b>56</b> , 2132 (1986)
$87.2 \pm 0.5 \pm 0.8$	$\pm 0.9$	29.0	Mark II	W. B. Schmidke <i>et al.</i> , Phys. Rev. Lett. <b>57</b> , 527 (1986)
$84.7 \pm 0.8 \pm 0.6$	$\pm 1.0$	29.0	TPC	H. Aihara <i>et al.</i> , Phys. Rev. D <b>35</b> , 1553 (1987)

Trimmed mean 50%

Correlation between measurements

Weighted resampling  $\text{Int}(1/\sigma^2)$  times

The error on measurements is not considered

Scope of the analysis: to test whether errors only or the data itself are unreliable

TABLE V. (a) Independent measurement of the  $\tau^- \rightarrow e^- \bar{\nu}_e \nu_\tau$  and  $\tau^- \rightarrow \mu^- \bar{\nu}_\mu \nu_\tau$  branching fractions  $B_e$  and  $B_\mu$  in percent. The statistical error is given first, the systematic error second. (b) Constrained or correlated measurements of the  $\tau^- \rightarrow e^- \bar{\nu}_e \nu_\tau$  and  $\tau^- \rightarrow \mu^- \bar{\nu}_\mu \nu_\tau$  branching fractions  $B_e$  and  $B_\mu$  in percent. The statistical error is given first, the systematic error second.

$B_e$		$B_\mu$		Energy	Experimental	Reference
Measurement	Combined error	Measurement	Combined error	(GeV)	group	
(a)						
		17.5±2.7±3.0	±4.0	3.8–7.8	Mark I	M. L. Perl <i>et al.</i> , Phys. Lett. <b>70B</b> , 487 (1977)
		22	$^{+10}_{-7}$	4.8		M. Cavalli-Storza <i>et al.</i> , Lett. Nuovò Cimentò <b>20</b> , 337 (1977)
16.0	±1.3	15	±3.0	3.6–5.0	PLUTO	J. Burmester <i>et al.</i> , Phys. Lett. <b>68B</b> , 297 (1977)
		22	$^{+7}_{-8}$	3.1–7.4	DELCO	W. Bacino <i>et al.</i> , Phys. Rev. Lett. <b>41</b> , 13 (1978)
		21±5±3	±6	6.4–7.4	Iron Ball	J. G. Smith <i>et al.</i> , Phys. Rev. D <b>18</b> , 1 (1978)
19	±9.0	35	±14	3.6–7.4	DELCO	W. Bacino <i>et al.</i> , Phys. Rev. Lett. <b>42</b> , 6 (1979)
		17.8±2.0±1.8	±2.7	12–31.6	TASSO	R. Brandelik <i>et al.</i> , Phys. Lett. <b>92B</b> , 199 (1980)
18.3±2.4±1.9	±3.1	17.6±2.6±2.1	±3.3	9.4–31.6	PLUTO	Ch. Berger <i>et al.</i> , Phys. Lett. <b>99B</b> , 489 (1981)
20.4±3.0 $^{+1.4}_{-0.9}$	$^{+3.3}_{-3.1}$	12.9±1.7 $^{+0.7}_{-0.5}$	±1.8	34.0	CELLO	H. J. Behrend <i>et al.</i> , Phys. Lett. <b>127B</b> , 270 (1983)
13.0±1.9±2.9	±3.5	19.4±1.6±1.7	±2.3	13.9–43.1	TASSO	M. Althoff <i>et al.</i> , Z. Phys. C <b>26</b> , 521 (1985)
				34.6	PLUTO	Ch. Berger <i>et al.</i> , Z. Phys. C <b>28</b> , 1 (1985)
				average		
		17.4±0.6±0.8	±1.0	14.0–46.8	Mark J	B. Adeva <i>et al.</i> , Phys. Lett. B <b>179</b> , 177 (1986)
17.0±0.7±0.9	±1.1	18.8±0.8±0.7	±1.1	34.6	JADE	W. Bartel <i>et al.</i> , Phys. Lett. B <b>182</b> , 216 (1986)
				average		
19.1±0.8±1.1	±1.4	18.3±0.9±0.8	±1.2	29.0	Mark II	P. R. Burchat <i>et al.</i> , Phys. Rev. D <b>35</b> , 27 (1987)
(b)						
18.9±1.0±2.8	±3.0	18.3±1.0±2.8	±3.0	3.8–7.8	Mark I	M. L. Perl <i>et al.</i> , Phys. Lett. <b>70B</b> , 487 (1977)
22.7	±5.5	22.1	±5.5	4.1–7.4	Lead-Glass Wall	A. Barbaro-Galtiero <i>et al.</i> , Phys. Rev. Lett. <b>39</b> , 1058 (1977)
18.5±2.8±1.4	±3.1	18.0±2.8±1.4	±3.1	3.9–5.2	DASP	R. Brandelik <i>et al.</i> , Phys. Lett. <b>73B</b> , 109 (1978)
17.6±0.6±1.0	±1.3	17.1±0.6±1.0	±1.3	3.5–6.7	Mark II	C. A. Blocker <i>et al.</i> , Phys. Lett. <b>109B</b> , 119 (1982)
18.2±0.7±0.5	±0.9	18.0±1.0±0.6	±1.2	3.8	Mark III	R. M. Baltrusaitis <i>et al.</i> , Phys. Rev. Lett. <b>55</b> , 1842 (1985)
17.4±0.8±0.5	±0.9	17.7±0.8±0.5	±0.9	29.0	MAC	W. W. Ash <i>et al.</i> , Phys. Rev. Lett. <b>55</b> , 2118 (1985)
18.4±1.2±1.0	±1.6	17.7±1.2±0.7	±1.4	29.0	TPC	H. Aihara <i>et al.</i> , Phys. Rev. D <b>35</b> , 1553 (1987)

# Results

TABLE VI. Means and standard deviations (SD) for  $B_1$ ,  $B_\rho$ ,  $B_\pi$ ,  $B_e$ , and  $B_\mu$ . Both quantities are in percent.

Branching fraction	Bootstrap (method A)		Analysis method Bootstrap with weighted measurements (method C)		Normal-error method from Ref. 1	
	Mean, 25% trimmed	SD	Mean, 25% trimmed	SD	Mean, not trimmed	Formal error
$B_1$	85.8	0.63	86.9	0.36	86.6	0.28
$B_\rho$	22.5	0.35	22.5	0.19	22.5	0.85
$B_\pi$	10.2	0.55	10.8	0.45	10.8	0.60
$B_e$	18.3	0.38	17.8	0.30	17.6	0.44
$B_\mu$	18.2	0.56	17.8	0.21	17.7	0.41

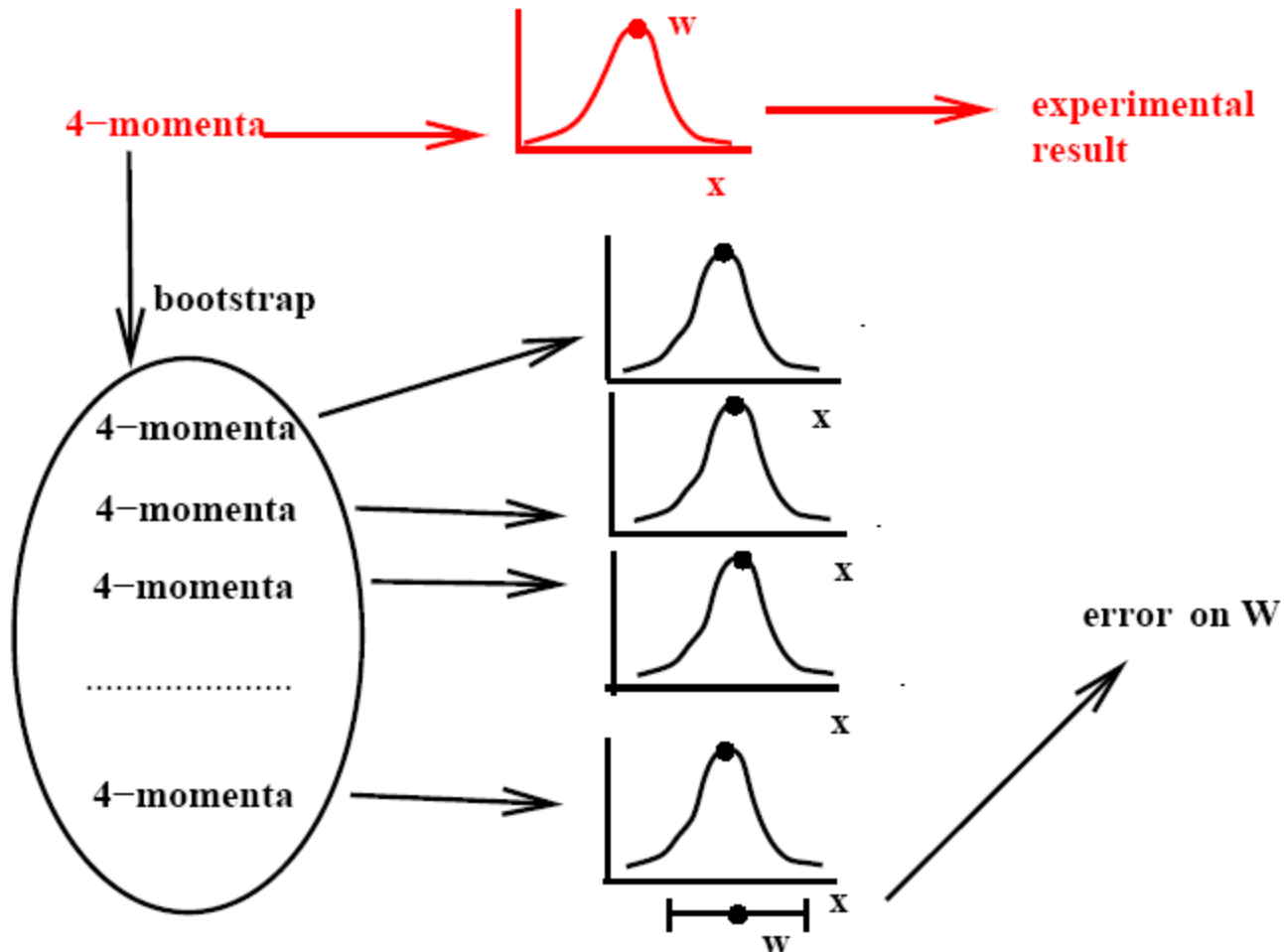
Bootstrap:  $\frac{85.8 - 81.3}{\sqrt{1.3^2 + 0.6^2}} = 3.1$

Standard analysis:  $\frac{86.6 - 80.6}{\sqrt{1.5^2 + 0.3^2}} = 3.9$

Some **data** are unreliable

# The non parametric BOOTSTRAP

A possible use of the Bootstrap in Nuclear physics



## BOOTSTRAP FOR COMPARING TWO POPULATIONS

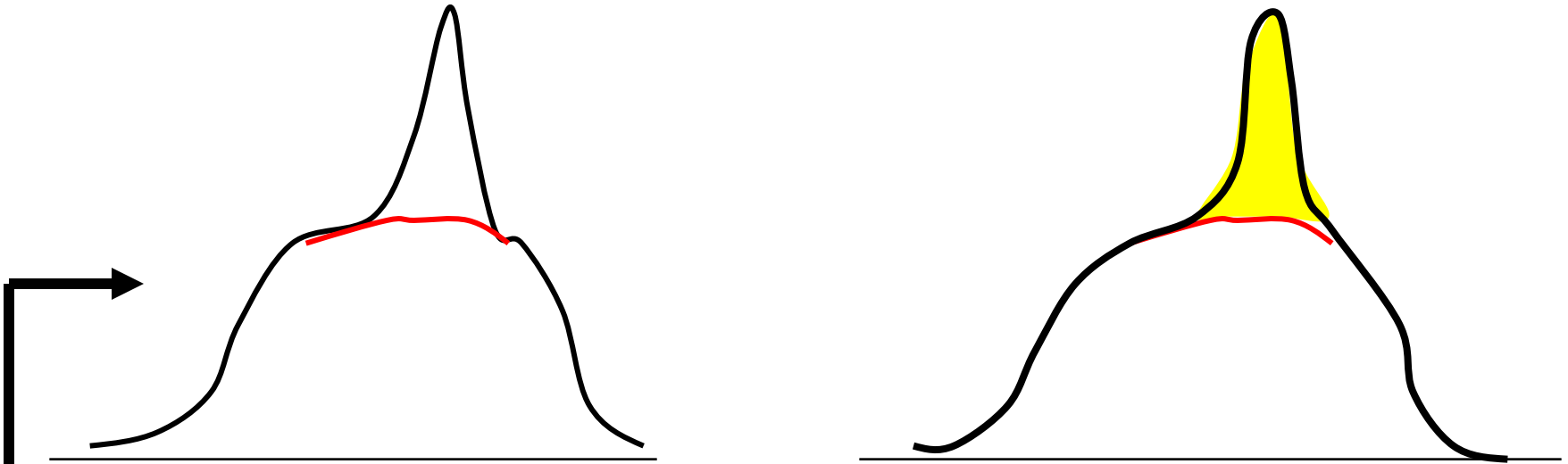
Given independent SRSs of sizes  $n$  and  $m$  from two populations:

1. Draw a resample of size  $n$  with replacement from the first sample and a separate resample of size  $m$  from the second sample. Compute a statistic that compares the two groups, such as the difference between the two sample means.
2. Repeat this resampling process hundreds of times.
3. Construct the bootstrap distribution of the statistic. Inspect its shape, bias, and bootstrap standard error in the usual way.

Useful when the two samples are  
**signal** and **background**....



# The dual Bootstrap



Fix the background on one sample and  
calculated the peak signal  
with another sample to avoid biases !!

Repeat on bootstrap samples (dual bootstrap)

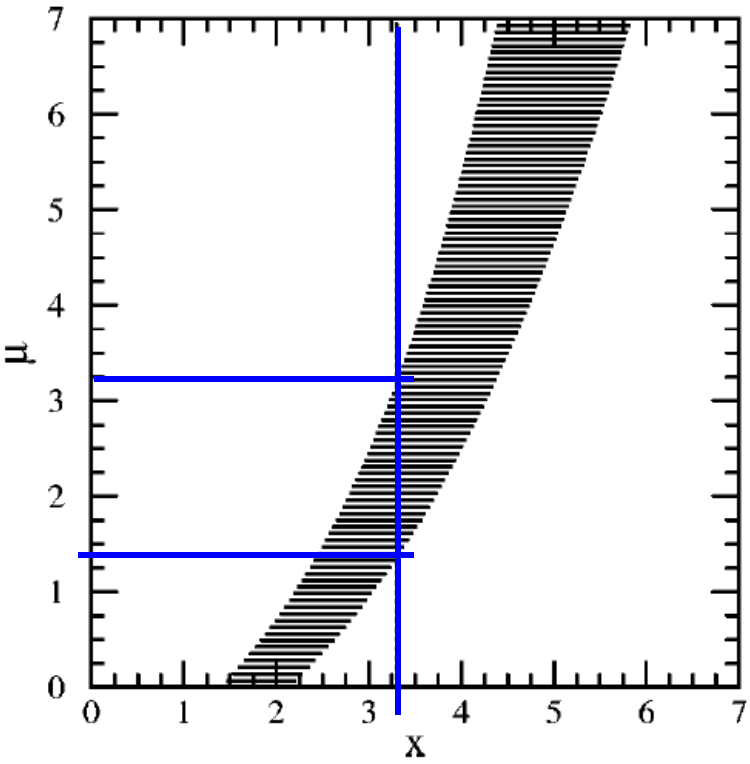
## Standard analysis in nuclear physics experiments

- the 4-momenta are reconstructed and the analysis is performed
- errors are calculated following the standard (gaussian) theory
- a MC toy model is invented and the analysis procedure is checked on this model
- at this point the procedure could be further checked on bootstrapped data!

# Conclusions

- **Poissonian Counting**: most of the tests do not consider the error on background and overestimate the signal. Often true (mean) values and measured values are improperly confused.
- **Binomial counting**: a general theory there exists and should be applied.
- The **errors** should be calculated by MC methods and the procedure checked with MC toy models
- **Nonparametric Bootstrap** methods should be used also by physicists

# Some problems with frequentism and their cure



We restart from the Neyman construction

True value

Observed value



**Neyman's prescription:**

Before doing an experiment, for each possible Value of theory parameters determine a region of data that occurs C.L. of the time, say 90%.

## Some frequentist problems - I

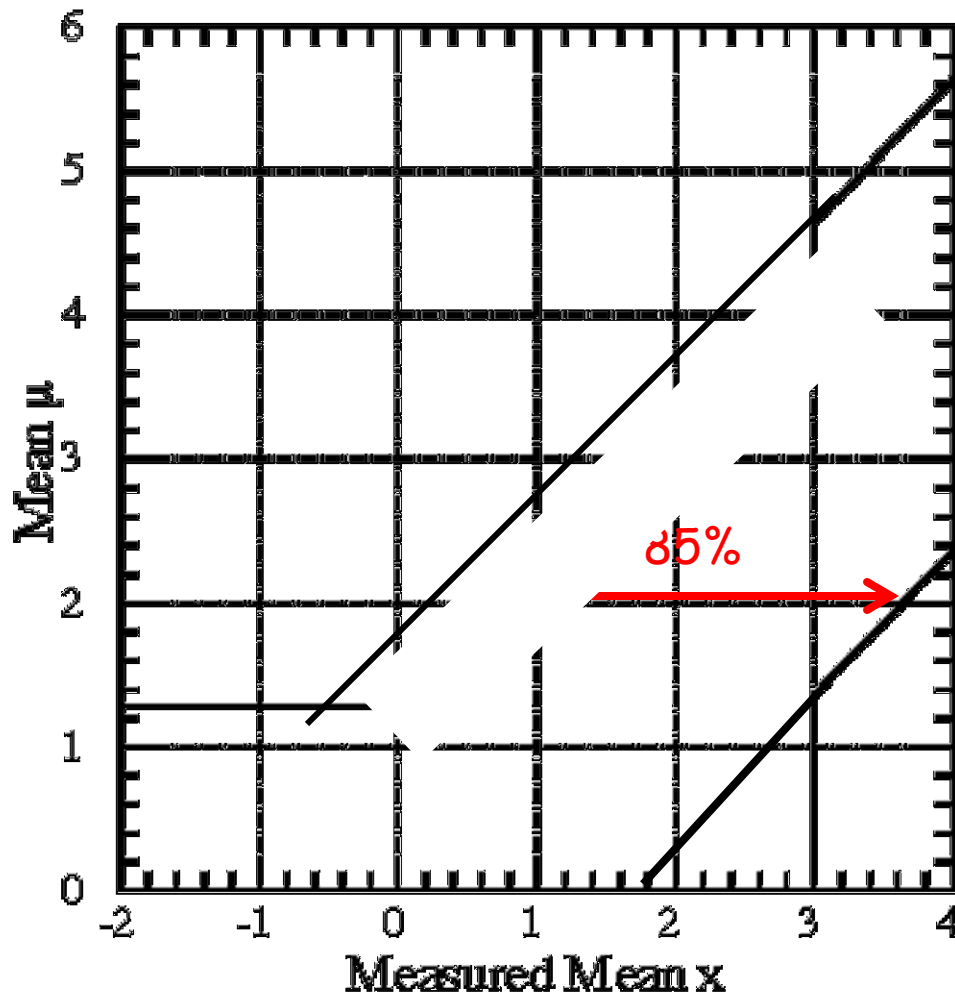
A Gaussian upper limit estimate with  $CL = 90\%$  when physics says that **the true value is  $\mu \geq 0$** .

If a negative value  $x < -1.28\sigma$  is obtained, we find an unphysical upper limit  $\mu < 0$  !

A solution, the FLIP-FLOP technique:

when  $x < 0$  one assumes the upper limit for  $x = 0$ , that is  $\mu = 1.28\sigma$

**WRONG!:** one finds an 85% upper limit



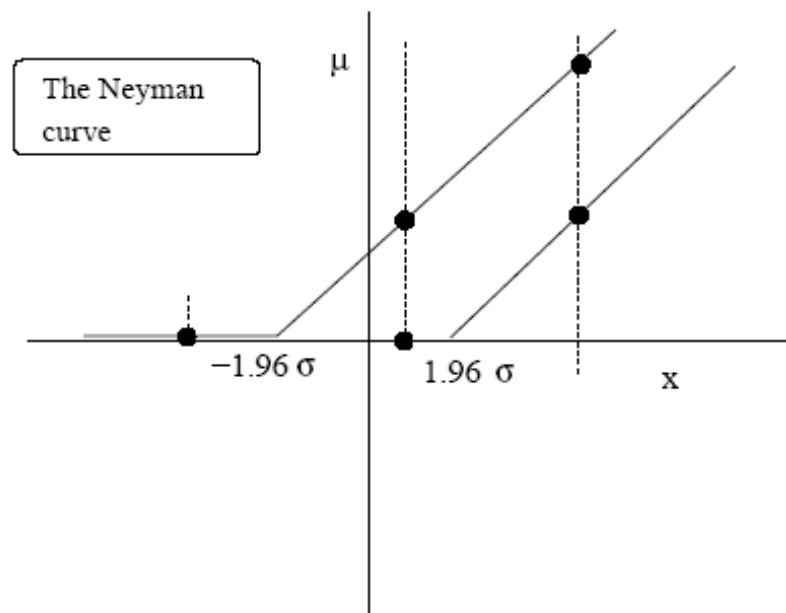
When  $\mu = 2$  there is only 85% coverage!  
 Due to flip-flopping (deciding whether to use an upper limit  
 or a central confidence region based on the data)  
 these are not valid confidence intervals.

## Some frequentist problems - I

If  $\mu > 0$  an interval with correct coverage  
(i.e.  $CL = 95\%$ ) is

$$\mu \in \begin{cases} (x - 1.96\sigma, x + 1.96\sigma) & x > 1.96\sigma \\ (0, x + 1.96\sigma) & \text{WHEN } -1.96\sigma < x < 1.96\sigma \\ 0 & x < -1.96\sigma \end{cases}$$

Here the coverage is correct

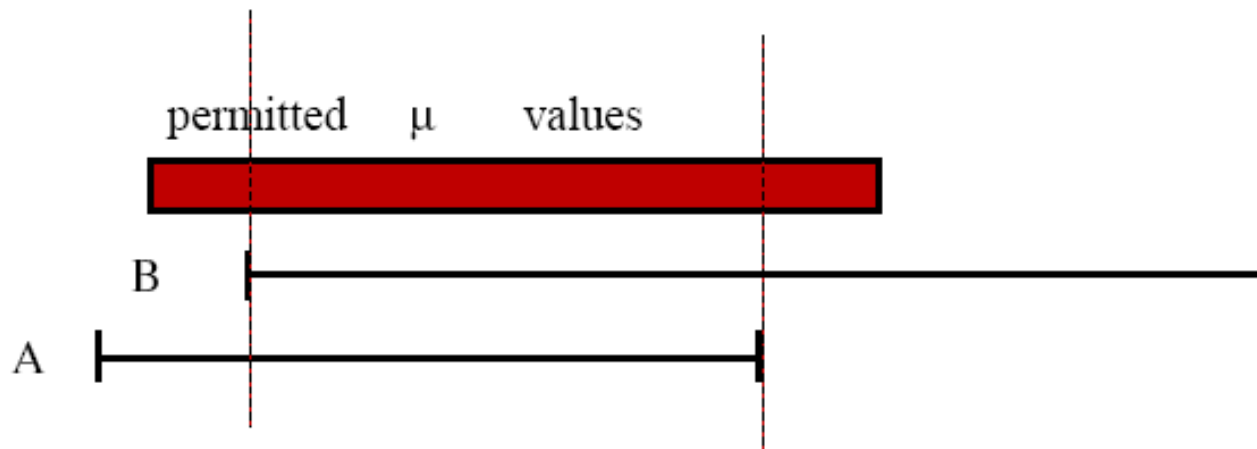


BUT, when  $x < -1.96\sigma$  we have  $\mu = 0$

Are we Happy?



## Not only the COVERAGE!!



**A and B have the same coverage but**

**A minimizes the probability to contain  
wrong  $\mu$  values**

**The A interval is the result of a  
more powerful estimator  
New concepts are necessary**

## Some frequentist problems - II

A counting experiment with background

$$P(n; \mu, b) = \frac{(n + b)^n}{n!} e^{-(\mu+b)}$$

The background  $b$  is known, the counts  $n$  are measured.

Find the **upper limit** for the  $\mu$  parameter with a fixed  $CL$ , for example 90%

$b/n$	0	1	2	3	4
0	2.30	3.89	5.32	6.68	7.99
1	1.30	2.89	4.32	5.58	6.99
2	0.30	1.89	3.32	4.68	5.99
3	<b>-0.79</b>	0.89	2.32	3.68	4.99

When no events are counted, an experiment with an expected background of 3 events measures a negative upper limit for the expected value of the counts!!

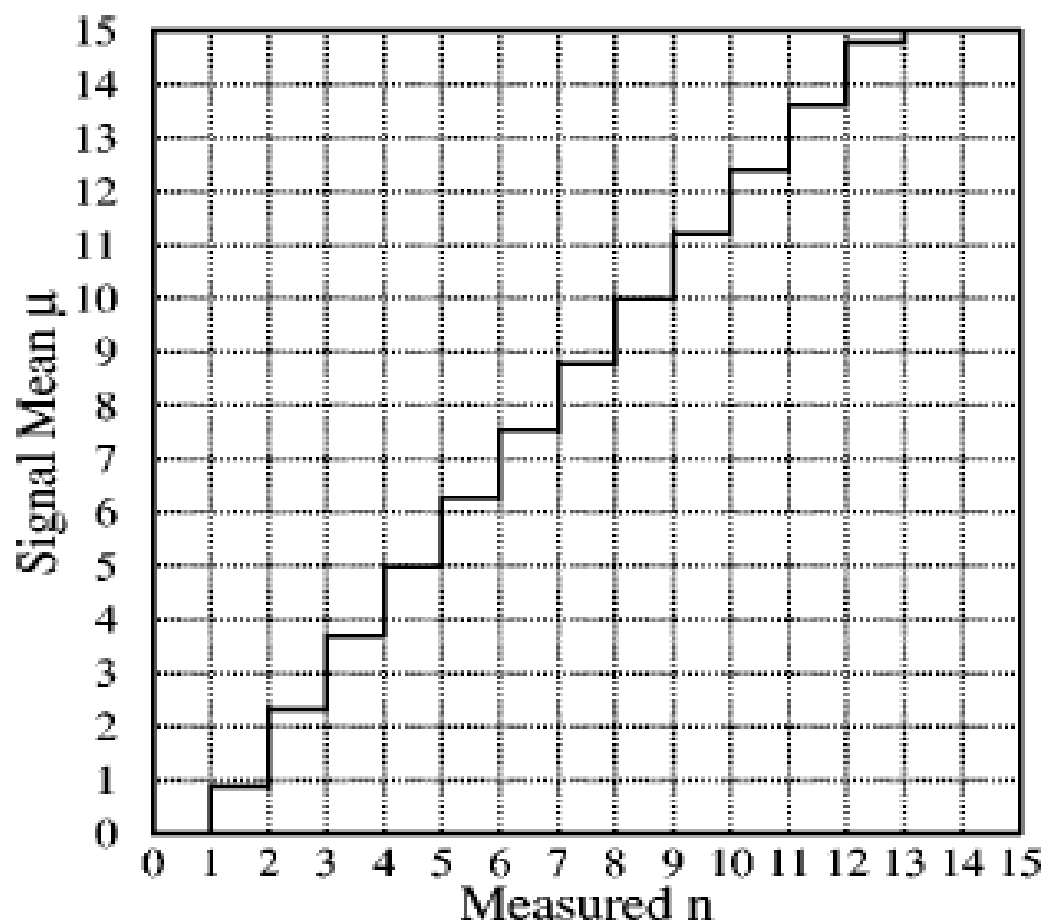


FIG. 5. Standard confidence belt for 90% C.L. upper limits, for unknown Poisson signal mean  $\mu$  in the presence of a Poisson background with known mean  $b = 3.0$ . The second line in the belt is at  $n = +\infty$ .

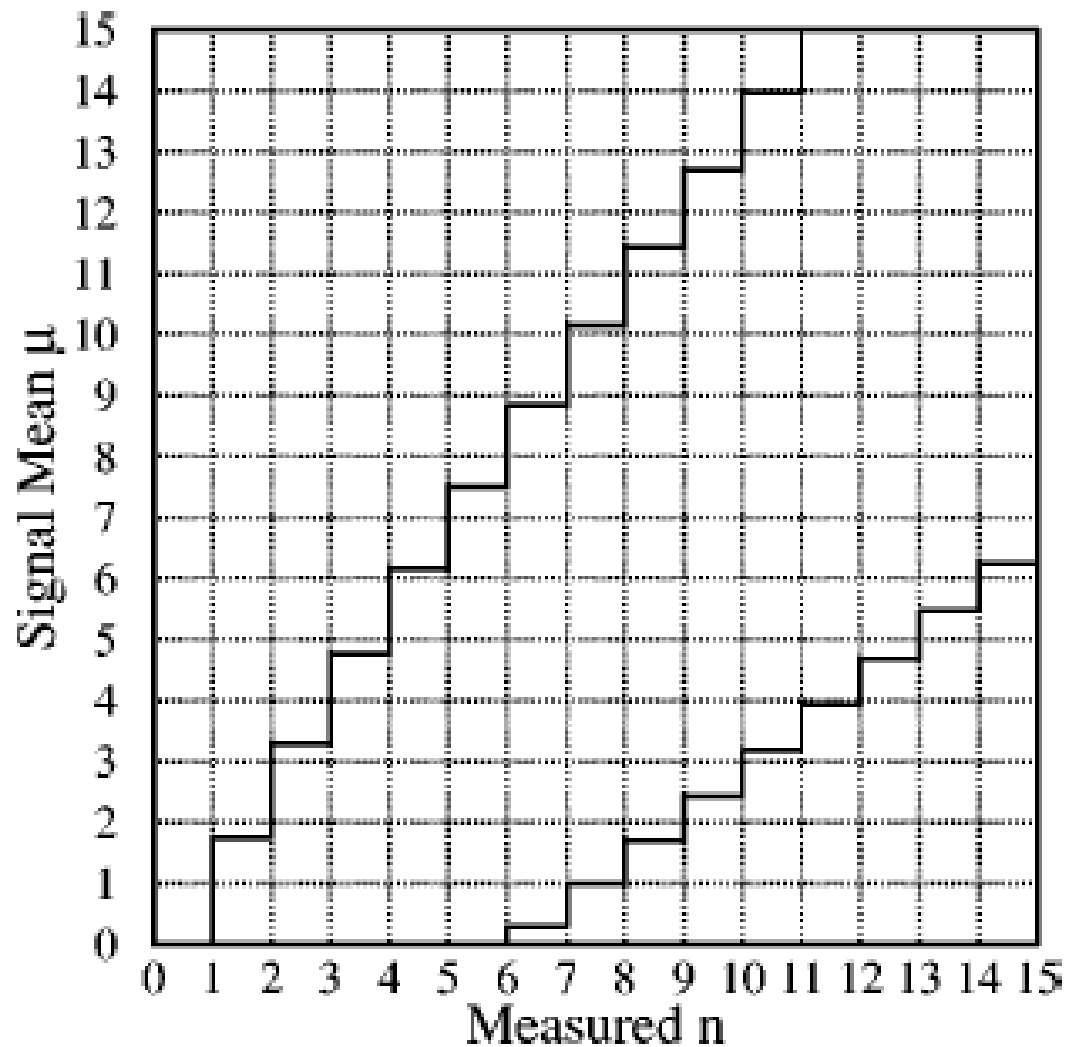


FIG. 6. Standard confidence belt for 90% C.L. central confidence intervals, for unknown Poisson signal mean  $\mu$  in the presence of a Poisson background with known mean  $b = 3.0$ .

**Unified approach to the classical statistical analysis of small signals**

Gary J. Feldman\*

*Department of Physics, Harvard University, Cambridge, Massachusetts 02138*

Robert D. Cousins†

*Department of Physics and Astronomy, University of California, Los Angeles, California 90095*

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We give a classical confidence belt construction which unifies the treatment of upper confidence limits for null results and two-sided confidence intervals for non-null results. The unified treatment solves a problem (apparently not previously recognized) that the choice of upper limit or two-sided intervals leads to intervals which are not confidence intervals if the choice is based on the data. We apply the construction to two related problems which have recently been a battleground between classical and Bayesian statistics: Poisson processes with background and Gaussian errors with a bounded physical region. In contrast with the usual classical construction for upper limits, our construction avoids unphysical confidence intervals. In contrast with some popular Bayesian intervals, our intervals eliminate conservatism (frequentist coverage greater than the stated confidence) in the Gaussian case and reduce it to a level dictated by discreteness in the Poisson case. We generalize the method in order to apply it to analysis of experiments searching for neutrino oscillations. We show that this technique both gives correct coverage and is powerful, while other classical techniques that have been used by neutrino oscillation search experiments fail one or both of these criteria.

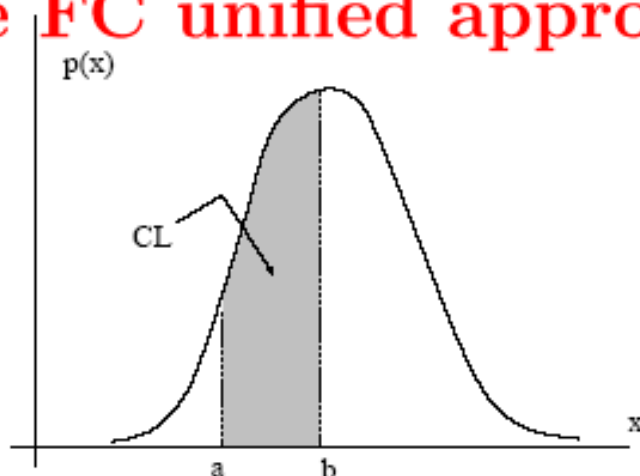
[S0556-2821(98)00109-X]

PACS number(s): 06.20.Dk, 14.60.Pq

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## The FC unified approach



$$R = \frac{p(x; \mu)}{\max [p(x; \mu)]} = \frac{p(x; \mu)}{p(x; \hat{\mu})}$$

$$CL = \sum_R p(x; \mu) \rightarrow \int_R p(x; \mu) dx$$

This **frequentist** approach is called **unified**:

- the technique for the one-sided and the two-sided intervals is the same (by FC)
- the approach merges the parameter estimate and the hypothesis testing techniques

For a **given  $CL$  and  $\mu$** , there are many  $(a, b)$  choices. The FC **ordering Principle (FCOP)**, inspired to the **NP theorem**, is to **choose the extremes  $a$  and  $b$  that cover the points ordered for decreasing values of**

# The FC Neyman curve

The idea is to use the **likelihood ratio**

$$R = \frac{p(x; \mu)}{p(x; \hat{\mu})} = \frac{L(\mu; x)}{L(\hat{\mu}; x)}$$

- $R \simeq 1 \rightarrow \mu \simeq \hat{\mu}$
- $R \simeq 0 \rightarrow \mu$  far from the ML estimate
- constraints on  $\mu$  are fully considered
- $P\{\mu \in I_{\text{FC}}\}$  minimum when  $\mu \neq \mu_{\text{true}}$

The method is officially recommended from PDG 1998

# The FC idea

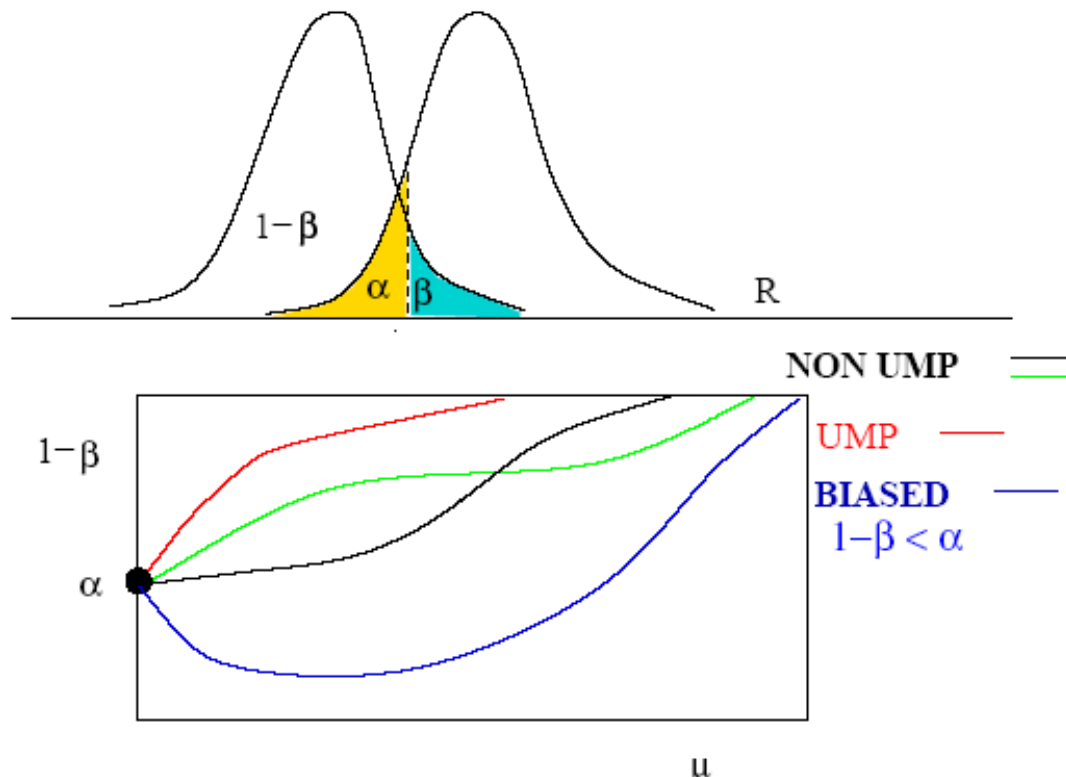
The ratio

$$R = \frac{L(\mu; x)}{L(\hat{\mu}; x)}$$

minimizes  $\beta$  and maximizes  $(1 - \beta)$

The  $R$  test tends to be **Uniformly Most Powerful**.

**The probability that  $I$  contains false  $\mu$  values is minimized**





# Poisson with background

## The FC method

$$P(n; \mu, b) = \frac{(n+b)^n}{n!} e^{-(\mu+b)}$$

$$\frac{\partial}{\partial \mu} \{(\mu+b)^n e^{-(\mu+b)}\} = e^{-(\mu+b)} [n(\mu+b)^{n-1} - (\mu+b)^n] = 0$$

Hence

$$\hat{\mu} = \begin{cases} n - b & \text{if } n > b \\ 0 & \text{otherwise} \end{cases} \rightarrow \hat{\mu} = \max(0, n - b)$$

The method when  $\mu = 0.5$ ,  $b = 3$ ,  $CL = 90\%$

This is only ONE POINT on the Neyman curve



$n$	$P(n; \mu, b)$	$\hat{\mu}$	$P(n; \hat{\mu}, b)$	$R$	score 90%
0	0.030	0	0.050	0.607	6
1	0.106	0	0.149	0.708	3
2	0.185	0	0.224	0.826	3
3	0.216	0	0.224	0.963	2
4	0.189	1	0.195	0.966	1
5	0.132	2	0.175	0.753	4
6	0.077	3	0.161	0.480	7
7	0.039	4	0.149	0.259	
8	0.017	5	0.140	0.121	
9	0.007	6	0.125	0.018	
10	0.002	7	0.125	0.006	

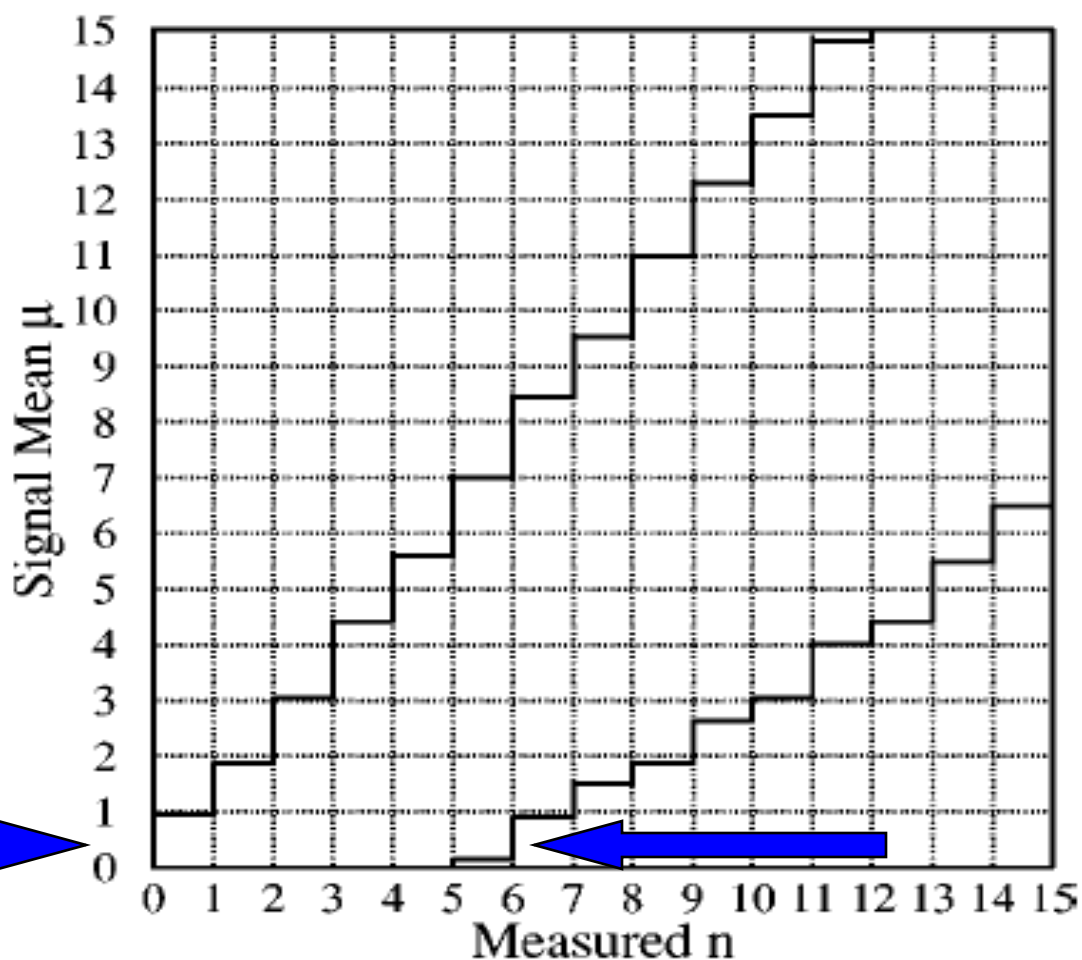


FIG. 7. Confidence belt based on our ordering principle, for 90% C.L. confidence intervals for unknown Poisson signal mean  $\mu$  in the presence of a Poisson background with known mean  $b = 3.0$ .

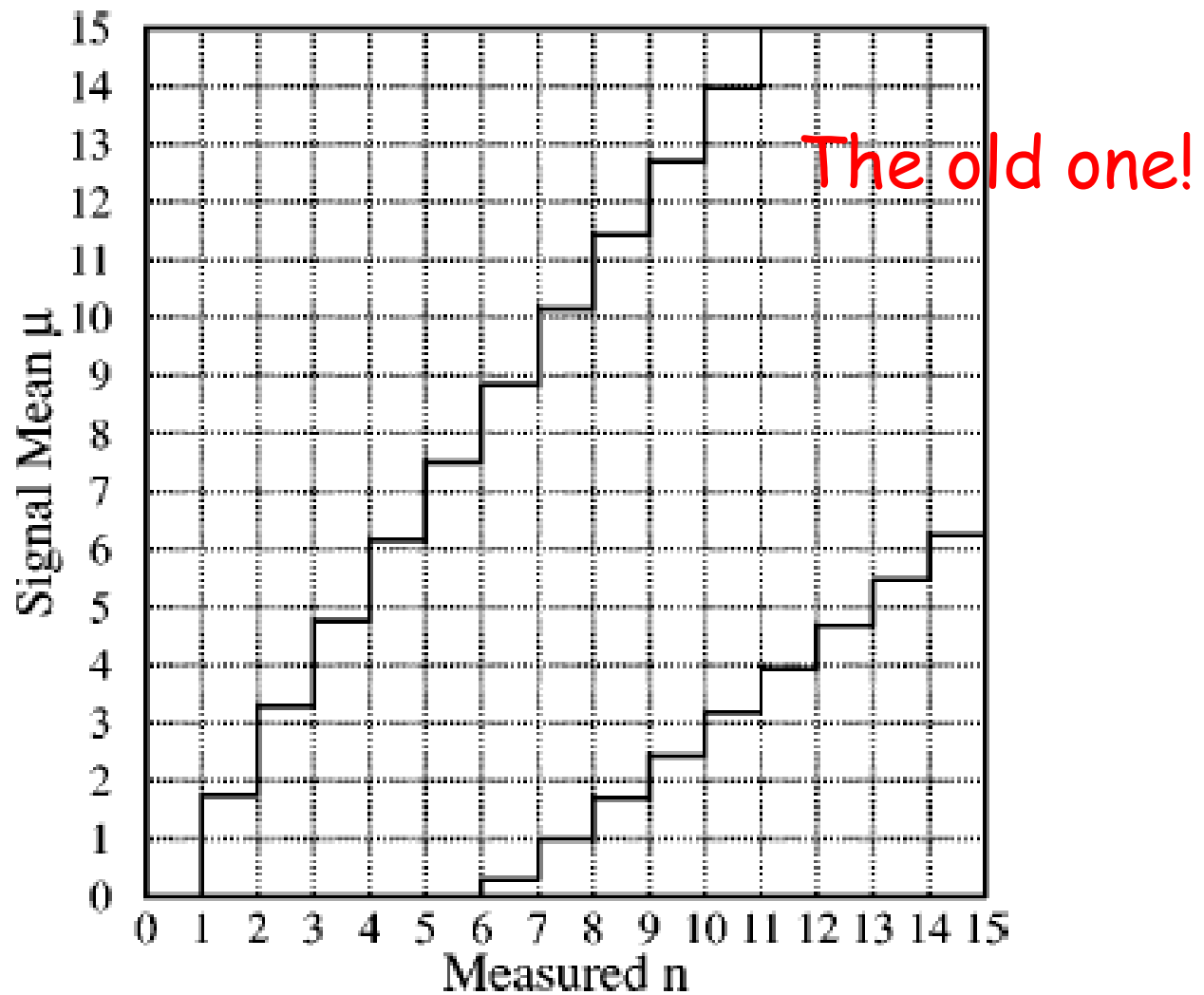
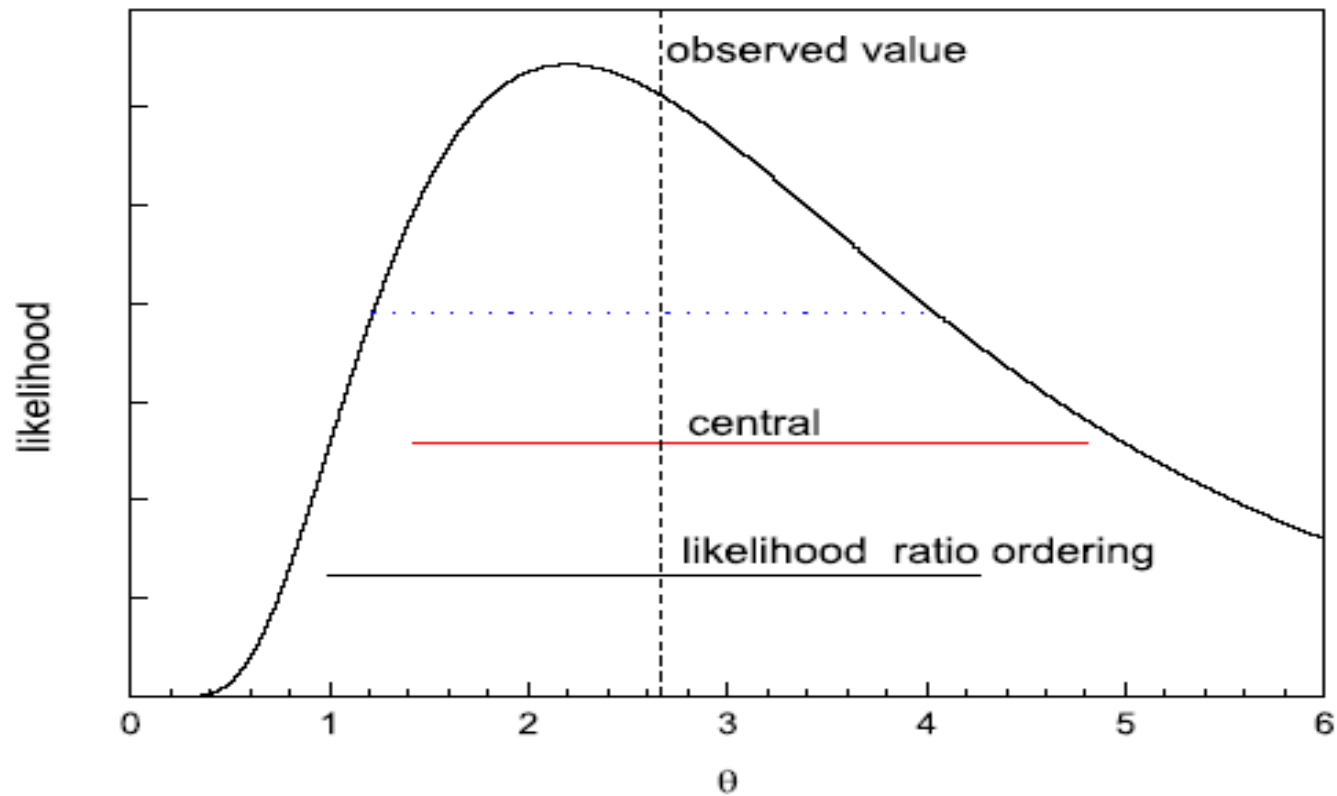


FIG. 6. Standard confidence belt for 90% C.L. central confidence intervals, for unknown Poisson signal mean  $\mu$  in the presence of a Poisson background with known mean  $b = 3.0$ .



**Fig. 4.** Position measurement from drift time. The error is due to diffusion. Classical confidence intervals are shown together with the likelihood function

# Gaussian with constraints

## The FC method

$$\frac{\partial}{\partial \mu} \left[ \exp \left[ -\frac{1}{2} \frac{(x - \mu)^2}{\sigma^2} \right] \right] = 0 \rightarrow \hat{\mu} = \begin{cases} x & \text{if } x \geq 0 \\ 0 & \text{if } x \leq 0 \end{cases} \rightarrow \max(0, x)$$

$$R = \frac{g(x; \mu)}{g(x; \hat{\mu})}, \quad \text{where } g(x; \hat{\mu}) = \begin{cases} \frac{1}{\sqrt{2\pi}} & x \geq 0 \\ \frac{\exp(-x^2/2)}{\sqrt{2\pi}} & x < 0 \end{cases}$$

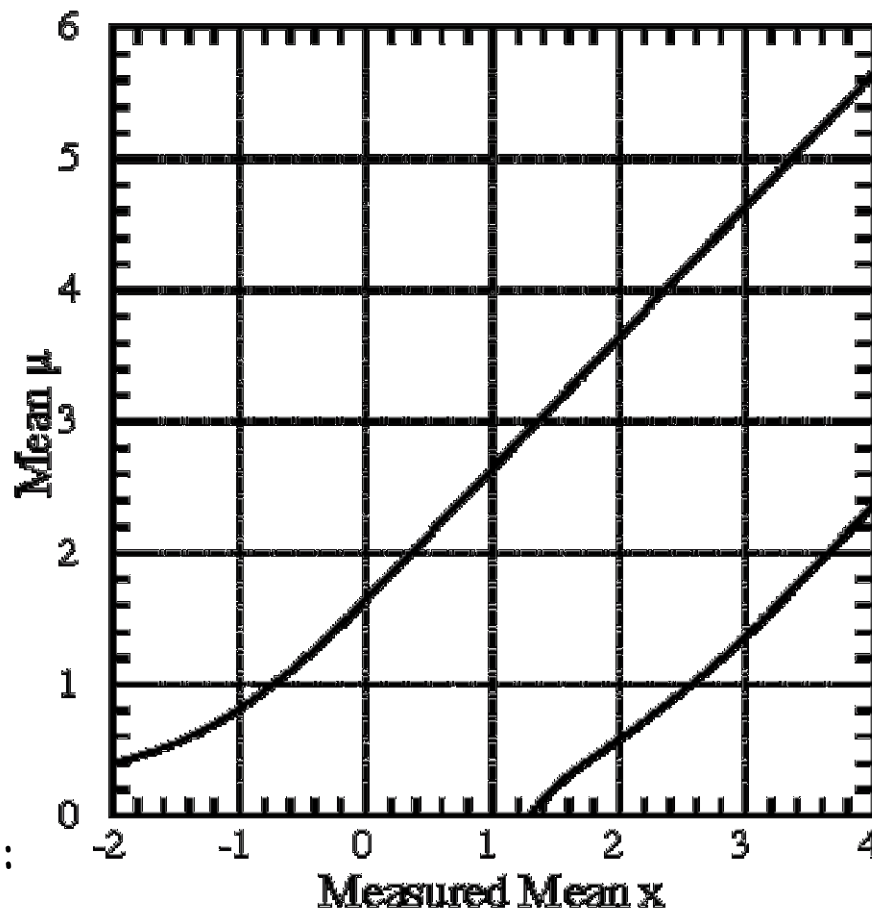
$$R = \begin{cases} e^{-(x-\mu)^2/2} & x \geq 0 \\ e^{(x\mu-\mu^2/2)} & x < 0 \end{cases} \quad \begin{matrix} \mathbf{m} > \\ \mathbf{0} \end{matrix}$$

**Then, the Neyman construction:**

One determines the order in which the values of  $x$  are integrated.

That is, **for any value of  $\mu$** , one determines the interval  $[x_1, x_2]$  such that  $R(x_1) = R(x_2)$  and that

$$\int_{x_1}^{x_2} g(x; \mu) dx = CL$$



From Feldman notes:

- (1) This approaches the central limits for  $x \gg 1$ .
- (2) The upper limit for  $x = 0$  is 1.64, the two-sided rather than the one-sided limit.
- (3) From the defining 1937 paper of Neyman, this is the only valid confidence belt, since there are 4 requirements for a valid belt:
  - (a) It must cover.
  - (b) For every  $x$ , there must be at least one  $\mu$ .
  - (c) No holes (only valid for single  $\mu$ ).
  - (d) Every limit must include its end points.

## A famous Paradox

An experiment that measures less events than the **expected** background, will report

**a better (lower) upper limit**

than an identical experiment which measures a number of events equal to the background

If no events are detected, the experiment with expected background will find

**a better upper limit**

than the experiment with no background.

## A famous Paradox

Standard frequentist result:  
counts with background,  $CL = 90\%$ , the  
upper limits improves when  $\mu_b$  increases

$\frac{n \rightarrow}{\mu_b}$	0	1	2	3	4
0.0	2.30	3.89	5.32	6.68	7.99
0.5	1.80	3.39	4.82	6.18	7.49
1.0	1.30	2.89	4.32	5.58	6.99
2.0	0.30	1.89	3.32	4.58	5.99

**A paradox?**

**YES** from the Bayesian point of view

$$P(H|\text{data})$$

**NO** from the frequentist point of view

$$P(\text{data}|H)$$

It implies simply that the upper limit  
“improves”, but in a small number  
of experiments, when  $n < \mu_b$



## A frequentist remedy: the Sensitivity

- a  $\mu_b$  value is fixed
- some Poisson data are generated via MC

$$p(x; \mu_b) = \frac{\mu_b^x}{x!} e^{-\mu_b}$$

- the FC average upper limit is found for a given  $CL$

# The sensitivity

Our suggestion for doing this is that in cases in which the measurement is less than the estimated background, the experiment reports both the upper limit and the “sensitivity” of the experiment, where the “sensitivity” is defined as the **average** upper limit that would be obtained by an ensemble of experiments with the expected background and no true signal. Table XII gives these values, for the case of a measurement of a Poisson variable.

TABLE XII. Experimental sensitivity (defined as the average upper limit that would be obtained by an ensemble of experiments with the expected background and no true signal), as a function of the expected background, for the case of a measurement of a Poisson variable.

$b$	68.27% C.L.	90% C.L.	95% C.L.	99% C.L.
0.0	1.29	2.44	3.09	4.74
0.5	1.52	2.86	3.59	5.28
1.0	1.82	3.28	4.05	5.79
1.5	2.07	3.62	4.43	6.27
2.0	2.29	3.94	4.76	6.69
2.5	2.45	4.20	5.08	7.11
3.0	2.62	4.42	5.36	7.49
3.5	2.78	4.63	5.62	7.87
4.0	2.91	4.83	5.86	8.18
5.0	3.18	5.18	6.32	8.76
6.0	3.43	5.53	6.75	9.35
7.0	3.63	5.90	7.14	9.82
8.0	3.86	6.18	7.49	10.27
9.0	4.03	6.49	7.81	10.69
10.0	4.20	6.76	8.13	11.09
11.0	4.42	7.02	8.45	11.46
12.0	4.56	7.28	8.72	11.83
13.0	4.71	7.51	9.01	12.22
14.0	4.87	7.75	9.27	12.56
15.0	5.03	7.99	9.54	12.90

# The Unified Approach in two (or more) dimensions

One has to estimate the  $(x, y)$  CL regions and sometimes the  $z$  confidence region

$$z = f(x, y)$$

having measured  $x_m$  and  $y_m$ .

- the **Likelihood Ratio** is chosen as:

$$R = \frac{L(x, y; \mu)}{L(x, y; \hat{\mu})} \rightarrow$$

$$-2 \ln R = -2[\ln L(x, y; \mu) - \ln L(x, y; \hat{\mu})] \simeq \chi^2(\hat{\mu})$$

- for a given  $CL$  a  $\mu_x$  and  $\mu_y$  **map** is made, calculating at each point the quantile

$$R \leq R_{1-CL}$$

where

$$\int_0^{R_{1-CL}} g(R) \, dR = 1 - CL$$

When the  $R$ -space is constrained or complicated MC integration must be used.

- when we have to find  $z = f(x, y)$  a second map must be generated (usually via MC) for each  $(\mu_x, \mu_y)$  with the values

$$z_{1-CL/2} \quad , \quad z_{1-(1-CL)/2}$$

# The Unified Approach in two (or more) dimensions

- Now the

$$(\mu_x, \mu_y)$$

plane is mapped with three numbers:

$$R_{1-CL} \quad , \quad z_{1-CL/2} \quad , \quad z_{1-(1-CL)/2}$$

- the acceptance region  $(\mu_x, \mu_y)_{CL}$  is defined by

$$R(x_m, y_m) < R_{1-CL}$$

$$z_{1-CL/2} \leq z_m = f(x_m, y_m) \leq z_{1-(1-CL)/2}$$

# The Unified Approach in two (or more) dimensions

When we have  $x_i$  **gaussian variables**  $\sim N(\mu_i, \sigma_i^2)$

$$-2 \ln R = \Delta \chi^2 = \sum_i \left[ \frac{(x_i - \mu_i)^2}{\sigma_i^2} - \frac{(x_i - \hat{\mu}_i)^2}{\sigma_i^2} \right]$$

When there are no cuts or constraints

$$\hat{\mu}_i = x_i$$

and we reobtain the usual  $\chi^2$ .

In the case of **Poisson variables** we have

$$-2 \ln \left[ \frac{\prod_i \mu_i^{x_i} e^{-\mu_i}}{\prod_i \hat{\mu}_i^{x_i} e^{-\hat{\mu}_i}} \right] = 2 \sum_i [\mu_i - x_i \ln \mu_i - \hat{\mu}_i + x_i \ln \hat{\mu}_i]$$

When there are no cuts or constraints:

$$-2 \ln R = 2 \sum_i [\mu_i - x_i \ln \mu_i - x_i + x_i \ln x_i]$$

# Example

Ratio of two gaussians  $z = x/y$ , comparison of three methods

- **standard**

$$\sigma[z] = \frac{x}{y} \sqrt{\frac{\sigma_x^2}{x^2} + \frac{\sigma_y^2}{y^2}}$$

- **bootstrap:**

sample from two gaussian of average  $x$  and  $y$  (measured value), take the ratio, make the histogram and find the two quantiles  $z_{1-CL/2}$  and  $z_{1-(1-CL)/2}$ .

- **unified method:** find

$$R(x_m, y_m) < R_{1-CL}$$

$$z_{1-CL/2} \leq z_m = f(x_m, y_m) \leq z_{1-(1-CL)/2}$$

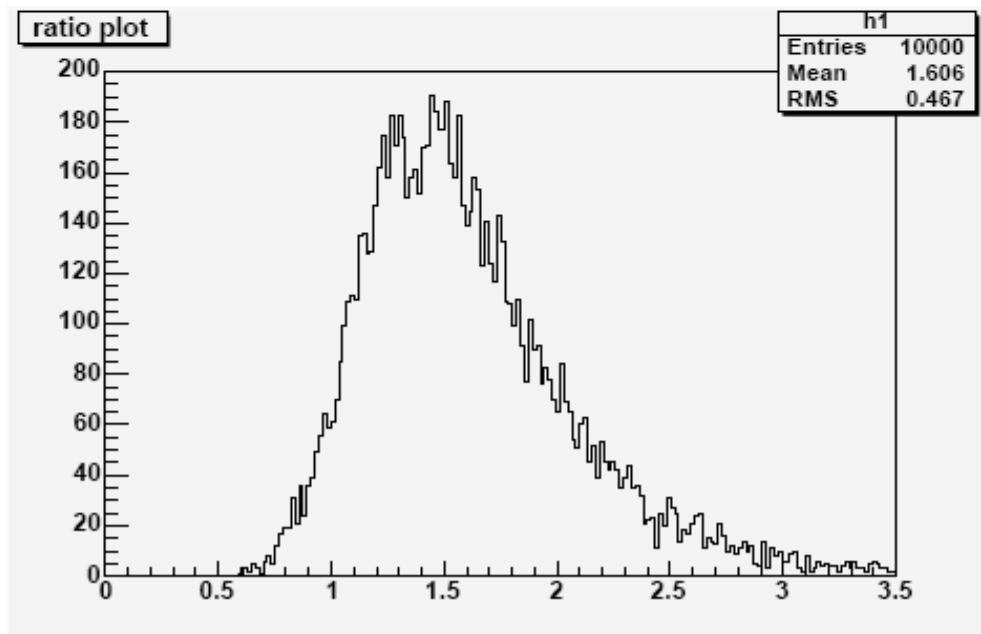
# Example

Measured

$$x = 20 \quad y = 13 \quad \sigma_x = \sigma_y = 3$$

$z = x/y$  interval with  $CL = 0.683$ ;  
coverage calculated with MC:

- **standard:**  $z = 0.730 \pm 0.002$ ;
- **bootstrap**  $z = 0.700 \pm 0.002$ ;
- **unified:**  $z = 0.696 \pm 0.002$ ;





# Example

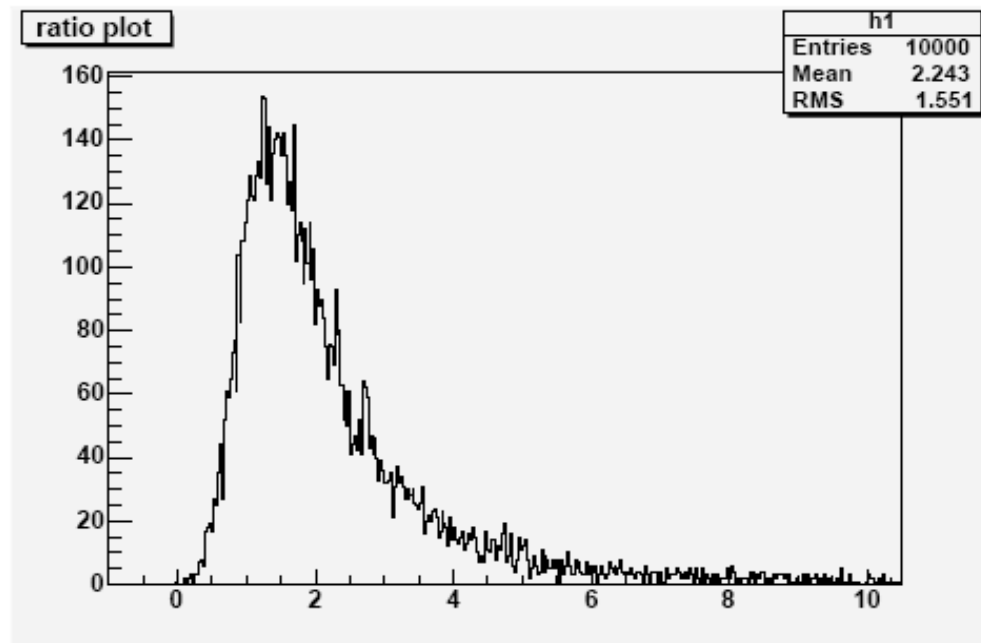
Measured

$$x = 11 \quad y = 6 \quad \sigma_x = \sigma_y = 3$$

$z = x/y$  interval with  $CL = 0.683$

with the cut  $y > 0$ :

- **standard:**  $z = 0.774 \pm 0.002$ ;
- **bootstrap**  $z = 0.736 \pm 0.002$ ;
- **unified:**  $z = 0.686 \pm 0.002$ ;



# Neutrino Oscillations

The QM probability is:

$$P(\nu_\mu \rightarrow \nu_e) = \sin^2(2\theta) \sin^2\left(\frac{1.27\Delta m^2 L}{E}\right)$$

$L$  is the distance (km),  $E$  is the energy in GeV and  $\Delta m^2 = |m_1^2 - m_2^2|$  is  $(\text{eV}/c^2)^2$ .

The result is plotted in the  $\Delta m^2$  vs.  $\sin^2(2\theta)$  plane

The goal is the search for an  $\nu_e$  excess (the signal) over the normal  $\nu_e$  background.

The data are usually a bin content, the signal  $n_i$  and the backg.  $b_i$ .

The expected number of event is:

$$\mathbf{m}_{\text{true}} = \mathbf{F} \left( \sin^2(2\theta) \sin^2\left(\frac{1.27\Delta m^2 L}{E}\right) \right)$$

The frequentist test is

$$\chi^2 = \sum_i \frac{(n_i - b_i - \mu_i)^2}{\sigma_i^2}$$

## Frequentist neutrino Monte Carlo

The starting point is the key formula:

$$2\Delta[\ln L] \equiv 2 \left( \ln L(\hat{\theta}) - \ln L(\theta) \right) = \chi_{\alpha}^2(1) ,$$

Recall that from probability calculus

$$\sum_i^n \frac{(X_i - \mu_{\text{true}})^2}{\sigma^2} \sim \chi^2(n)$$

and **asymptotically**, in statistics

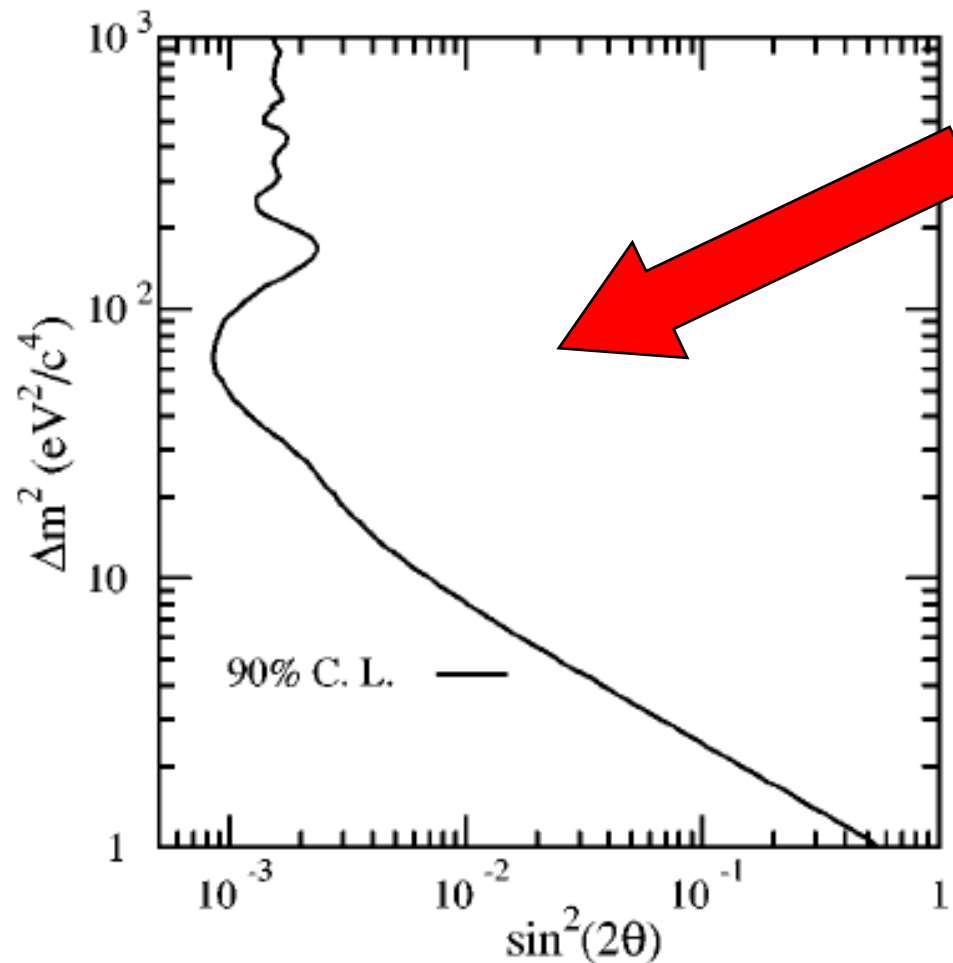
$$\underbrace{\sum_i^n \frac{(X_i - \mu(p)_{\text{true}})^2}{\sigma^2}}_{n \text{ d.o.f.}} - \underbrace{\sum_i^n \frac{(X_i - \hat{\mu}(p))^2}{\sigma^2}}_{(n-p) \text{ d.o.f.}} \sim \underbrace{\chi^2(p)}_{p \text{ d.o.f.}}$$

For  $CL = 90\%$  and two parameters

$$\chi^2(\sin^2(2\theta), \Delta m^2) - \chi^2(\text{best}) \leq 4.6$$

The region is given by the points with  $\chi^2$  within 4.6 of the minimum  
(**acceptances neglected**)

## The acceptance zone for no oscillations (Hypothesis)



if the experiment falls here, we can reject the hypothesis with 90% CL

FIG. 11. Calculation of the confidence region for an example of the toy model in which  $\sin^2(2\theta)=0$ . The 90% confidence region is the area to the left of the curve.

## Frequentist neutrino Monte Carlo

Another method is the **Raster Scan**  
A **grid** is made for each  $\Delta m^2$  value:

$$\Delta\chi^2 = \sum_i^n \frac{(n_i - b_i - \mu_i \text{ true}(\sin^2(2\theta)))^2}{\sigma_i^2}$$
$$- \sum_i^n \frac{(n_i - b_i - \hat{\mu}_i(\sin^2(2\theta)))^2}{\sigma_i^2} \leq (1.65)^2$$

$\chi^2$  is calculated as a function of  $\sin^2(2\theta)$   
Raster Scan gives an exact coverage  
but **does not give the optimum coverage**.

The point is that  $\hat{\mu}$  is found on one parameter only, without taking into account the compound probability of both  $(\sin^2(2\theta), \Delta m^2)$ , as required by the  $R$  test

# Unified Approach (FC)

## Monte Carlo

The correct method  
applies the FC ordering principle

$$2 \ln R = \Delta\chi^2 = \sum_i^n \frac{(n_i - b_i - \mu_i)^2}{\sigma_i^2} - \sum_i^n \frac{(n_i - b_i - \hat{\mu}_i)^2}{\sigma_i^2}$$

- $\forall[\sin^2(2\theta), \Delta m^2]$  a set of  $n_i, b_i$  values is simulated;
- for each point, the true value

$$\mu_i \rightarrow \sin^2(2\theta) \sin^2\left(\frac{1.27\Delta m^2 L}{E}\right)$$

is calculated with the model,

here the  
cuts are  
Taken into  
account



$$\mu_{\text{best}} \equiv \hat{\mu}$$

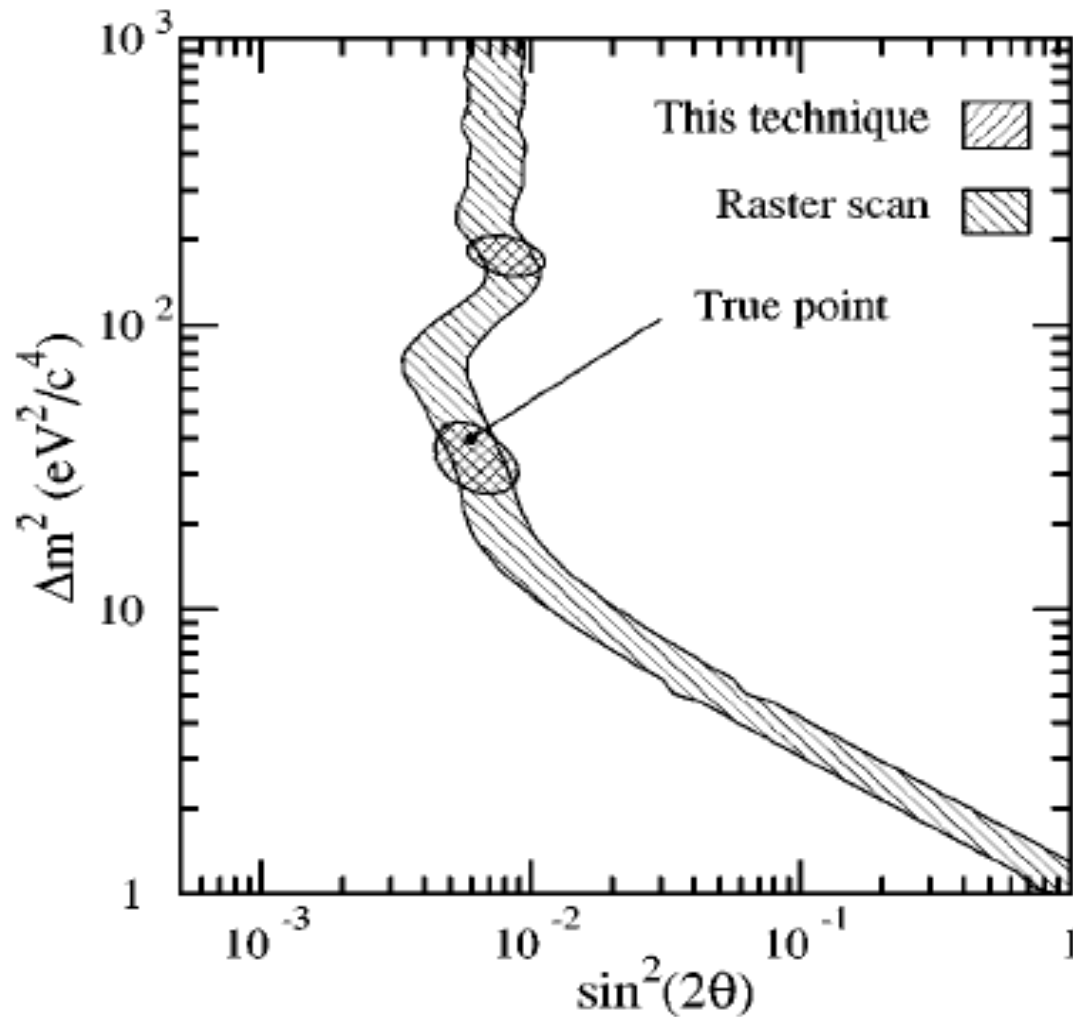
gives the highest probability for the physically allowed values

- $\forall[\sin^2(2\theta), \Delta m^2]$  the **quantile**  $\chi_{CL}^2$  is calculated

$$P\{\Delta\chi^2 \leq \Delta\chi_{CL}^2\} = CL$$

- when **one** experiment gives  $\{n_i, b_i\}$ , the acceptance region is

$$\Delta\chi^2(n_i, b_i; \sin^2(2\theta), \Delta m^2) \leq \chi_{CL}^2$$



**This is a really  
a good result!**

FIG. 12. Calculation of the confidence regions for an example of the toy model in which  $\Delta m^2 = 40 \text{ (eV}/c^2\text{)}^2$  and  $\sin^2(2\theta) = 0.006$ , as evaluated by the proposed technique and the raster scan.

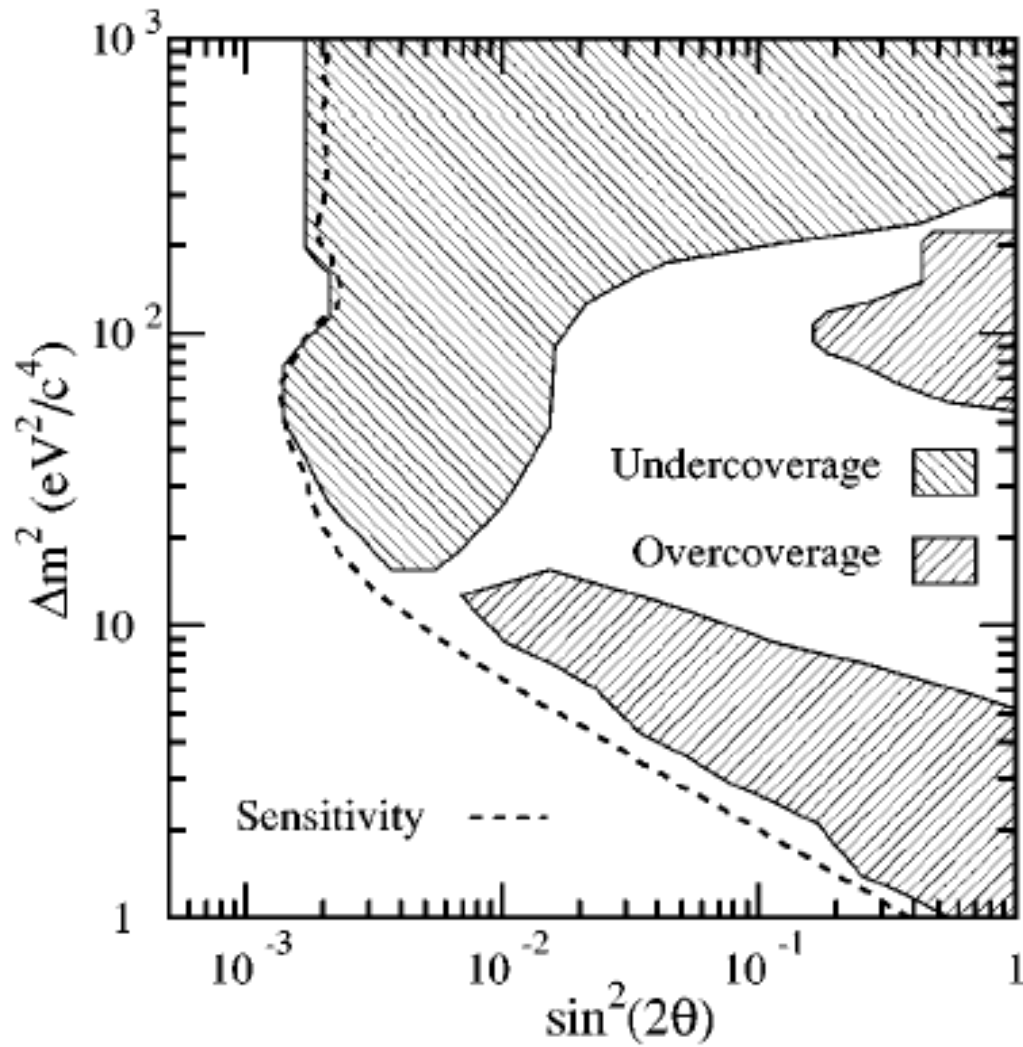


FIG. 14. Regions of significant under- and overcoverage for the global scan.



TABLE XI. Properties of the proposed technique for setting confidence regions in neutrino oscillation search experiments and three alternative classical techniques defined in the text.

Technique	Always gives useful results	Gives proper coverage	Is powerful
Raster scan		√	
Flip-flop raster scan			
Global scan			√
Proposed technique	√	√	√

# Some frequentist problems III

A lifetime measurement gives

$$t = 1 \text{ s}$$

Evaluate the lifetime  $\lambda$  with  $\alpha \equiv CL = 0.683$ .

We use the method of the **pivot quantity** (which is in this case  $q = \lambda t$ ):

$$p(t; \lambda) dt = \lambda e^{-\lambda t} dt = e^{-q} dq$$

Hence we use the pivotal equality

$$P\{q_1 < q(t; \lambda) < q_2\} = P\{\lambda_1(q_1) < \lambda < \lambda_2(q_2)\} = \alpha = CL$$

Then, the interval is

$$\int_{q_1}^{q_2} e^{-q} dq = e^{-q_1} - e^{-q_2} = \alpha \equiv CL$$

$$q_2 = -\ln(e^{-q_1} - \alpha)$$

$$\frac{q_1}{t} < \lambda < \frac{q_2}{t} = -\frac{\ln(e^{-q_1} - \alpha)}{t}$$

$\partial/\partial q_1 = 0$  gives the minimum interval as

$$0 < \lambda \leq -\frac{1}{t} \ln(1 - CL)$$

$$0 < \lambda \leq 1.15 \text{ s}^{-1}$$

# A Paradox: the lifetime measurement II

$$0 < \lambda \leq -\frac{1}{t} \ln(1 - CL)$$

$$0 < \lambda \leq 1.15 \text{ s}^{-1}$$

If one works in terms of  $\tau = 1/\lambda$  and repeats the same procedure, finds:

$$\frac{t}{-\ln(e^{-q_1} - \alpha)} \leq \tau \leq \frac{t}{q_1}$$

$\partial/\partial q_1 = 0$  gives the minimum interval as

$$0.15 < \lambda \leq 2.65 \text{ s}^{-1}$$

corresponding to

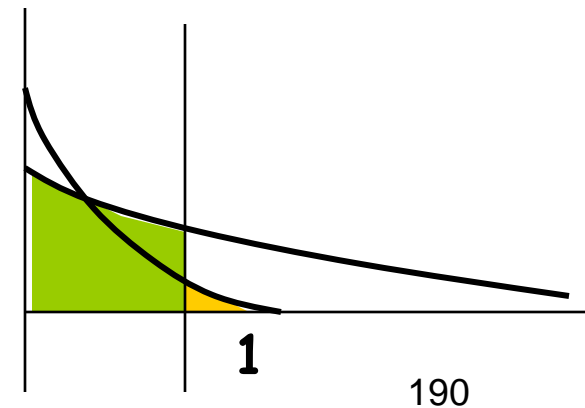
$$0.377 < \lambda \leq 5.88 \text{ s}^{-1}$$

Note that both the  $\lambda$  intervals give the right CL!!

$$\int_0^1 1.15 e^{-1.15t} dt = 0.683$$

$$\int_1^\infty 5.88 e^{-5.88t} dt = 0.0027, \quad \int_0^1 0.377 e^{-0.377t} dt = 0.3140$$

$$1 - 0.3140 - 0.0027 = 0.683$$



## A Paradox: the lifetime measurement III

The **likelihood ratio** is invariant w.r.t. any **changement of variable** (fundamental theorem).  
In this case, for a  $1\sigma$  interval

$$\ln \hat{L} - \ln L = 0.5$$

we have to find the  $\hat{\lambda}$  value

$$\frac{\partial}{\partial \lambda} \lambda e^{-\lambda} = 0 \rightarrow 1 - \lambda^2 = 0 \rightarrow \hat{\lambda} = 1$$

The confidence interval is the solution of the equation

$$\ln e^{-1} - \ln \lambda e^{-\lambda} = 0.5 \rightarrow \lambda - \ln \lambda = 1.5$$

The solution is

$$0.301 \leq \lambda \leq 2.358 \text{ s}^{-1}$$

# A Paradox: the lifetime measurement IV

$$0.301 \leq \lambda \leq 2.358 \text{ s}^{-1}$$

$$\int_1^\infty 2.358 e^{-2.358t} dt = 0.0946, \quad \int_0^1 0.301 e^{-0.301t} dt = 0.2599$$

$$1 - 0.2599 - 0.0946 = 0.645$$

The coverage is wrong

Some physicists use the LR technique instead of the frequentist or Bayesian approaches (see G. Zech, EPJ direct C12, 1-81 (2002))

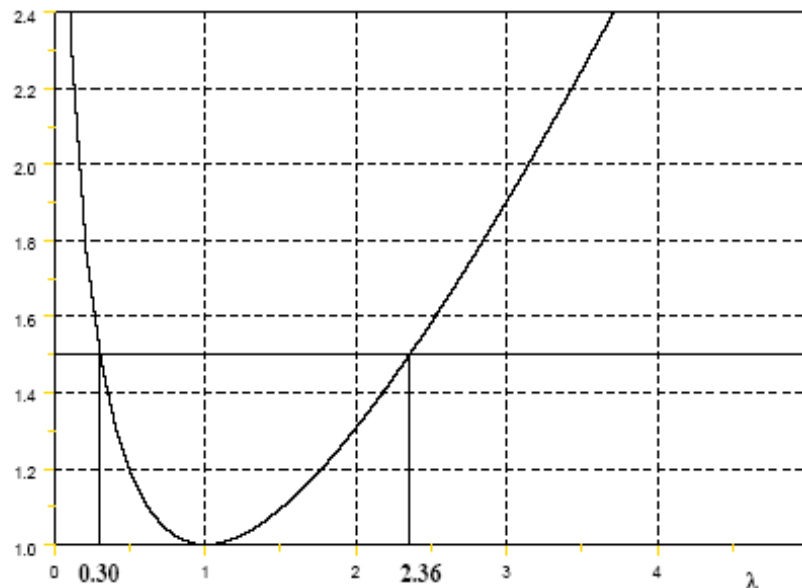
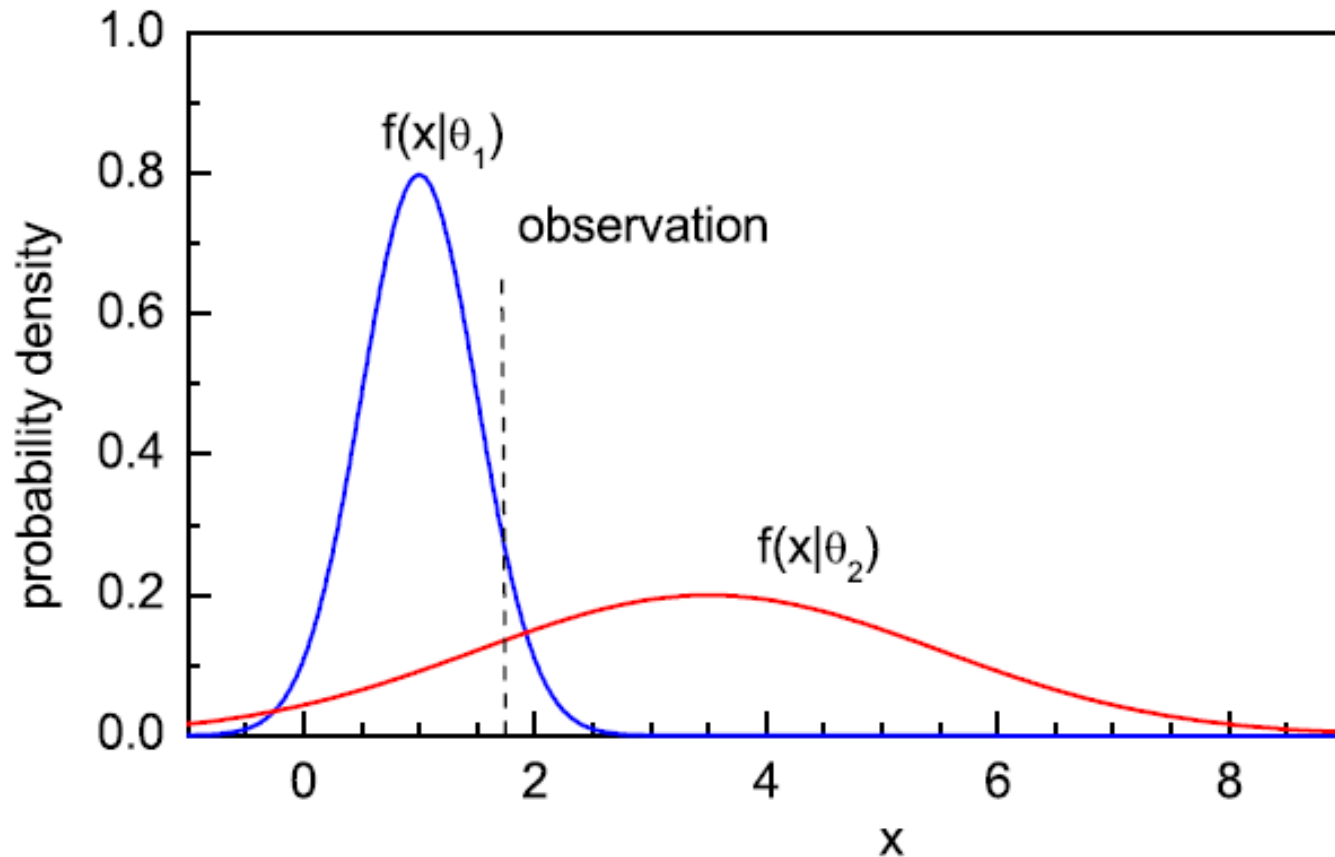


Figure 1:  $\lambda - \ln \lambda = 1.5$

## Frequentism, Bayes or likelihood ratio??

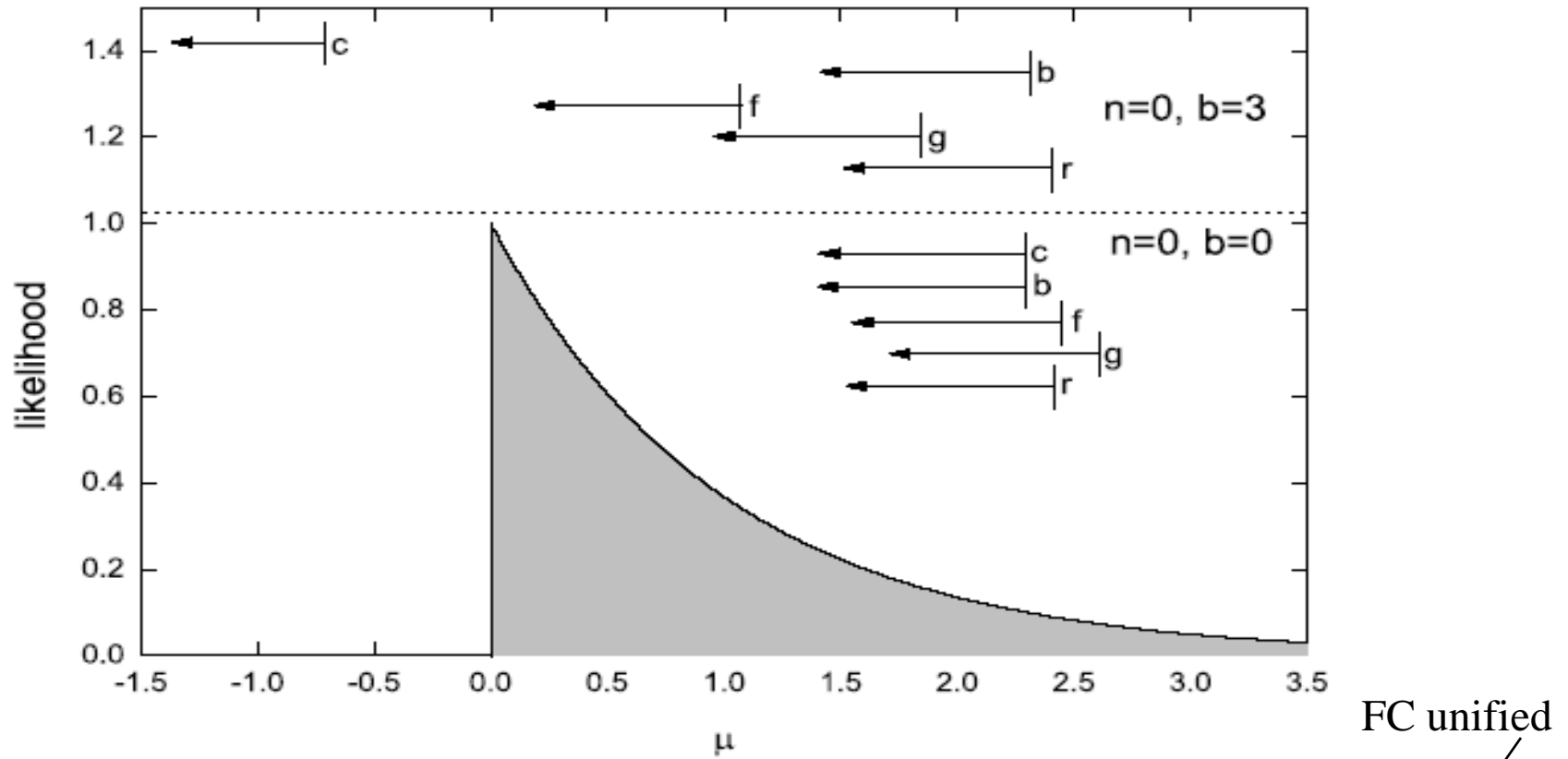


**Fig. 1.** The likelihood is larger for parameter  $\theta_1$ , but the observation is less than 1 st. dev. off  $\theta_2$ . Classical approaches include  $\theta_2$  and exclude  $\theta_1$  within a 68.3% confidence interval

# Draw the conclusions by yourself .....

Table 4. Comparison of different approaches to define error intervals, see text

method:	classical	unified	likelihood	Bayesian u.p.	Bayesian a.p.
consistency	--	--	++	+	+
precision	--	-	+	+	+
universality	--	--	-	+	++
simplicity	-	--	++	+	+
variable transform.	-	++	++	--	--
nuisance parameter	-	-	-	+	+
error propagation	-	-	+	+	+
combining data	-	-	++	+	-
coverage	+	++	--	--	--
objectivity	-	-	++	+	-
discrete hypothesis	-	-	+	+	+



**Fig. 16.** Likelihood function for zero observed events and 90% confidence upper limits with and without background expectation. The labels refer to [9] (f), Bayesian (b), [41] (g) and [42] (r) classical (c)



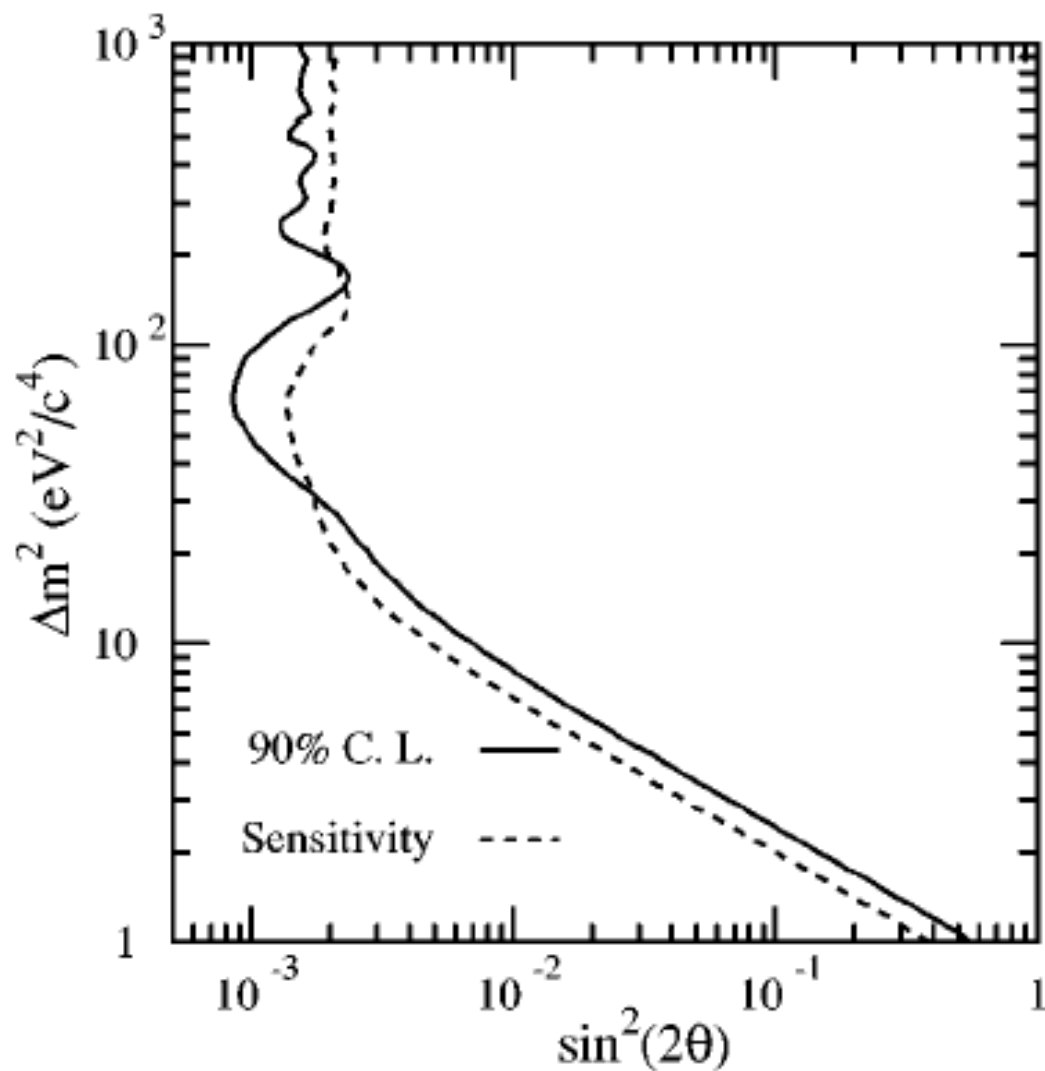


FIG. 15. Comparison of the confidence region for an example of the toy model in which  $\sin^2(2\theta)=0$  and the sensitivity of the experiment, as defined in the text.

# STATISTICA PER FISICI

1. Calcolo delle probabilità
- 2a. Statistica frequentista
- 2b. Statistica bayesiana
3. Likelihood
- 4a. Fondo e segnale
- 4b. Metodi Bootstrap
5. Approccio Unificato
6. *Unfolding*

# Folding theorem

$$Z = f(X_1, X_2) .$$

$Z_1 \equiv Z$  e  $Z_2 = X_2$  auxiliary variable

$$Z_1 = f(X_1, X_2) , \quad Z_2 = X_2 .$$

The jacobian is

$$|J| = \begin{vmatrix} \frac{\partial f_1^{-1}}{\partial z_1} & \frac{\partial f_1^{-1}}{\partial z_2} \\ 0 & 1 \end{vmatrix} = \left| \frac{\partial f_1^{-1}}{\partial z_1} \right| ,$$

From the general theorem one obtains

$$p_{\mathbf{Z}}(z_1, z_2) = p_{\mathbf{X}}(x_1, x_2) \left| \frac{\partial f_1^{-1}}{\partial z_1} \right| .$$

by integrating on the auxiliary variable :

$$p_{Z_1}(z_1) = \int p_{\mathbf{Z}}(z_1, z_2) dz_2 .$$

hence

$$\begin{aligned} p_Z(z) &= \int p_{\mathbf{X}}(x_1, x_2) \left| \frac{\partial f_1^{-1}}{\partial z} \right| dx_2 \\ &= \int p_{\mathbf{X}}(f_1^{-1}(z, x_2), x_2) \left| \frac{\partial f_1^{-1}}{\partial z} \right| dx_2 , \end{aligned}$$

which is the probability density

# Convolution theorem

For independent variables:

$$p_Z(z) = \int p_{X_1}(f_1^{-1}(z, x_2)) p_{X_2}(x_2) \frac{\partial f_1^{-1}}{\partial z} dx_2 .$$

when  $Z$  is given by the sum

$$Z = X_1 + X_2 ,$$

we have

$$X_1 = f_1^{-1}(Z, X_2) = Z - X_2 , \quad \frac{\partial f_1^{-1}}{\partial z} = 1 ,$$

and we obtain

$$p_Z(z) = \int_{-\infty}^{+\infty} p_{\mathbf{X}}(z - x_2, x_2) dx_2 .$$

When  $X_1$  and  $X_2$  are independent, we obtain the **convolution integral**

$$p_Z(z) = \int_{-\infty}^{+\infty} p_{X_1}(z - x_2) p_{X_2}(x_2) dx_2 ,$$

**In physics**

(  $\delta$  instrument function,  $f$  signal ) :

$$g(y) = \int_{-\infty}^{+\infty} f(y - x) \delta(x) dx ,$$

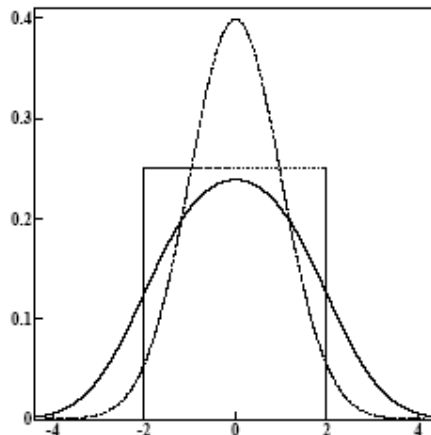
# Uniform\*Gaussian

When  $Z = X + Y$  where  
 $X \sim N(\mu, \sigma^2)$  e  $Y \sim U(a, b)$ .

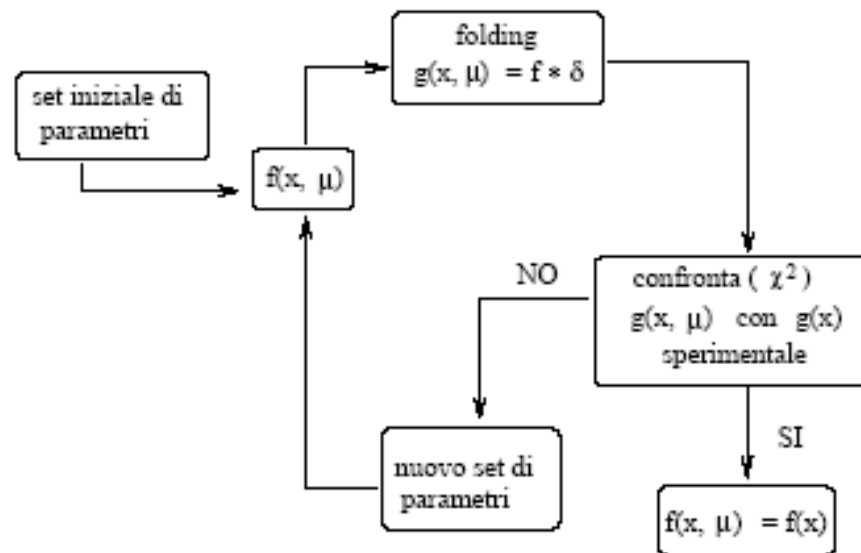
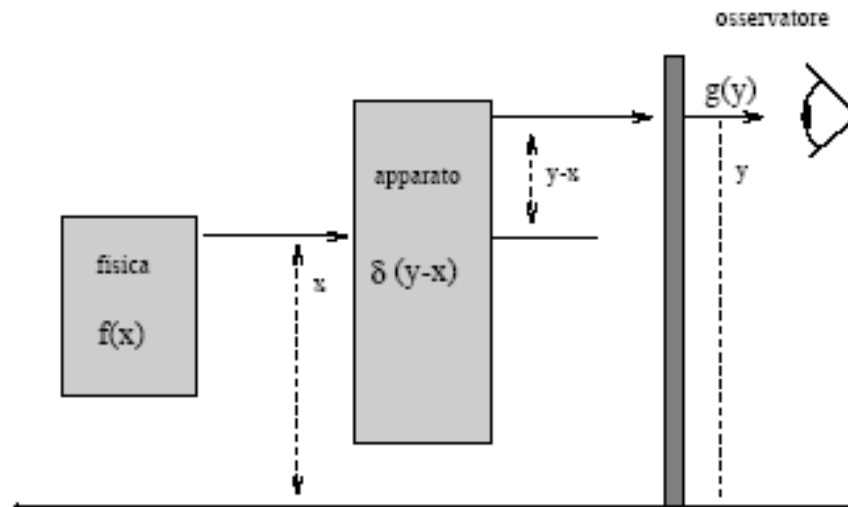
one has immediately

$$\begin{aligned} p_Z(z) &= \frac{1}{b-a} \int_a^b \frac{1}{\sigma\sqrt{2\pi}} \exp\left[-\frac{(z-y-\mu)^2}{2\sigma^2}\right] dy \\ &= \frac{1}{b-a} \int_a^b \frac{1}{\sigma\sqrt{2\pi}} \exp\left[-\frac{[y-(z-\mu)]^2}{2\sigma^2}\right] dy . \end{aligned}$$

$$p_Z(z) = \frac{1}{b-a} \left[ \Phi\left(\frac{b-(z-\mu)}{\sigma}\right) - \Phi\left(\frac{a-(z-\mu)}{\sigma}\right) \right]$$



$$g(y) = \int f(x) \delta(y - x) dx ,$$



# The 1D problem

In the reconstruction of an histogram,

- the **true histogram (image)** where the bin contents are the expected **values**

$$\boldsymbol{\mu} = (\mu_1, \mu_2, \dots, \mu_N) , \quad \mu_j = \mu_{\text{tot}} p_j = \mu_{\text{tot}} \int_{\text{bin } i} f_t(y) dy$$



# The problem in 2-D

A picture in a  $x - y$  plane is the result of a double dimensional folding, where the true points are smeared out by detector effects.

$$N = \sum_{ij=1}^{n_c} N_{ij}(\text{exp}) , \quad (93)$$

$N$  is the total number of events and  $N_{ij}(\text{exp})$  is the recorded number of event in the pixel placed at the  $i$ th-row and  $j$ th-column.

The observed  $N_{ij}(\text{exp})$  events have to be compared with the **expected values**  $N_{ij}(\text{th})$  predicted by a model.

$$N_{ij}(\text{th}) = N P_{ij}(\text{obs}) = N \sum_{i'j'} P_{i'j'}(\text{true}) P_v(\text{obs}_{ij}|\text{true}_{i'j'}) , \quad (94)$$

that is, the number of events observed in the  $ij$ th-cell is due to the presence into the  $i'j'$ th-cell, times the probability  $P_v$  that the PSF shifts the point from the  $i'j'$  to the  $ij$ -cell. One has to sum on all the cells near the  $ij$ -one.

In the case of a two dimensional Gaussian point spread function **PSF**:

$$P_v(\text{obs}_{ij}|\text{true}_{i'j'}) = \frac{1}{2\pi \sigma_x \sigma_y} \exp \left[ -\frac{(x_{ij} - x_{i'j'})^2}{2 \sigma_x^2} - \frac{(y_{ij} - y_{i'j'})^2}{2 \sigma_y^2} \right] , \quad (96)$$



# Fourier techniques

$$f(x) = \int F(t) e^{2\pi i x t} dt$$

**Convolution:**

$$f(x) = \int g(y)\delta(x - y) dy$$

$$\int F(t) e^{2\pi i x t} dt = \int G(t) e^{2\pi i y t} \Delta(t) e^{2\pi i (x-y)t} dt$$

$$\int F(t) e^{2\pi i x t} dt = \int G(t) \Delta(t) e^{2\pi i x t} dt \rightarrow F(t) = G(t) \Delta(t)$$

**Correlation**

$$\text{Corr}(g, \delta) \equiv \int g(x + y) \delta(y) dy \rightarrow G(t)\Delta^*(t)$$

if the functions are **real**

$$G(t) = G(-t)^* , \quad \text{Corr}(g, \delta) \rightarrow G(t)\Delta(-t)$$

**Autocorrelation (Wiener theorem)**

$$\text{Corr}(g, g) \rightarrow |G(t)|^2$$

**Total Power:**

$$P(f) \equiv \int |f(x)|^2 dx = \int |F(t)|^2 dt$$

**Power Spectral Density (in the Fourier space):**

$$PSD(f) \equiv |F(t)|^2 + |F(-t)|^2 \xrightarrow{f(x) \text{ real}} 2|F(t)|^2 \quad 0 \leq t \leq \infty$$

# Image Deconvolution

$$D(\mathbf{x}) = \int d\mathbf{y} I(\mathbf{y}) \delta(|\mathbf{x} - \mathbf{y}|)$$

In the absence of noise

$$I = F^{-1} \left[ \frac{F(D)}{F(\delta)} \right]$$

where  $F$  is the Fourier transform.

For a real image  $I(n_1, n_2)$  the Fourier transform is:

$$F(k_1, k_2) = \sum_{n_2=0}^{N_2-1} \sum_{n_1=0}^{N_1-1} e^{2\pi i k_2 n_2 / N_2} e^{2\pi i k_1 n_1 / N_1} I(n_1, n_2)$$

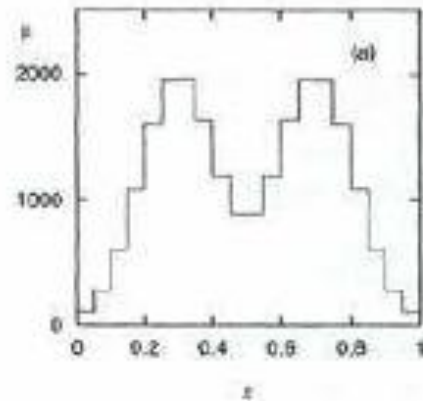
$$F(k_1, k_2) = FFT_2[FFT_1[I(n_1, n_2)]]$$

For the routines see for example *Numerical Recipes*

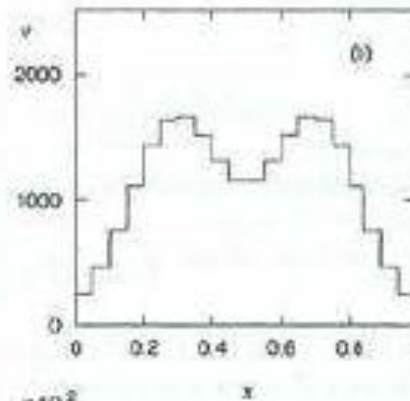
# The problem with fluctuations

Inverting the response matrix 161

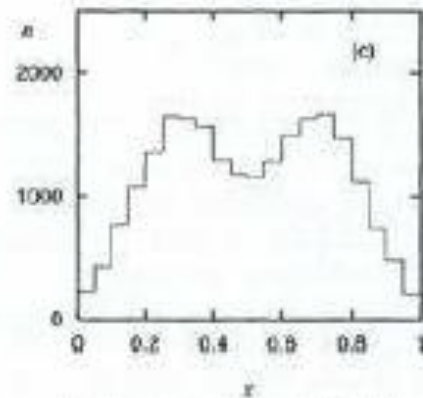
original



Gaussian smearing



Poisson statistics



Fourier (un)restored

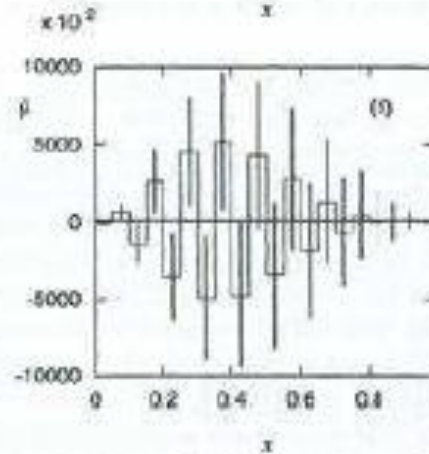
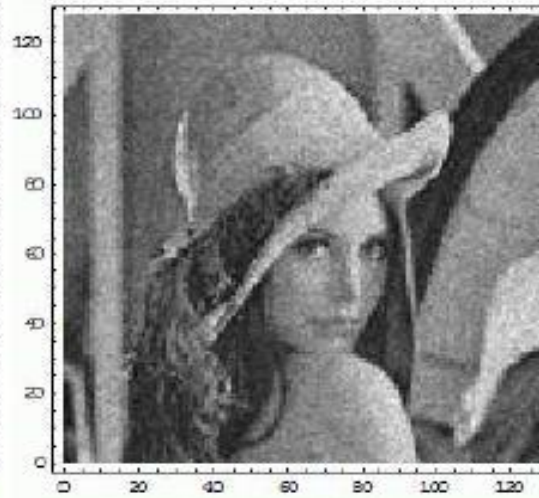


Fig. 11.1 (a) A hypothetical true histogram  $\mu$ , (b) the histogram of expectation values  $\nu = R\mu$ , (c) the histogram of observed data  $n$ , and (d) the estimators  $\hat{\mu}$  obtained from inversion of the response matrix.

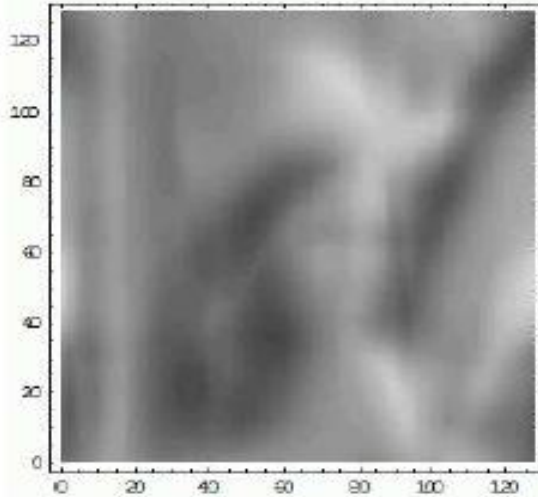
original



Poisson  
statistics



Gaussian  
smearing



Fourier  
restored

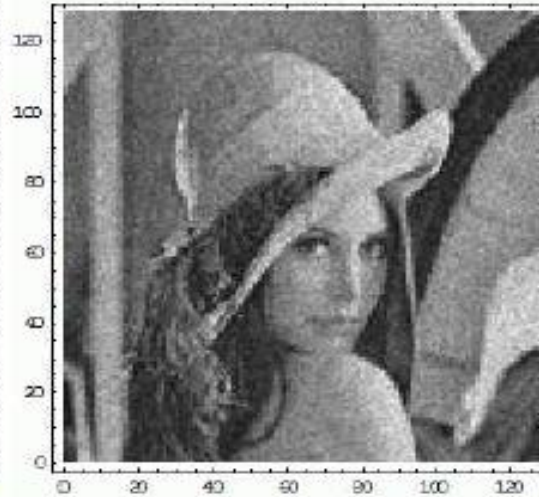
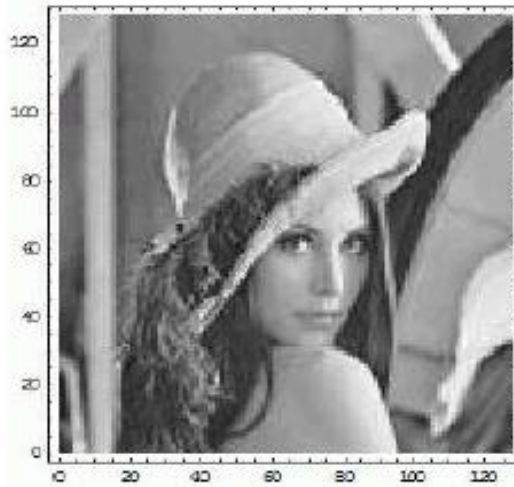
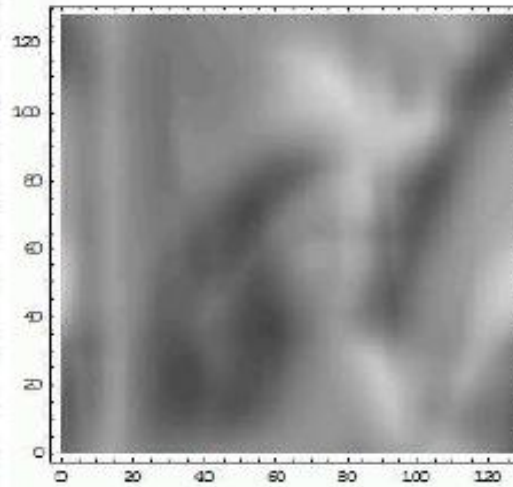


Figure 11: **Lena restored by FFT:** The original image (top left) is sampled with Poisson statistics (top right) and smeared with a 2D 10-bins Gaussian PSF (bottom left): the Fourier restored image (bottom right) is similar to the Poisson sampled image. In this case the noise term  $N$  is neglected.

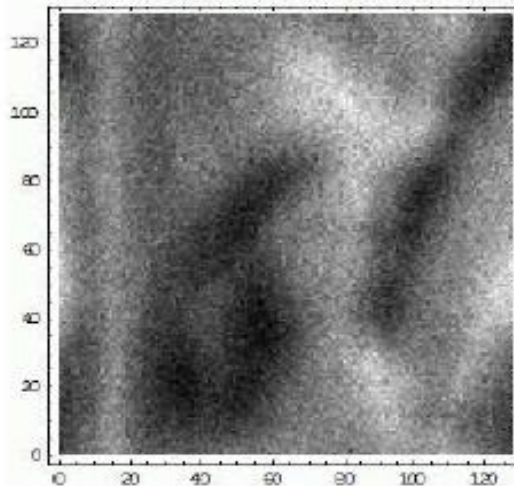
original



Gaussian smearing



Poisson statistics



Fourier (un)restored

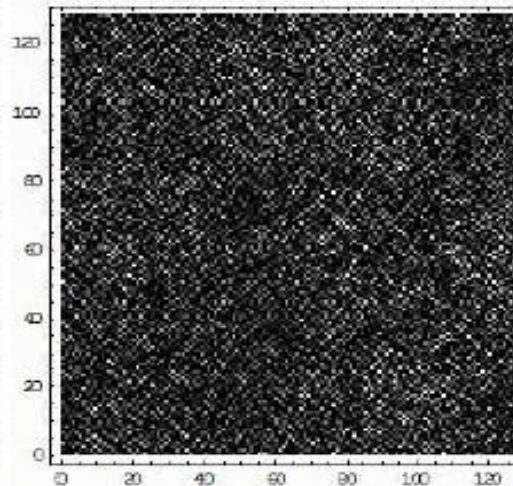
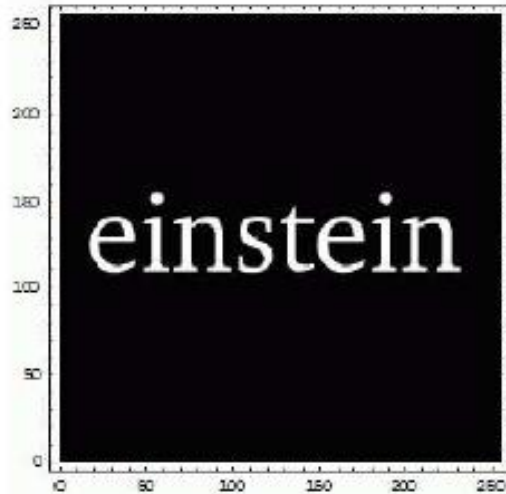


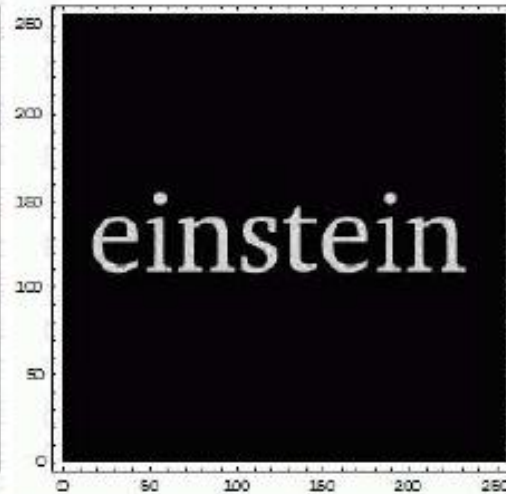
Figure 12: **Lena not restored by FFT:** In this case the noise term  $N$  is not ignored: the original image (top left) is smeared with a 2D 10-bins Gaussian PSF (top right) and the result is sampled with Poisson statistics (bottom left): the Fourier restored image (bottom right) cannot recover the information lost in the noise. Another approach, statistical in nature, is required.



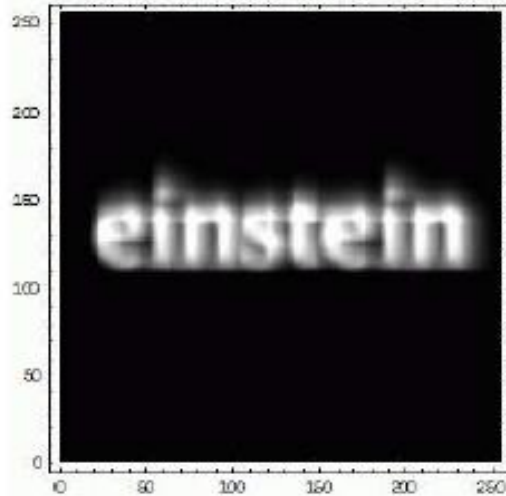
original



Poisson  
statistics



Gaussian  
smearing



Fourier  
restored

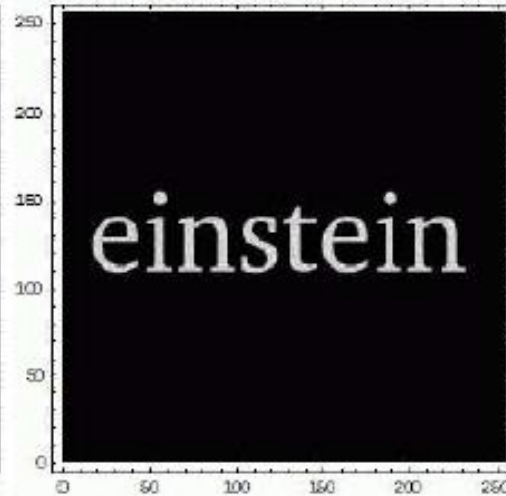
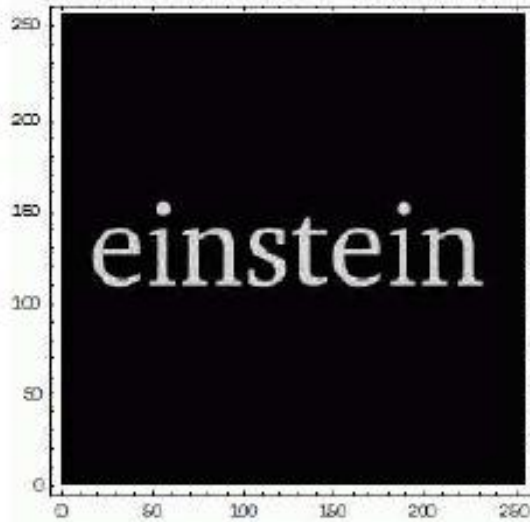
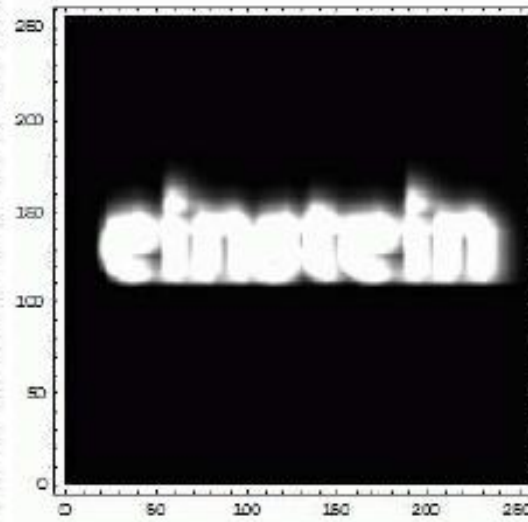


Figure 13: Einstein restored by FFT: explanation as in Figure 1.

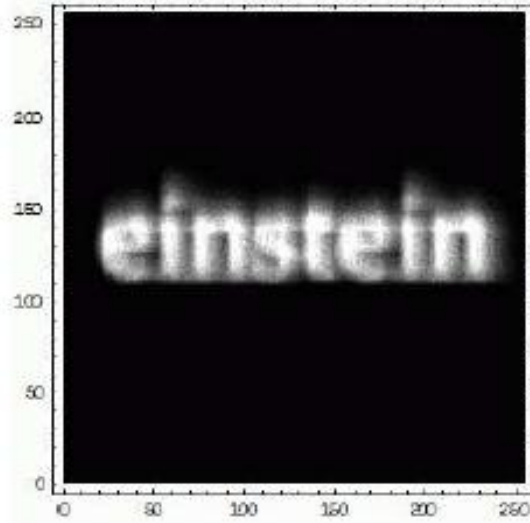
original



Gaussian  
smearing



Poisson  
statistics



Fourier  
(un)restored

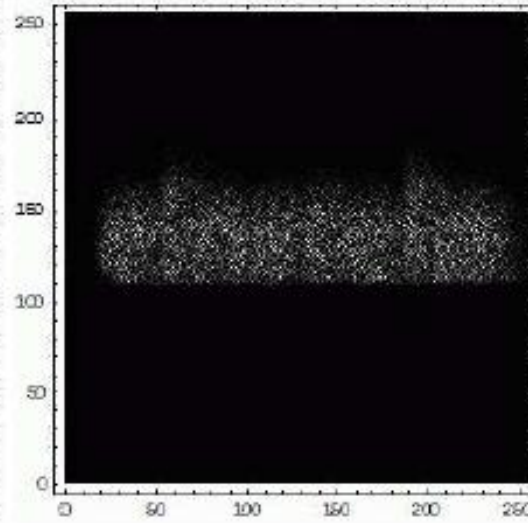


Figure 14: Einstein not restored by FFT: explanation as in Figure 2.

When  $\text{true} \rightarrow \text{obs} \equiv \mu \rightarrow \nu$  deterministic methods (FFT) can be used

$$\nu = R * \mu \quad (19)$$

When  $\text{true} \rightarrow \text{smeared} \rightarrow \text{obs} \equiv \mu \rightarrow \nu \rightarrow n$  statistical methods must be used

$$n = \nu + \rho = R * \mu + \rho$$

In the poissonian or binomial case we have to minimize:

$$-\ln L(\mu) = -\sum_i \ln P(n_i, \nu_i)$$

In the gaussian case we must minimize

$$\chi^2(\mu) = \sum_{ij} (\nu_i - n_i)(V^{-1})_{ij}(\nu_j - n_j)$$

In 2-D, when  $N_{ij}(\text{exp})$  contains fluctuations, we have to minimize:

$$-2 \ln L(n|\nu, \mu) \simeq \chi^2 = \sum_{ij} \frac{[N_{ij}(\text{exp}) - NP_{ij}(\text{obs})]^2}{NP_{ij}(\text{obs})} \quad (20)$$

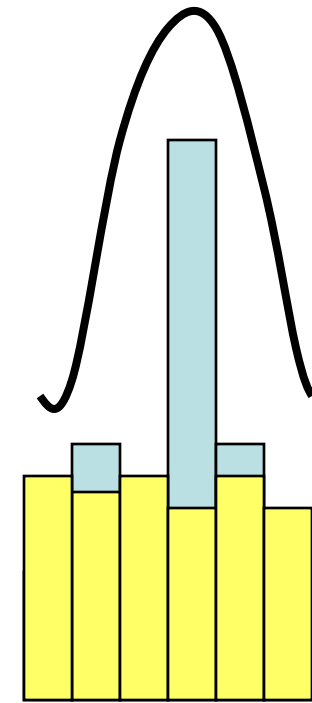
where

$$P(\text{obs}) = P(\nu|\mu) P(\mu)$$

If all the pixel contents  $\mu$  are the free parameters to be determined **the problem has zero DoF**

**This is a ILL-POSED problem with many (and more probable) unrealistic solution!!**

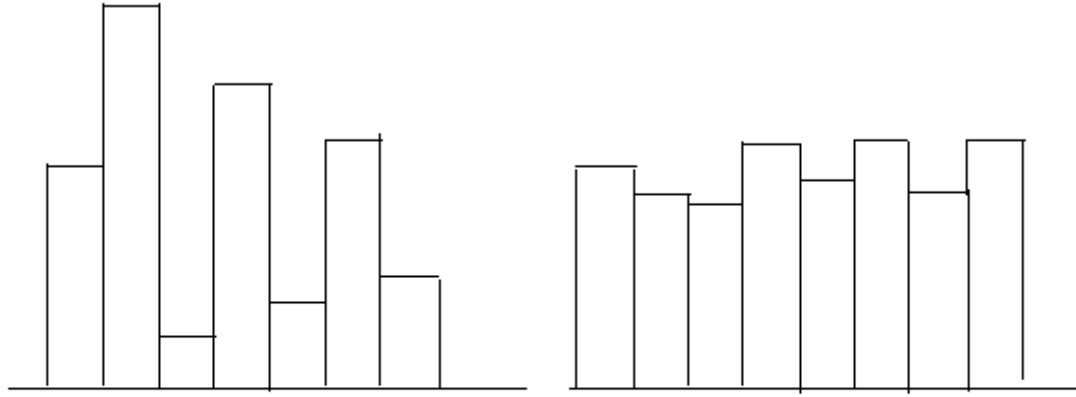
# Image restoration



Unlike!



# Explanation:



spike solution

**HIGLY PROBABLE**

smooth solution

**UNLIKE**

many solutions give a good  $\chi^2$

the spike ones are more probable!

**Cure:** to add to  $\chi^2$  an **empirical** regularization term  $C[p]$ .

$$\chi^2 \rightarrow \alpha \chi^2 + C[P(\text{true})]$$

**or**

$$\chi^2 \rightarrow \chi^2 + \alpha C[P(\text{true})]$$

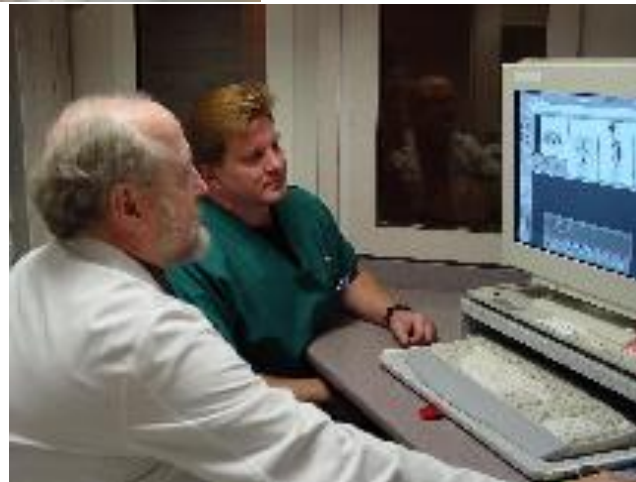
The smeared distributions of two input distributions cannot be distinguished if they agree on a large scale of  $x$  but differ by oscillations on a "microscopic" scale much smaller than the experimental resolution

**or**

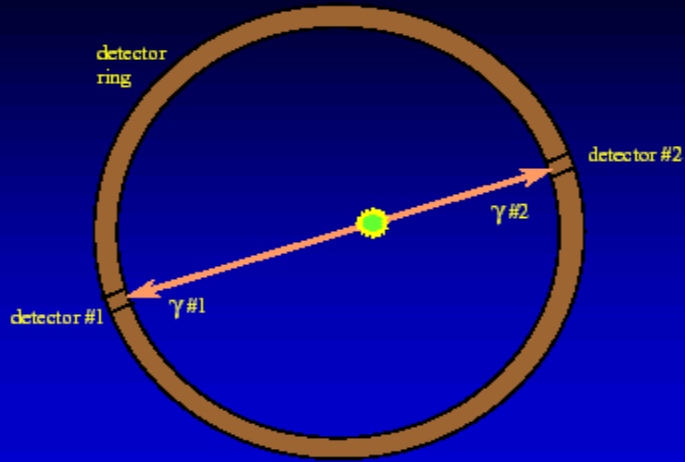
**to increase the DoF by using a parametric model**

$$P(v | \mu)P(\mu) \rightarrow P(v | \mu')$$

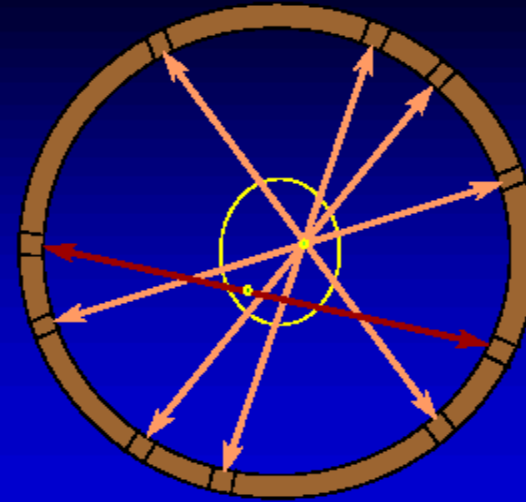
# PET: positron emission thomography



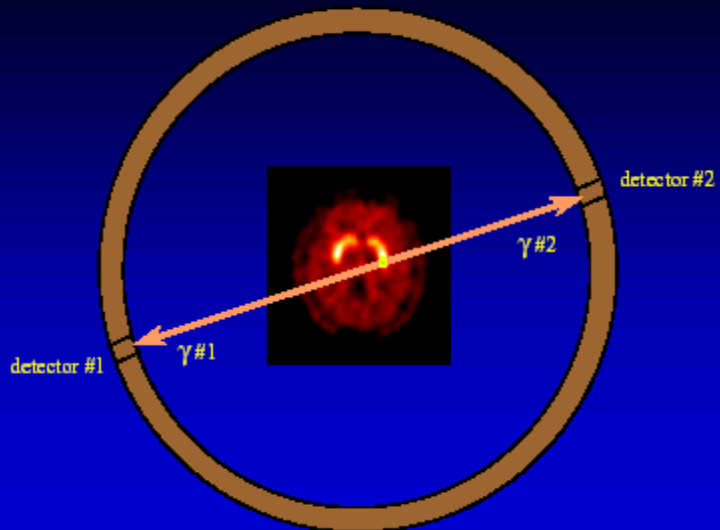
# Positron Emission Tomography



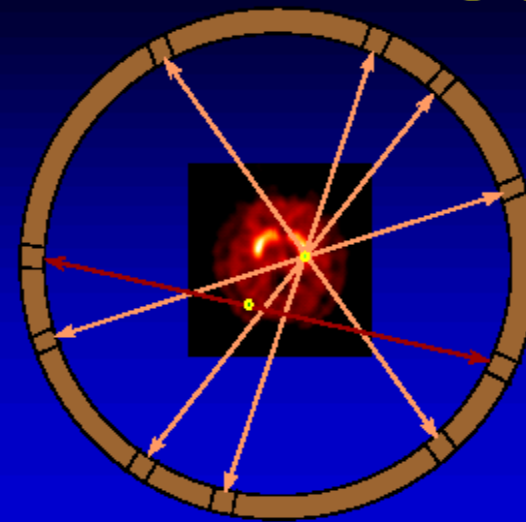
# Positron Emission Tomography



# Positron Emission Tomography



# Positron Emission Tomography



## Remember

$$\mu_i \xrightarrow{PSF} \nu_i \xrightarrow{\text{random}} n_i$$

and consider (95) as a form of the Bayes theorem

$$P(\text{true}_{ij}|\text{obs}) \propto \sum_{i',j'} P_{i'j'}(\text{true}) P_v(\text{obs}_{ij}|\text{true}_{i'j'}) = L(\mathbf{n}|\boldsymbol{\mu})P(\boldsymbol{\mu})$$

Bayesians say: **posterior = likelihood  $\times$  prior** One maximizes  $P(\text{true}_{ij}|\text{obs}) \equiv F(\boldsymbol{\mu})$  (or minimize  $-F(\boldsymbol{\mu})$ ):

$$F(\boldsymbol{\mu}) = \ln L(\mathbf{n}|\boldsymbol{\mu}) + \ln P(\boldsymbol{\mu}) \quad (99)$$

following the **Maximum Likelihood (ML)** principle.

The practical (no Bayesian) experimentalist introduces an empirical regularization parameter  $\alpha$  and considers the **prior**  $P(\boldsymbol{\mu})$  as a regularization function  $C(\boldsymbol{\mu})$ :

$$F(\boldsymbol{\mu}) = \alpha \ln L(\mathbf{n}|\boldsymbol{\mu}) + C(\boldsymbol{\mu}) \quad (100)$$

By keeping fixed the normalization:

$$\nu_T = \sum_i \sum_j R_{ij} \hat{\mu}_j + \rho_i = n_T$$

the objective function is

$$F(\boldsymbol{\mu}) = \alpha \ln L(\mathbf{n}|\boldsymbol{\mu}) + C(\boldsymbol{\mu}) + \lambda(n_T - \sum_i \nu_i) \quad (101)$$

where  $\lambda$  is a Lagrange multiplier

$$\frac{\partial F}{\partial \lambda} = 0 \rightarrow \sum_i n_i = n_T$$

The frequentist assumes

$$P(\boldsymbol{\mu}) = 1$$

## Regularization terms

The objective function to be minimized is

$$-F(\boldsymbol{\mu}) = -2 \ln L(\mathbf{n}|\boldsymbol{\mu}) - \alpha C(\boldsymbol{\mu}) + \lambda(n_T - \sum_i \nu_i) \quad (23)$$

$$\mu_j = \mu_{\text{tot}} p_j = \mu_{\text{tot}} \int_{\text{bin}_j} f_t(y) dy$$

where  $\alpha > 0$ . Some regularization terms:

- minimum second derivative (Tichonov)

$$C(\boldsymbol{\mu}) = - \int [f_t''(y)]^2 dy \simeq - \sum_{i=1}^{M-2} [-\mu_i + 2\mu_{i+1} - \mu_{i+2}]^2$$

- minimum variance:

$$C(\boldsymbol{\mu}) = -\text{Var}[\boldsymbol{\mu}] \equiv \|C\boldsymbol{\mu}\|^2 = - \sum_i \mu_i^2$$

- maximum entropy (MaxEnt)

$$C(\boldsymbol{\mu}) = - \sum_i p_i \ln p_i = - \sum_i \frac{\mu_i}{\mu_T} \ln \frac{\mu_i}{\mu_T}$$

- cross-entropy

$$C(\boldsymbol{\mu}) = - \sum_i p_i \ln \frac{p_i}{q_i} = - \sum_i \frac{\mu_i}{\mu_T} \ln \frac{\mu_i}{\mu_T q_i}$$

where  $\mathbf{q} = (q_1, q_2, \dots, q_n)$  is the most likely a priori shape for the true distribution  $\mu_i$ .

The objective function to be minimized is

$$-F(\boldsymbol{\mu}) = -2 \ln L(\mathbf{n}|\boldsymbol{\mu}) - \alpha C(\boldsymbol{\mu}) + \lambda(n_T - \sum_i \nu_i) \quad (24)$$

Some choices of  $\alpha > 0$  are:

- Bayesian

$$\alpha = \frac{1}{\mu_T}$$

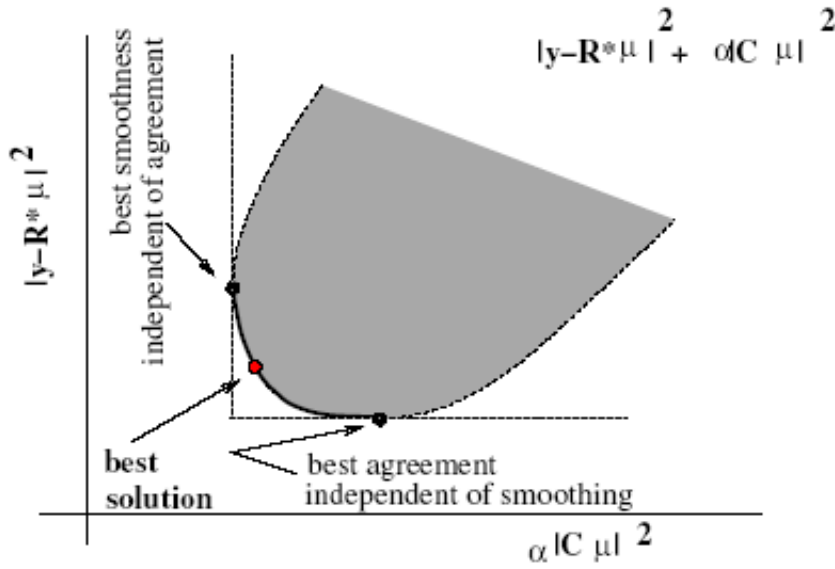
usually too much smoothing

- $A = \chi^2 + \alpha \|C\boldsymbol{\mu}\|^2 > 0$

we can regularize the solution by choosing  $\chi^2 \simeq DoF \equiv$  number of pixel  $N$ , with the condition:

$$\alpha = \frac{A - N}{\|C\boldsymbol{\mu}\|^2}$$

# Regularization parameter



# Regularization parameter

Two-peak deconvolution with the regularized ML methods (Glen Cowan, Statistical Data Analysis, Oxford (2000))

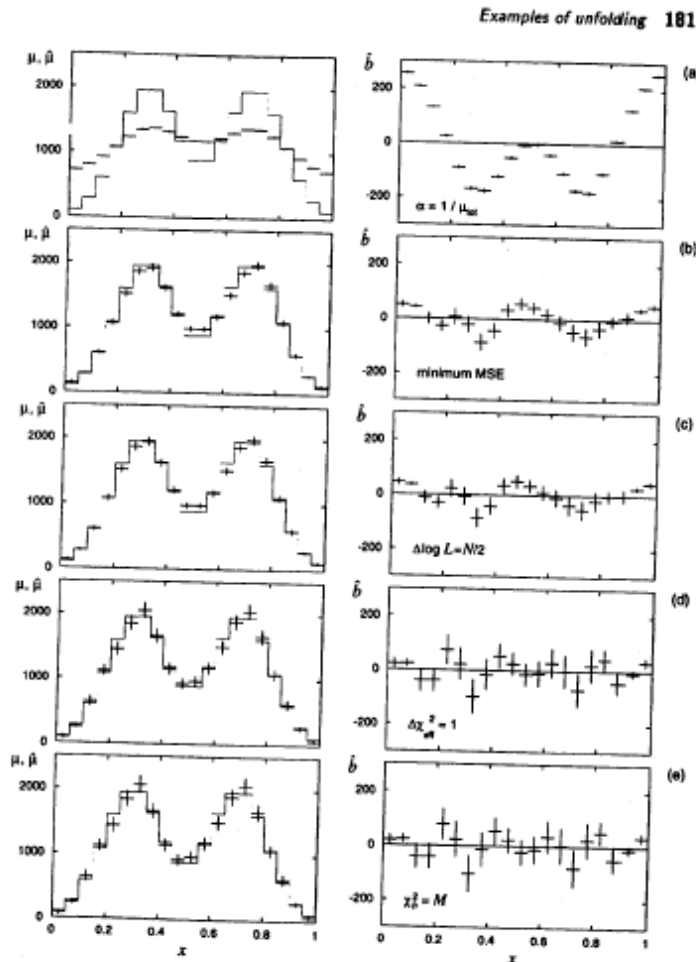
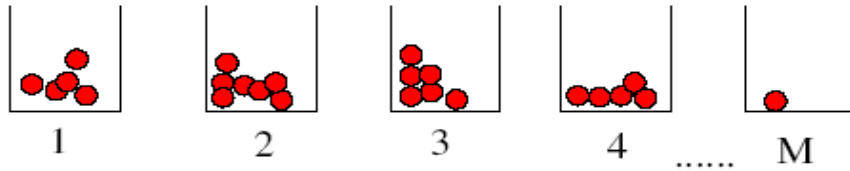


Fig. 11.3 MaxEnt unfolded distributions shown as a histogram (left) and the estimated biases (right) for different values of the regularization parameter  $\alpha$ . The five plots correspond to (a) the Bayesian prescription  $\alpha = 1/\hat{\mu}_{\text{tot}}$ , (b) the minimum MSE method, (c) the Bayesian prescription  $\Delta \log L = N/2$ , (d) the Bayesian prescription  $\Delta x_m^2 = 1$ , and (e) the Bayesian prescription  $x_m^2 = M$ .

We have  $M$  boxes and a monkey that throws  $N$  ball randomly into them.

What is the box-balls configuration of highest probability? Probability of a configuration:

$$p = \frac{1}{M^N} \frac{N!}{n_1! n_2! \dots n_N!} = e^{\ln p}$$



M boxes and N balls

equal to

N balls labelled randomly from 1 to M



$$\ln p = -N \ln M + \ln N! - \sum_i \ln(n_i!)$$

**Stirling formula:**  $n! = \sqrt{2\pi n} n^n e^{-n} \rightarrow \ln n! \simeq n \ln n - n$

$$\ln p = -N \ln M + N \ln N - N + \sum n_i - \sum_i n_i \ln n_i$$

$$\sum p_i = 1, \quad p_i = \frac{n_i}{N}, \quad \ln p = -N \ln M - N \sum_i p_i \ln p_i$$

The most probable configuration means to maximize

$$\ln p(\boldsymbol{\mu}) = S = - \sum_i p_i \ln p_i$$

What is MaxEnt ???



$$N_{ij}(\text{th}) = NP_{ij}(\text{obs}) = N \sum_{i'j'} P_{i'j'}(\text{true}) P_v(\text{obs}_{ij} | \text{true}_{i'j'}) \quad (25)$$

We write this equation considering the operator  $R$ :

$$n = R * \mu$$

The iterative method (Van Cittert 1930) adds with a weight  $\beta$  the residual  $r_k$  to the current solution

$$\mu_{k+1} = \mu_k + \beta[n - R * \mu_k] \quad (26)$$

The method is based on the known equation

$$\sum_{i=0}^k q^i = \frac{1 - q^{k+1}}{1 - q} \quad (27)$$

for  $k \rightarrow \infty$  the series converges if  $|q| < 1$ .

By applying iteratively (26)

$$\begin{aligned} \mu_{k+1} &= \beta n + (1 - \beta R)\mu_k = \beta n + (1 - \beta R)(\beta n + (1 - \beta R)\mu_{k-1}) \\ &= \beta n + \beta(1 - \beta R)n + (1 - \beta R)^2 \mu_{k-1} \\ &= \beta n + \beta(1 - \beta R)n + \beta(1 - \beta R)^2 n + (1 - \beta R)^3 \mu_{k-2} \dots \\ &= \sum_{i=0}^k \beta(1 - \beta R)^i n . \end{aligned}$$

From (27):

$$\mu_{k+1} = \frac{1 - (1 - \beta R)^{k+1}}{\beta R} \beta n \rightarrow R^{-1}n = \mu , \quad \text{for } k \rightarrow \infty .$$

if  $|1 - \beta R| < 1$

The iterative principle

In summary, we use

$$\mu_{k+1} = \mu_k + \beta[n - R * \mu_k] \quad (28)$$

with the initial condition

$$\mu_0 = n .$$

The convergence is assured if

$$|I - \beta R| < 1$$

Since  $|1 - \beta x| < 1$  implies  $0 < \beta < 2/x$ , in the case of the operator  $R$ , which can be transformed in a square matrix

$$R' = (R * \mu) \mu^{-1}$$

we obtain the condition:

$$0 < \beta < \frac{2}{\max \text{ eigenvalue of } R'}$$

Note that we works always with square matrices  $R * \mu$ ,  $\mu$ ,  $\mu^{-1}$  and  $R'$ .

However, this step must be repeated at each iteration

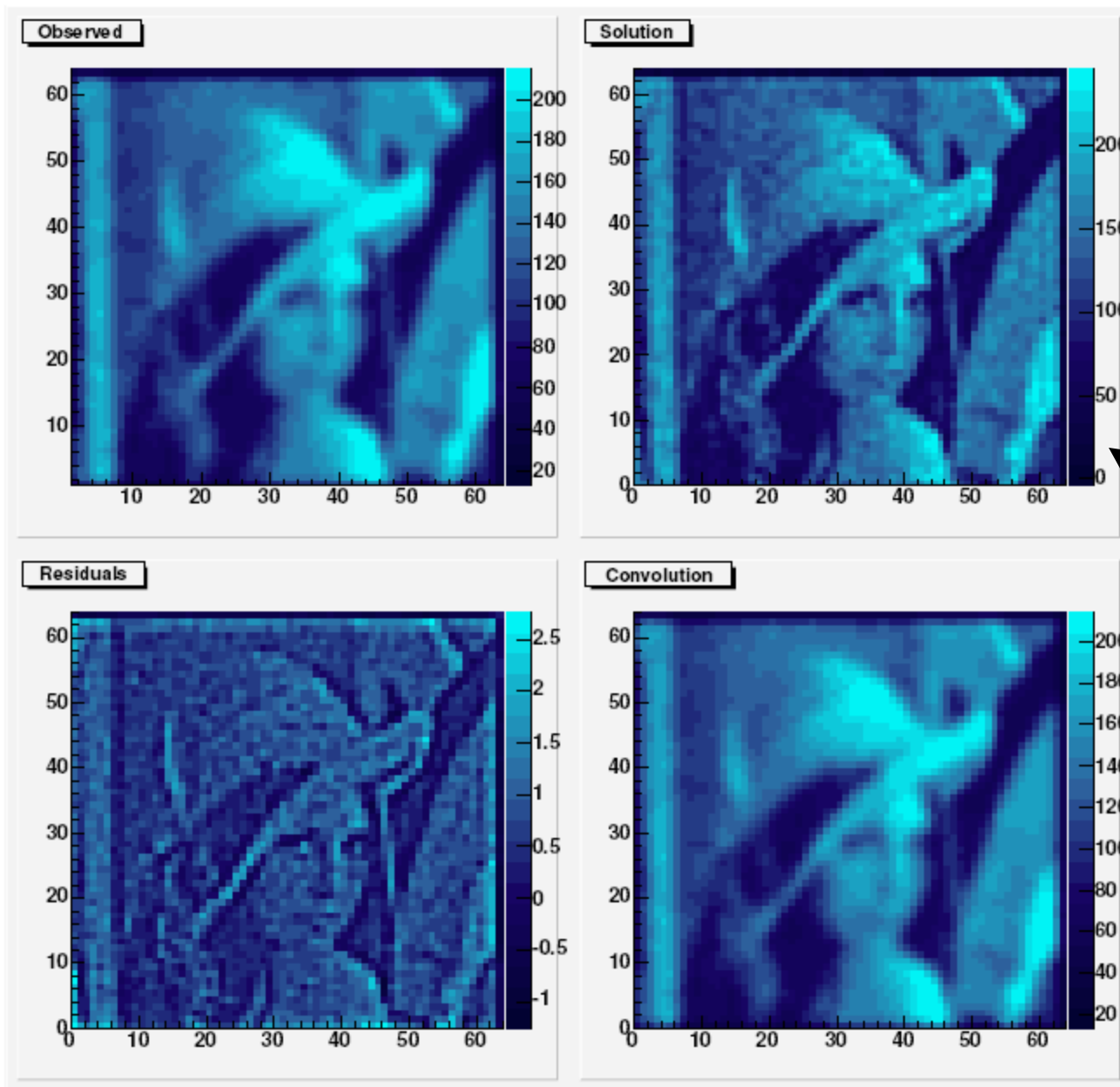
**This method sometimes gives spectacular result!**

**However, often it gives irregular solutions.**

**The iterative principle**

Without  $\beta$

$$\mu_{k+1} = \mu_k + [n - R * \mu_k]$$

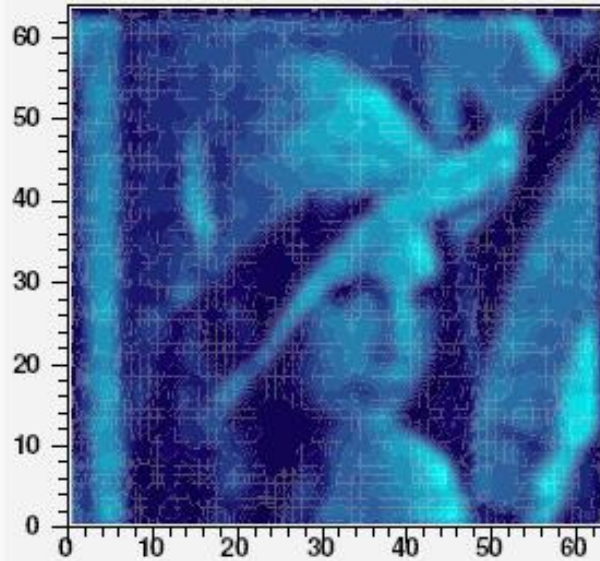


The iterative Principle without best fit

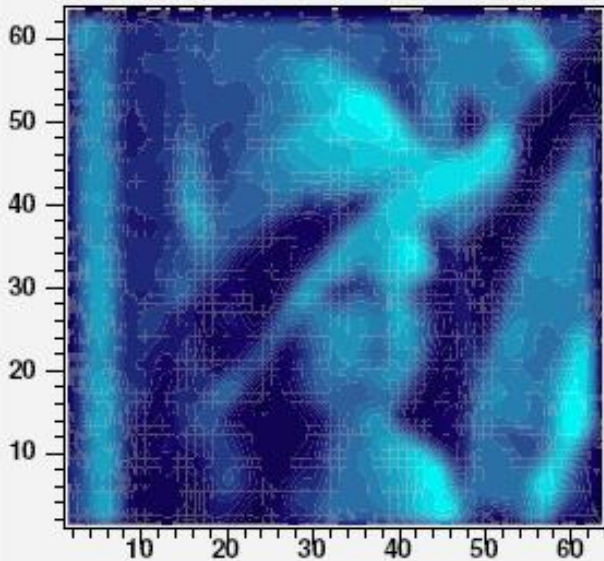
Good!



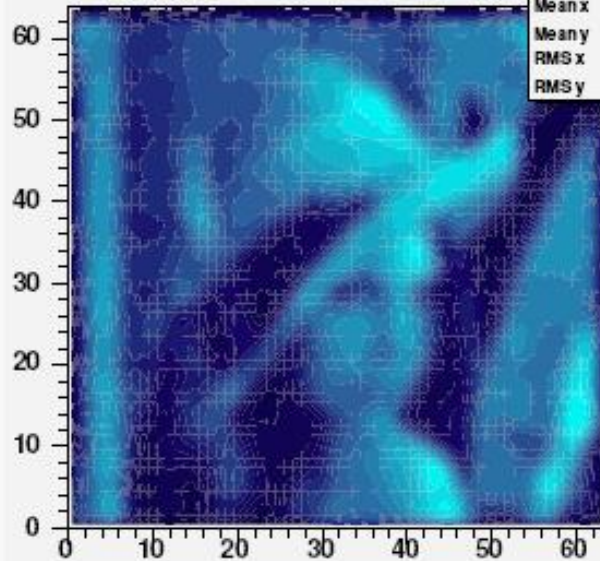
Solution



Observed



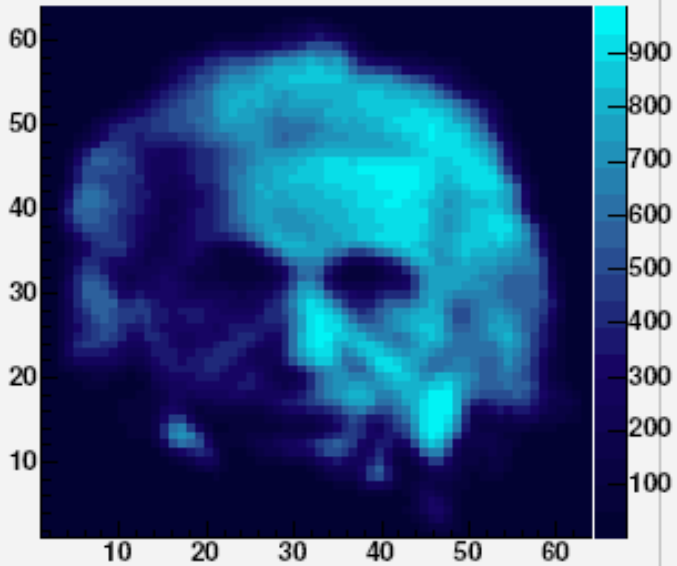
Convolution



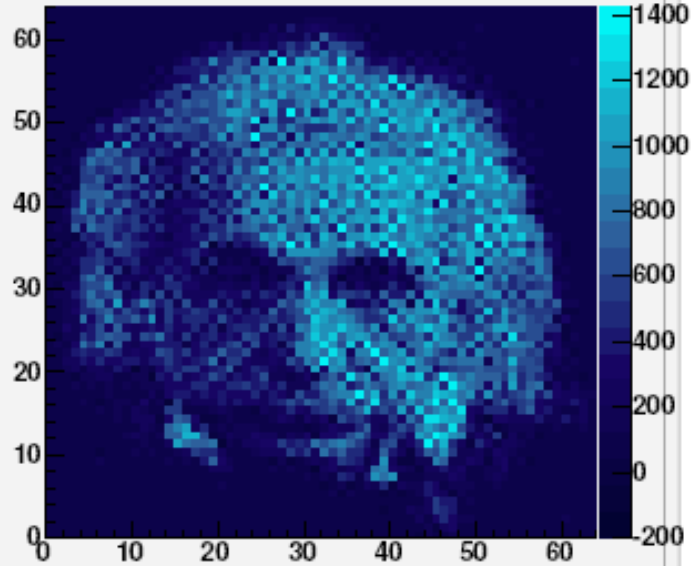
hobbs	
Entries	4094
Mean x	32.94
Mean y	32.8
RMS x	18.09
RMS y	18.07

The  
iterative  
Principle  
without  
best fit +  
smoothing

Observed

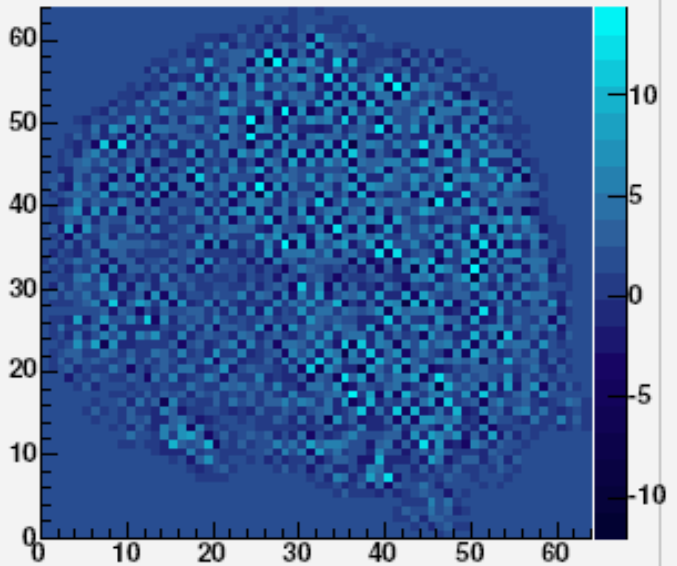


Solution

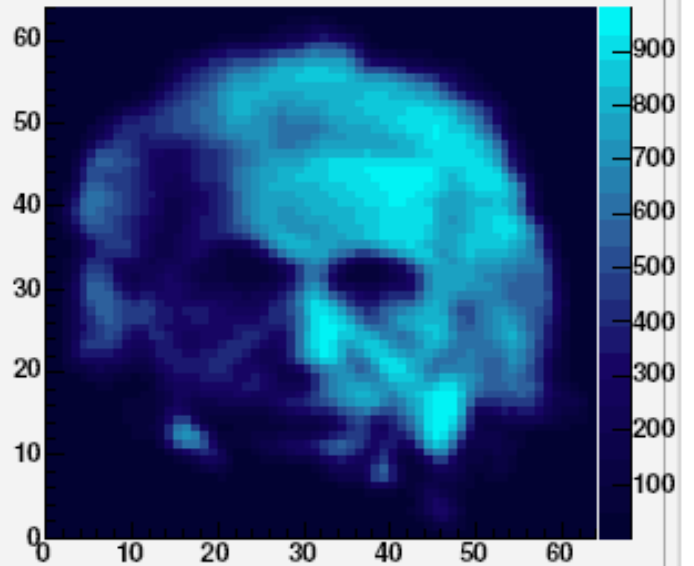


The iterative Principle without best fit

Residuals



Convolution



Bad!

Consider the case with statistical fluctuations

$$\mu_i \xrightarrow{PSF} \nu_i \xrightarrow{random} n_i$$

$$\mathbf{n} = \mathbf{R} * \boldsymbol{\mu} + \mathbf{r}$$

To have regular solutions and to make the method **robust**, we must search for an iterative solution which **minimize the  $\chi^2$** :

$$\chi^2 = \|\mathbf{R} * \boldsymbol{\mu} - \mathbf{n}\|^2 = \frac{1}{2} \sum_{ik} (\sum_{mn} \mathbf{R}_{i-m,k-n} \mu_{mn} - n_{ik})^2 .$$

Note that is the case in which **the PSF depends on the pixel difference only (translational invariance)**

In this case we consider  $R$  as an operator and we can work with symmetric  $M \times N$  matrices.

Minimum  $\chi^2$  w.r.t  $\mu_{ik}$  gives the equations:

$$\frac{\partial \chi^2}{\partial \mu_{mn}} = \sum_{ik} (\sum_{rs} R_{i-r,k-s} \mu_{rs} - n_{ik}) R_{i-m,k-n} = 0$$

$0 < m < M, \quad 0 < n < N .$

Hence :

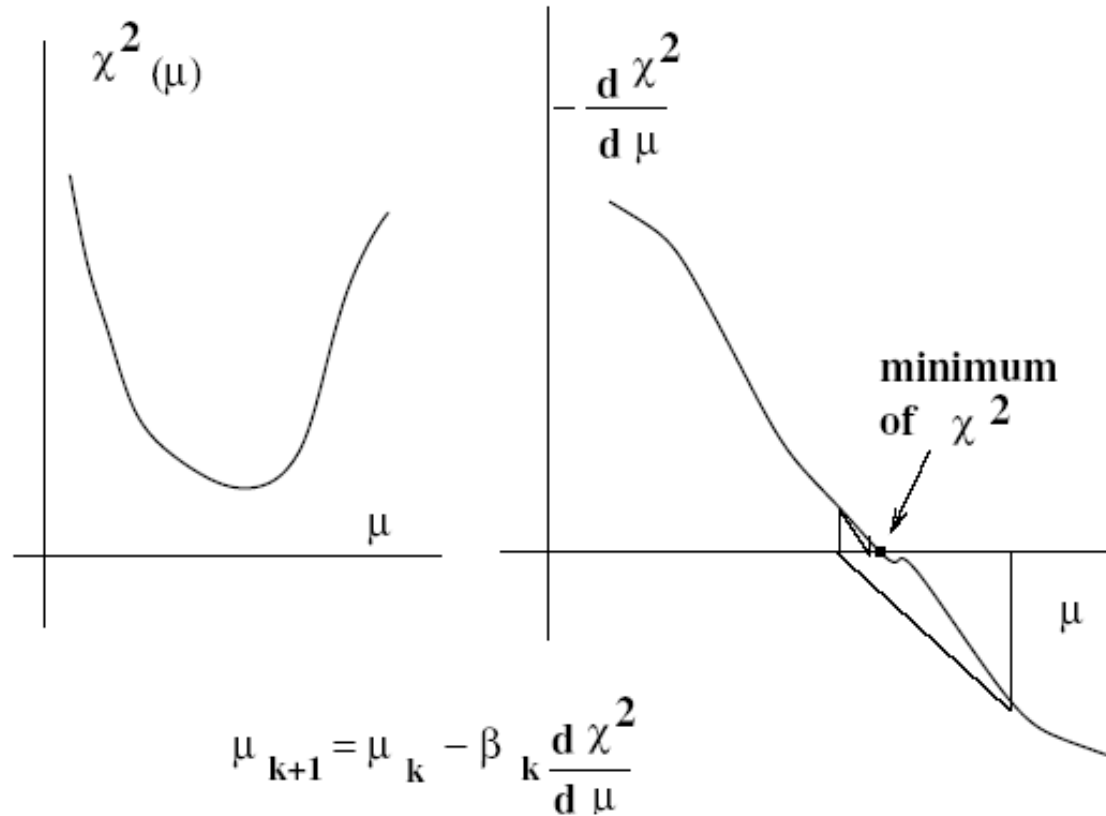
$$\frac{\partial \chi^2}{\partial \boldsymbol{\mu}} = \mathbf{R} * [\mathbf{R} * \boldsymbol{\mu} - \mathbf{n}] = 0 \tag{29}$$

The iterative solution toward the  $\mu$ 's that minimize  $\chi^2$  is obtained with the **Robbins-Monro** algorithm (1951).

The iterative algorithm + best fit



It belongs to the family of the Newton-Raphson methods From (29):



$$\mu_{k+1} = \mu_k - \beta_k \frac{d\chi^2}{d\mu}$$

$$\mu_{k+1} = \mu_k + \beta_k R * [n - R * \mu] \quad (30)$$

This formula minimizes  $\chi^2$ . For example when  $\beta_k = \beta$ :

$$\begin{aligned} \mu_{k+1} &= \mu_k + \beta R * [n - R * \mu_k] \\ &= \beta R * n + (I - \beta R^2) * \mu_k \\ &= \beta R * n + \beta (I - \beta R^2) * R * n + (I - \beta R^2)^2 * \mu_{k-1} \\ &= \sum_{i=0}^k \beta (I - \beta R^2)^i * R * n = \frac{I - (I - \beta R^2)^{k+1}}{\beta R^2} \beta R * n \rightarrow R^{-1} n \end{aligned}$$

The iterative algorithm + Best fit

$$\mu_{k+1} = \mu_k + \beta_k R * [n - R * \mu_k] \quad (31)$$

Previous method converges if

$$\|I - \beta R * R\| < 1$$

when  $\beta$  is independent of  $k$ . In this case

$$0 < \beta < \frac{2}{\text{max eigenvalue of } (R * R * \mu) * \mu^{-1}}$$

When  $\beta_k$  depends on  $k$  convergence is assured if (Robbins and Munro 1951)

$$\lim_{N \rightarrow \infty} \beta_N = 0, \quad \sum_{N=1}^{\infty} \beta_N = \infty, \quad \sum_{N=1}^{\infty} \beta_N^2 < \infty,$$

Next, the method must be regularized by adding a term to the  $\chi^2$ .

$$\chi^2 = \|R * \mu - n\|^2 + \alpha \|C * \mu\|^2 \quad (32)$$

For example,

$$\|C * \mu\|^2 = \sum_{ik} \mu_{ik}^2$$

$$\|C * \mu\|^2 = \left| \sum_{ik} \mu_{ik} \ln \mu_{ik} / \mu_{\text{tot}} \right|, \quad \alpha < 0$$

The iterative solution becomes

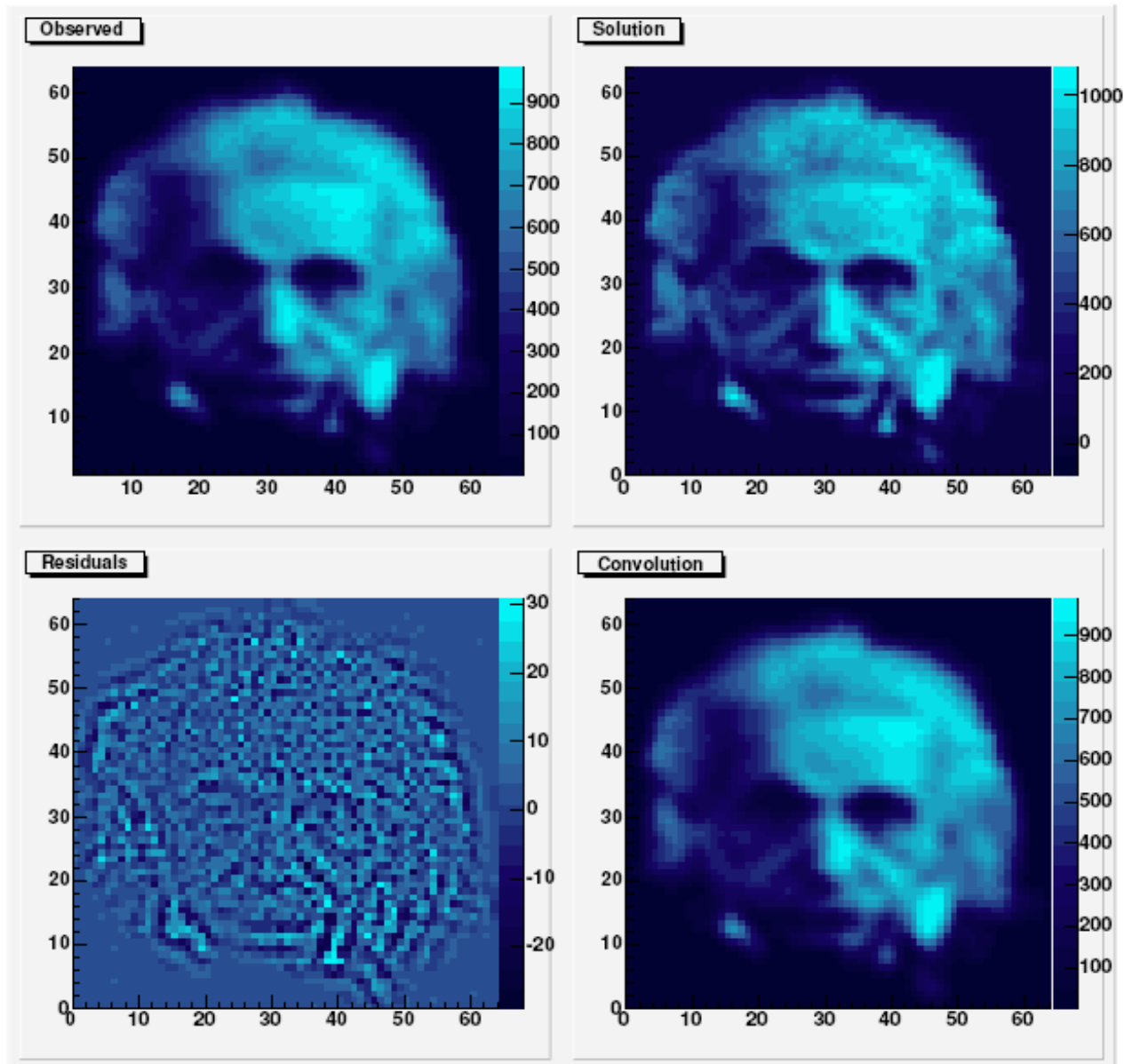
$$\mu_{k+1} = \mu_k + \beta_k [R * n - (R * R + \alpha C * C) \mu_k] \quad (33)$$

The iterative algorithm + best fit + regularization



$$\mu_{k+1} = \mu_k + \beta_k [R * n - [R * R * \mu_k + \alpha(\ln \mu_k / \mu_T + I)]]$$

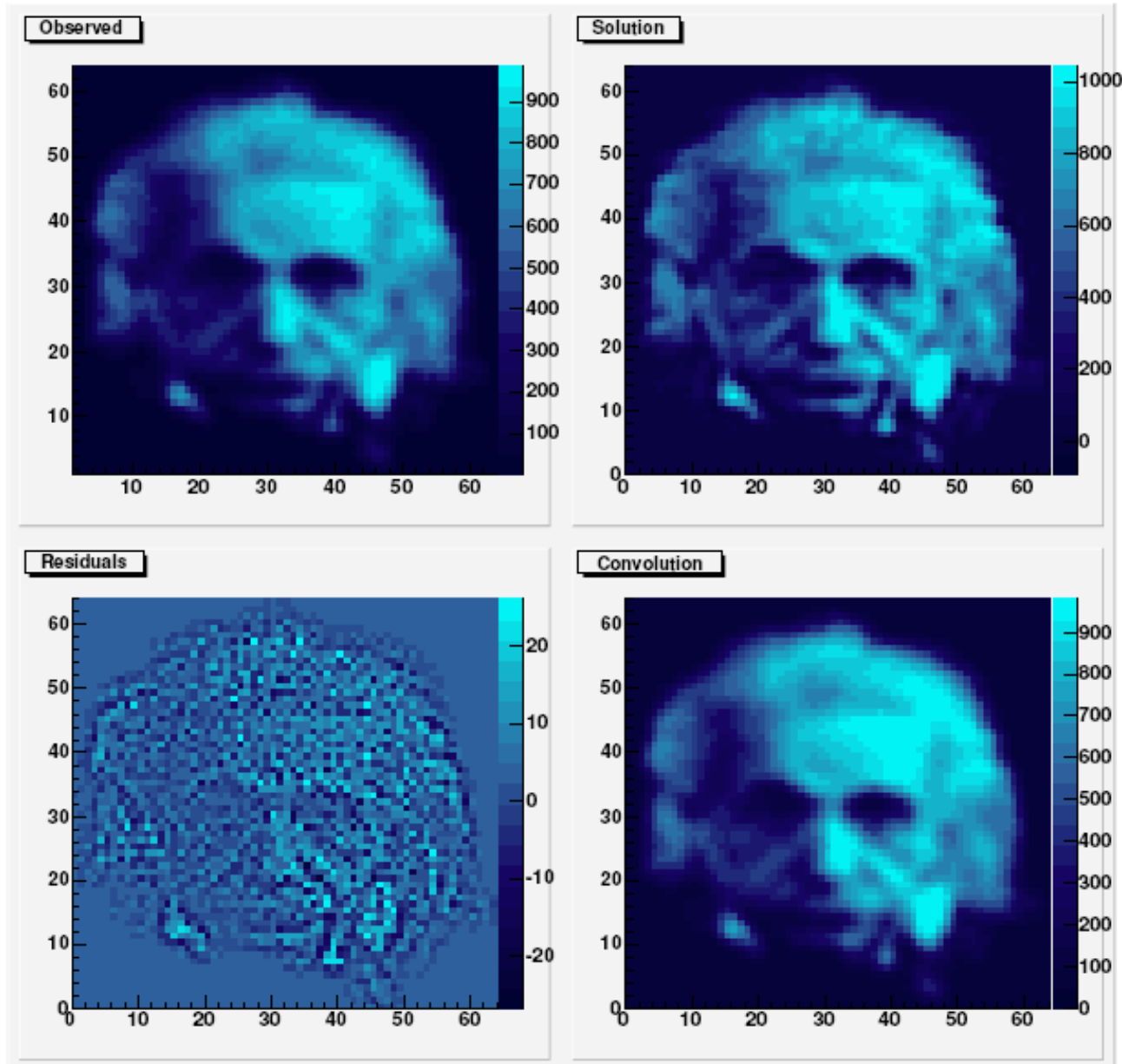
About 40 iterations, regularized with Maximum entropy



The iterative algorithm + best fit + MaxEnt regularization

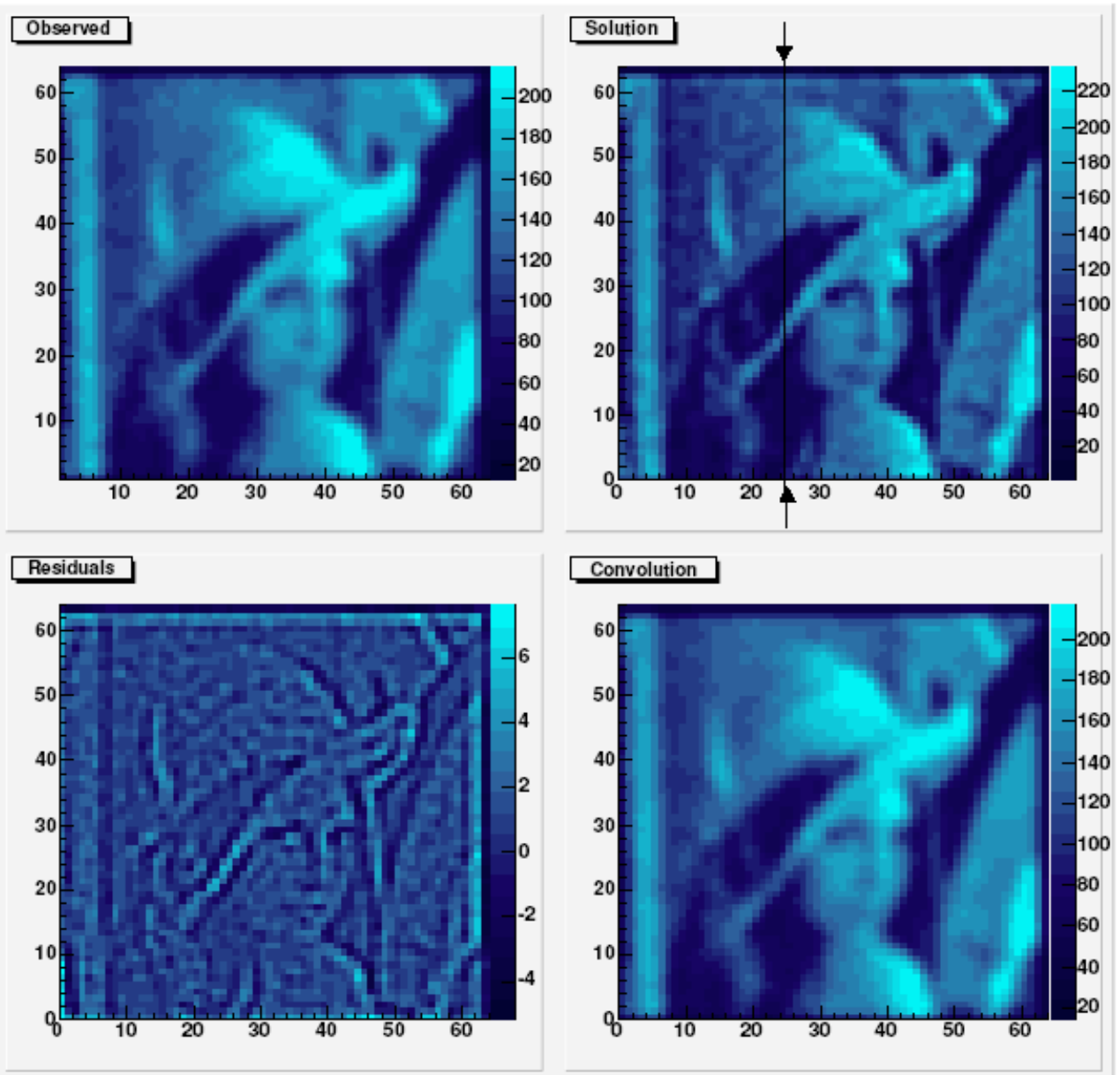
$$\mu_{k+1} = \mu_k + \beta_k [R * n - (R * R + \alpha I) * \mu_k]$$

About 100 iterations, regularized with the sum of squares



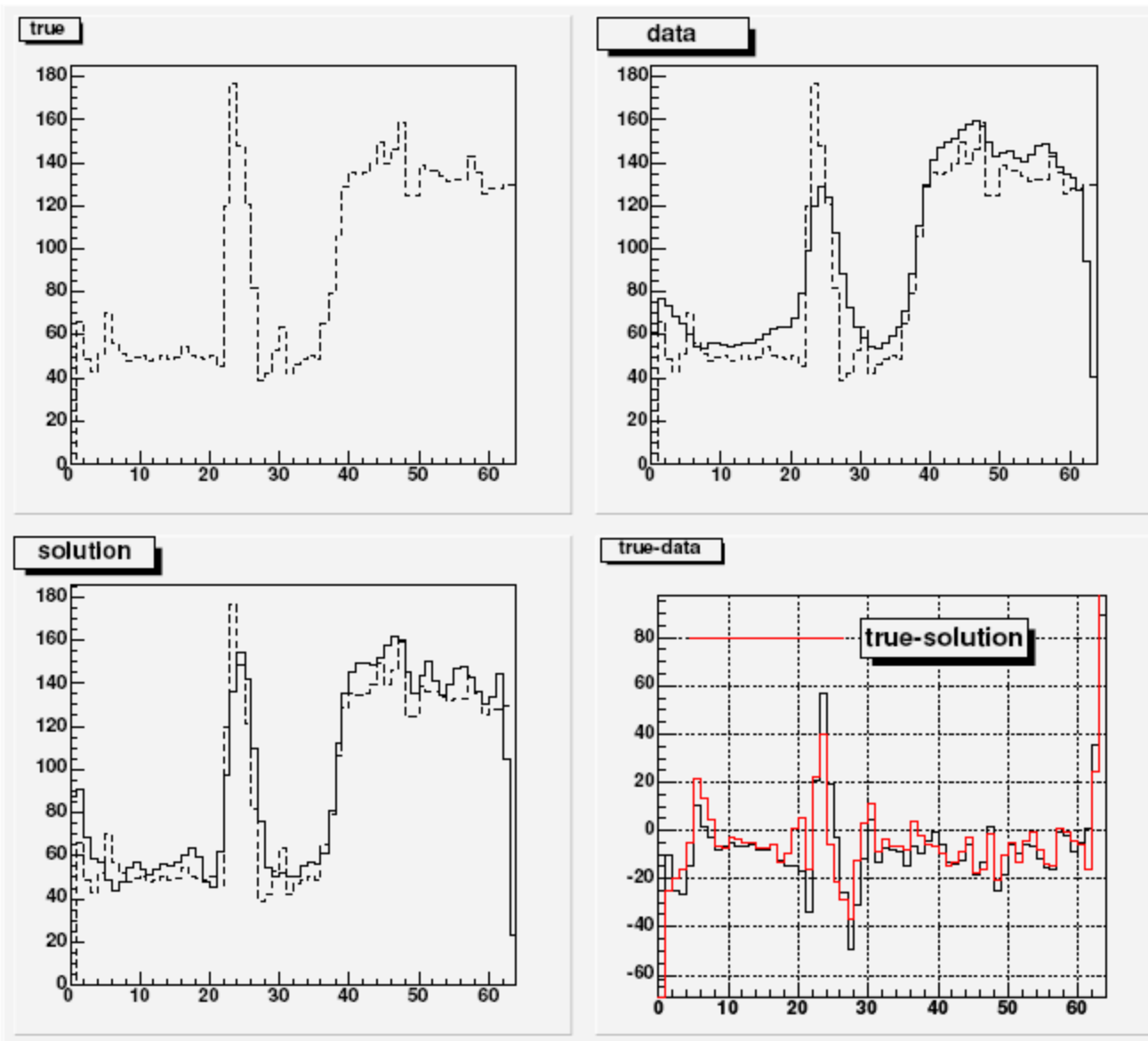
The iterative algorithm + best fit + Tichonov regularization

$$\mu_{k+1} = \mu_k + \beta_k [R * n - (R * R + \alpha I) * \mu_k]$$



The iterative algorithm + best fit + Tichonov regularization

$$\mu_{k+1} = \mu_k + \beta_k [R * n - (R * R + \alpha I) * \mu_k]$$



The iterative algorithm + best fit + Tichonov regularization

# Stopping Rules

- $\chi^2$  variation

$$\chi_k^2 = \|y - R * \mu_k\|^2 = \sum_i^{M \times N} \frac{(y_i - \sum_{ij} R_{ij} \mu_{j(k)})^2}{\sum_{ij} R_{ij} \mu_{j(k)}}$$

$$\frac{\chi_k^2 - \chi_{k-1}^2}{\chi_{k-1}^2} < 10^{-6}$$

If the regularization is good, one has  $\chi_k^2 \simeq \text{DoF}$ .

- Signal to noise ratio (usually measured in decibel)

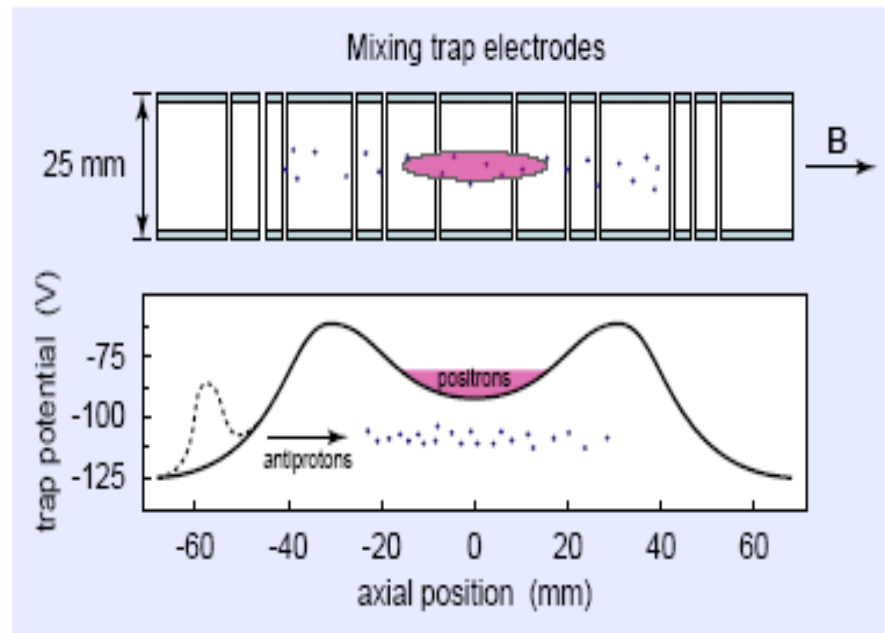
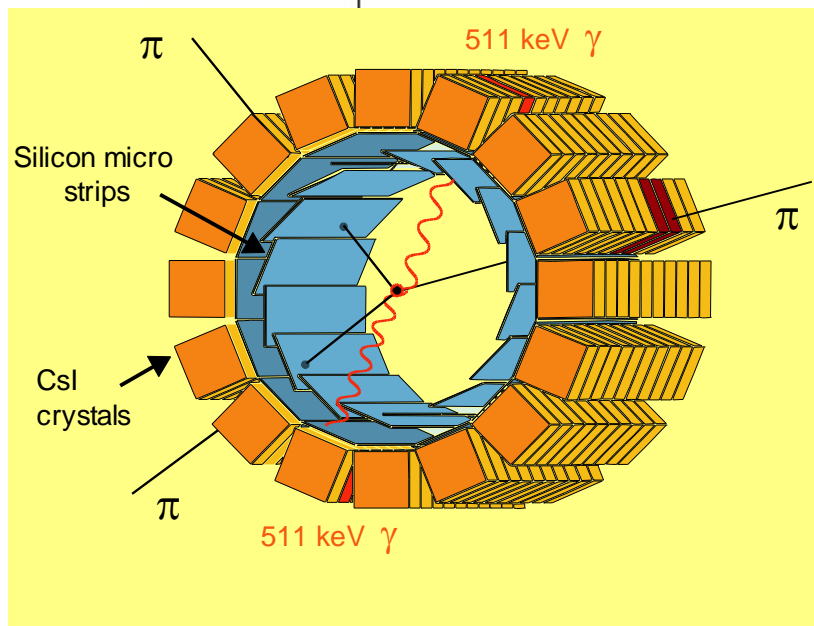
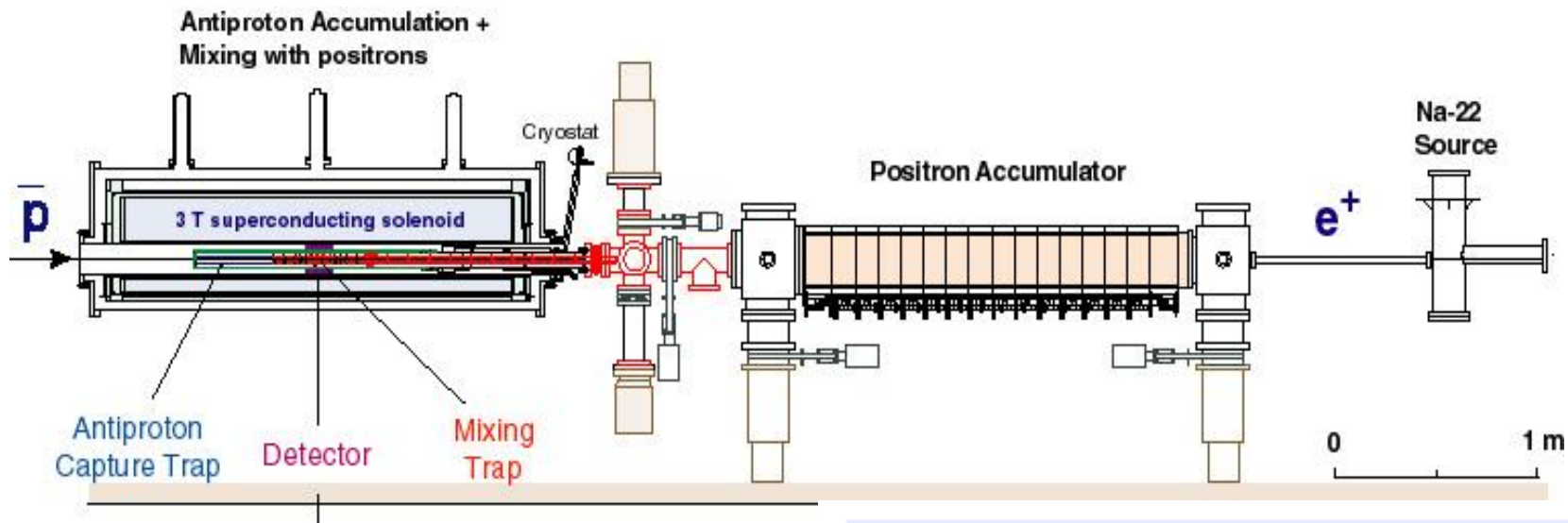
$$SNR = 10 \log_{10} \left[ \frac{\sum_i (\mu_i - y_i)^2}{\sum_i (\mu_i - \mu_{true\ i})^2} \right]$$

where  $\mu_{true}$  is the true image. This quantity is used in the MC simulations during when the true image is known.

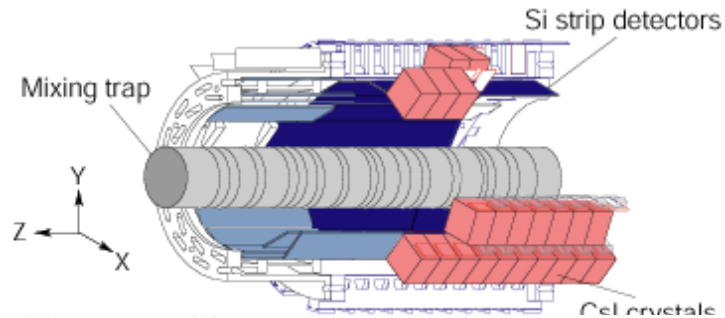
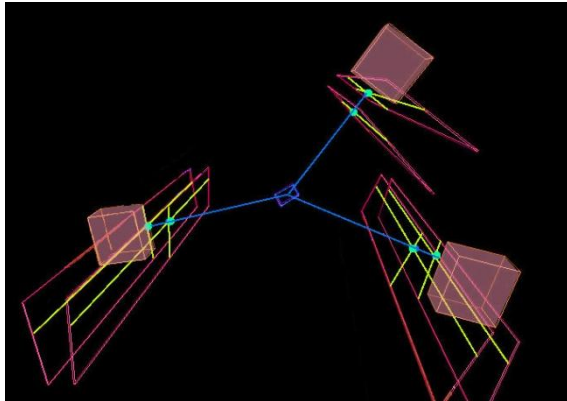
- convergence of the solution

$$\frac{\|\mu_k - \mu_{k-1}\|^2}{\|\mu_{k-1}\|^2} < 10^{-6}$$

# ATHENA apparatus

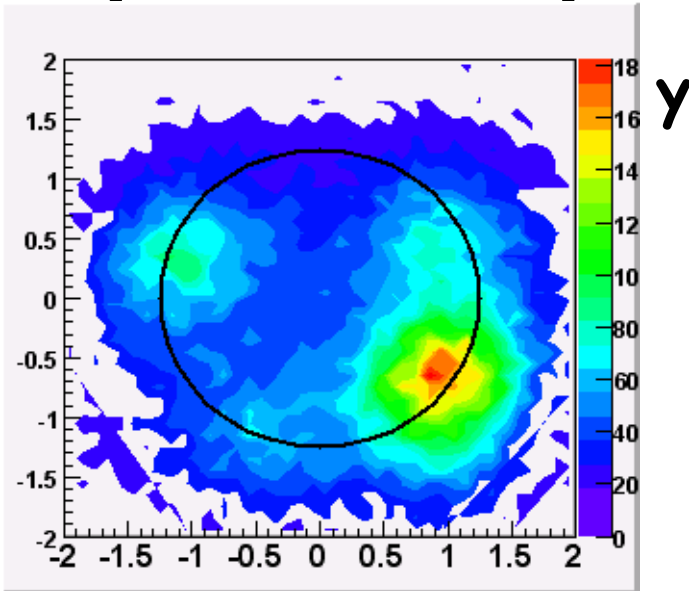


# From the ATHENA detector

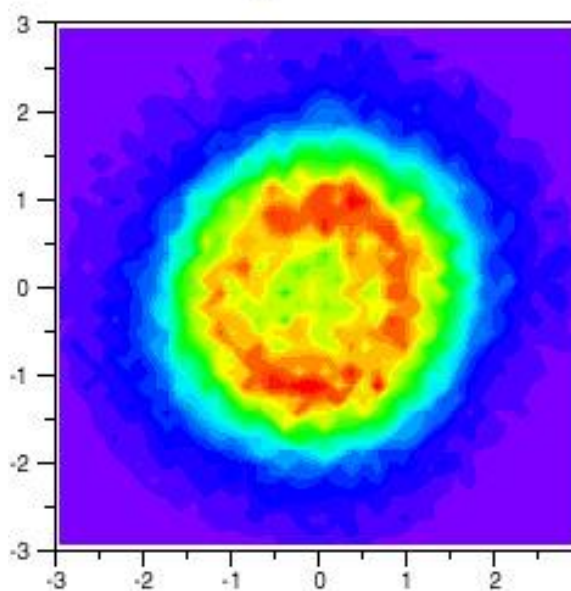


Distribution of annihilation vertices  
when antiprotons are mixed with ...

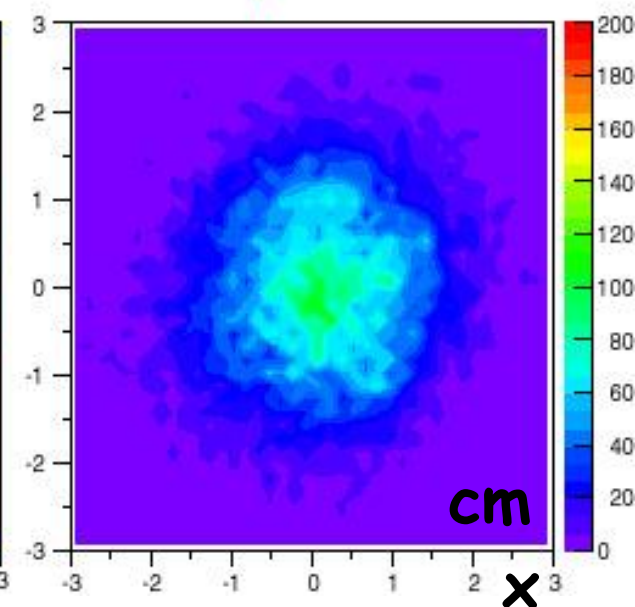
**Pbar-only  
(with electrons)**



**cold positrons**



**hot positrons**



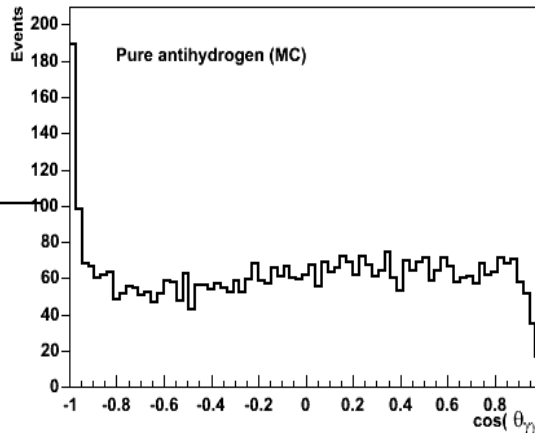
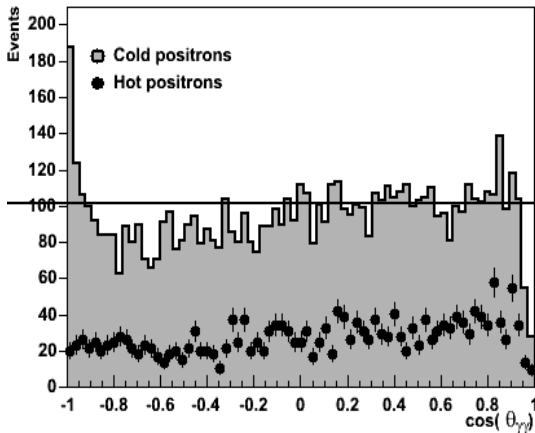
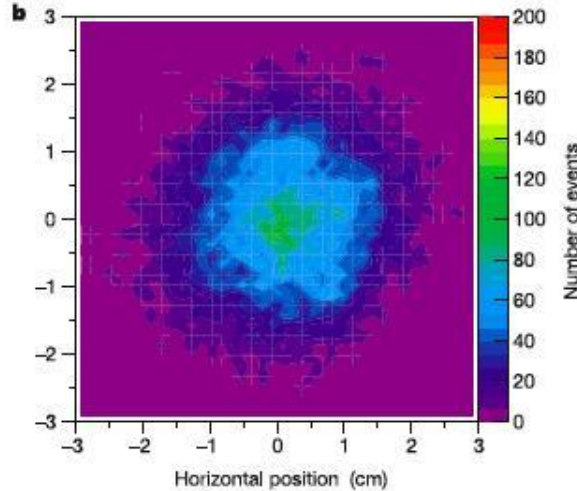
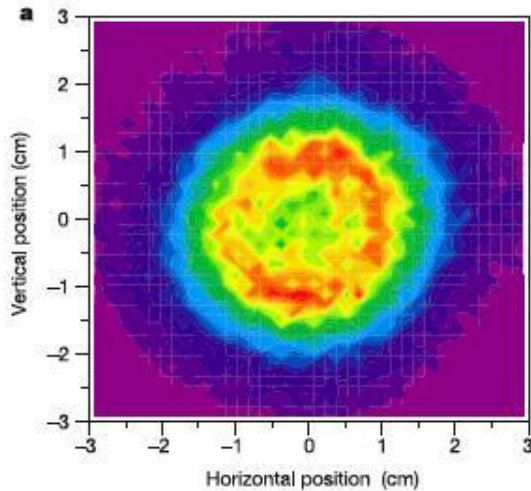


# antihydrogen !!!!!!!!!!!

## FIRST COLD ANTIHYDROGEN PRODUCTION & DETECTION (2002)

M. Amoretti et al., Nature 419 (2002) 456

M. Amoretti et al., Phys. Lett. B 578 (2004) 23



### SIGNAL ANALYSIS:

opening angle  
xy vertex distribution  
radial vertex distribution

65 % +/- 10% of  
annihilations  
are due to antihydrogen

between 2002 & 2004  
more than 2 millions  
antihydrogen atoms  
have been produced

that's about  $2 \times 10^{-15}$  mg  
.. or .. 1000 Giga years for a gram

$$\frac{80}{\sqrt{190 + 110}} = 4.7; \quad \frac{80}{\sqrt{190}} = 6.5; \quad \frac{80}{\sqrt{110}} = 8$$

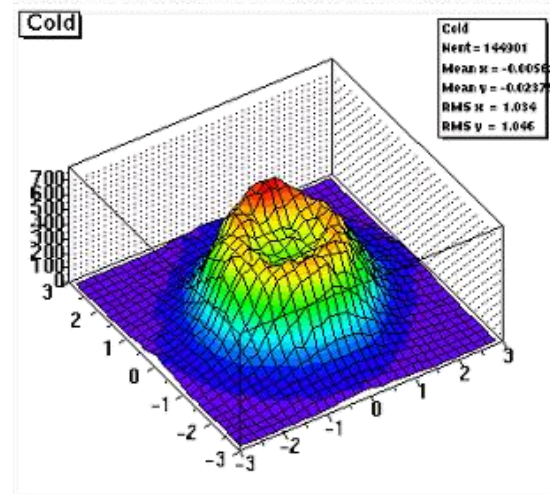
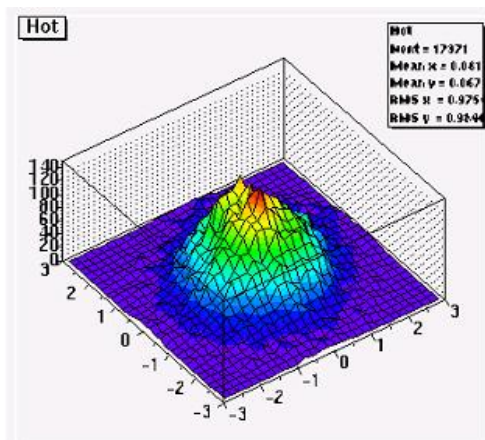
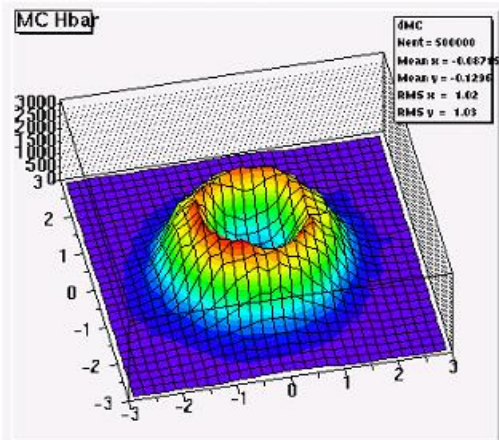


# Annihilation vertex in the trap x-y plane

Hbar (MC)

BCKG  
(HotMixData)

Cold Mix data



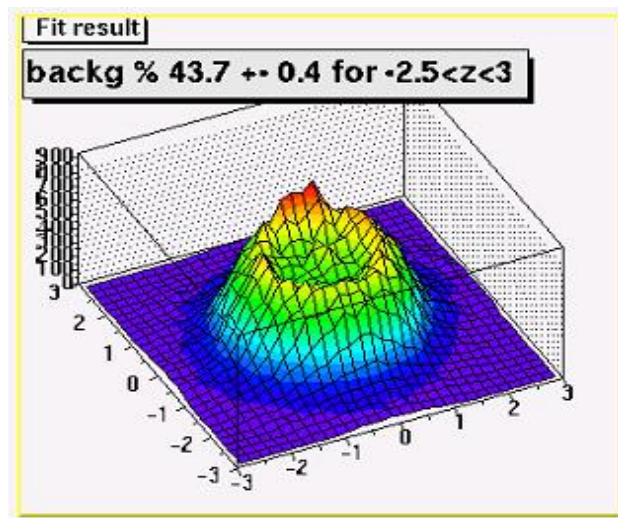
Pbar vertex XY projection (cm)

$$x \text{ Hbar} + (1-x) \text{ BCKG} =$$

ML Fit Result

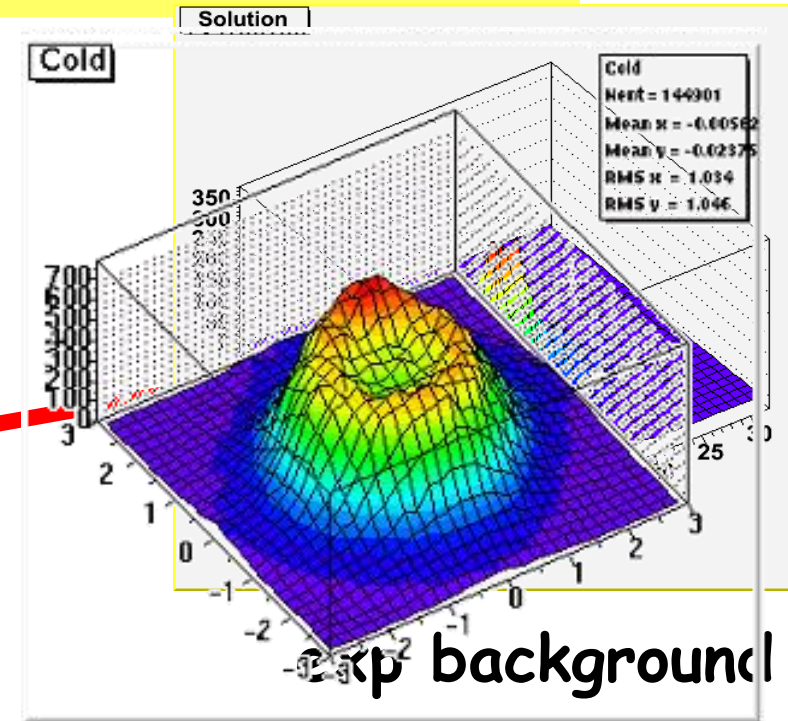
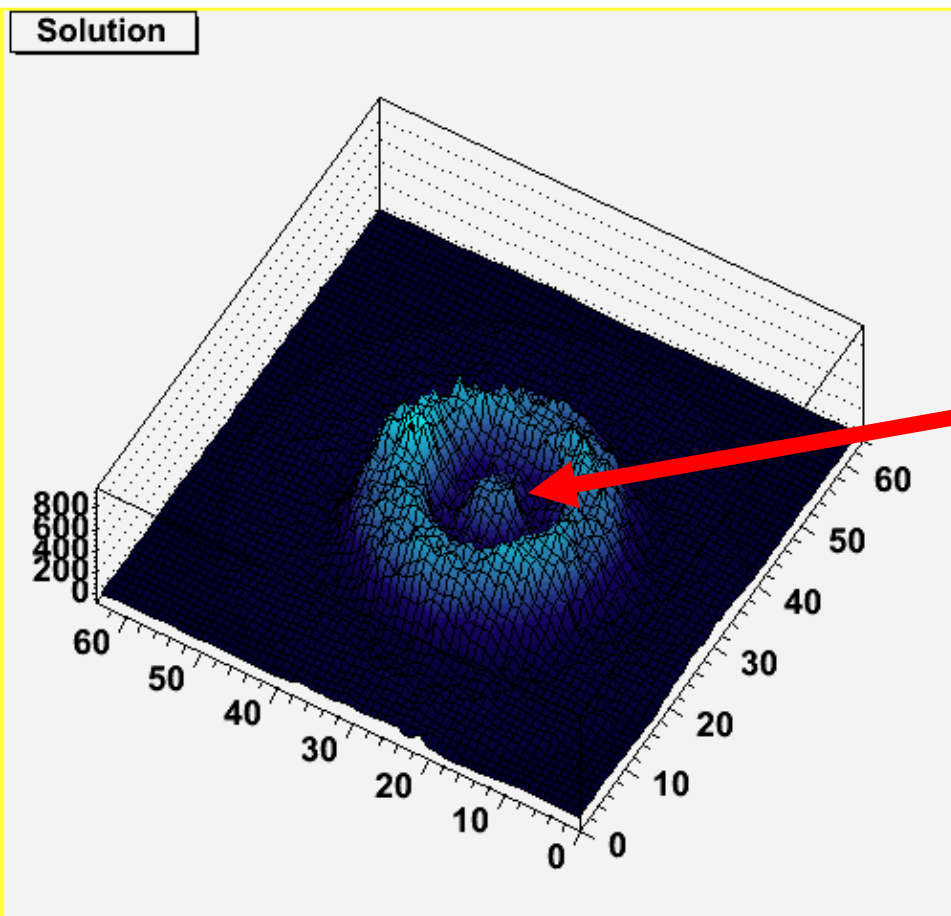
Hbar percentage

$$x = 0.65 \pm 0.05$$



# Iterative best fit method

Cold Mix data



Cold Mix

The vertex algorithm resolution function is gaussian with  $\sigma \cong 3$  mm

The 2D deconvolution reveals two different annihilation modes

## The iterative algorithms + best fit + regularization

- iterative algorithms are used in unfolding (ill posed) problems
- they need a Bayesian regularization term
- when there are degrees of freedom, one can use a best fit of a signal+background function to the data
- in this case there are no Bayesian terms (pure frequentist approach)

## Conclusions

- don't be **dogmatic**
- use Bayes to parametrize the **a priori knowledge** if any, not the **ignorance**
- in the case of **poor** a priori knowledge, use the **frequentist methods**