Data Analysis Methods

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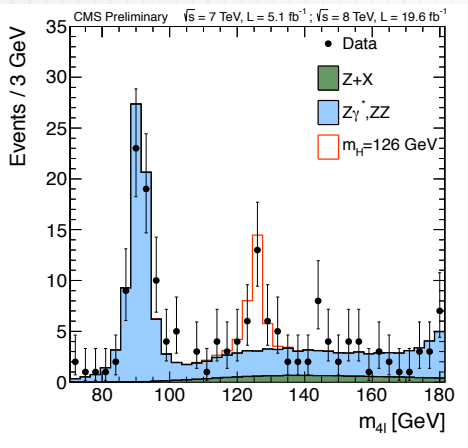
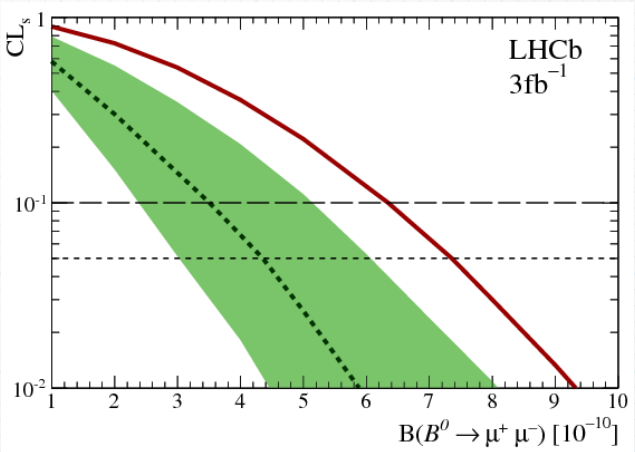
20/01/2015

Objectives

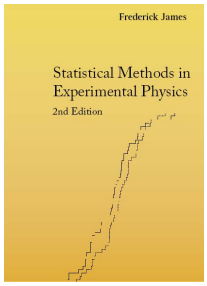


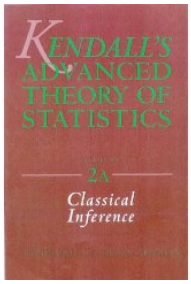


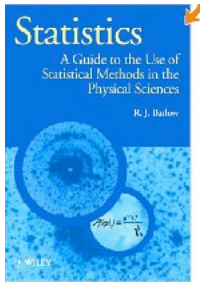
- Is there a new signal?
  - (In this case the Higgs boson)
- What is the limit on the production of a given process?
  - In this case the Branching ratio of $B \to \mu^+\mu^-$

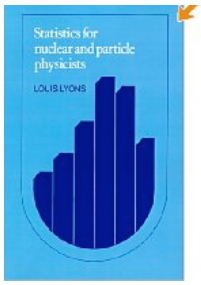
Bibliography

- Excellent lectures given by experts and related with HEP, that I use extensively here:
  - Glen Cowan: Freiburg lectures (2011)
    - http://www.pp.rhul.ac.uk/~cowan/stat_freiburg.html
  - Kyle Cranmer: CERN training lectures (2009)
  - Mike Willians: IDPASC Santiago de Compostela lectures (2013)
- Excellent books:









Objetives

- Introduction to Statistical Data Analysis Methods in High Energy Physics
  1. Classification of events into known categories
  2. Hypothesis testing: Is this incompatible with the null hypothesis? Do we reject the alternative hypothesis?
  3. Setting Confidence Level intervals or Upper Limits to physics parameters
  4. Parameter estimation (regression) and treatment of errors (statistical and systematic)

Objectives

- The physicist goals, depending on the experiment, are:
  - choose between different hypothesis (is there a Higgs boson?)
  - provide an upper limit or a C.L. interval of an observable: $B(\mathrm{Bs}\to\mu\mu)$
  - estimate the parameters of model (ϕs from $\mathrm{Bs}\to \mathrm{J}/\psi\phi$)
    - Estimate the statistical and systematic uncertainties
- To present or publish your result, you:
  - should indicate the methods used to obtain your measurements
  - use them correctly to not introduce bias or "incorrect" results
  - know what your measurement is and what is not!

Outlook

- Introduction and reminder

1. probability density functions (PDFs)
2. Bayes' theorem

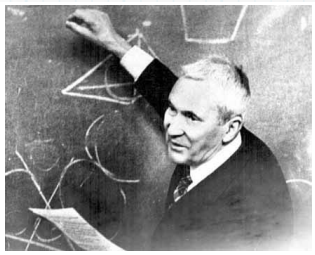
- Classification

3. Hypothesis testing
   - Neyman-Pearson Lema
   - MVA-methods
4. Goodness of the fit
5. C.L intervals

- Regression

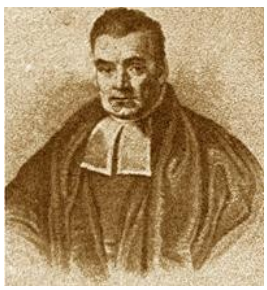
6. Parameter estimation
7. Uncertainties

Probability and Bayes



- Kolmogorov axioms:
  1. probability of an event is non-negative P(E)>=0
  2. probability for the entire space of events is 1
  3. if elements are disjoint, probability is additive P(E1)+P(E2)
- Corollaries
  1. $P(A \cup B) = P(A) + P(B) - P(A \cap B)$
  2. P(!A) = 1-P(A)

Bayes's theorem



- Marginal P(A) and conditional probability P(A|B)
- Bayes' theorem

$$P(A|B) = \frac{P(B|A)\,P(A)}{P(B)}$$

e Check bayes': two dices, probability they add to six if one is four, and that one is four if they add six.

$$\frac{1}{3}\frac{1}{6} = \frac{2}{5}\frac{5}{36} = \frac{1}{18}$$

Bayesians vs Frequentist

- The impossible divide:
  - **Frequentists:** they are objective, they obtain **P(data|theory),** they are deductive, they assume an experiment can be repeated n-large times in the same conditions
  - **Bayesians:** they are "subjective" (with some reasonable assumptions), obtain **P(theory | data)**, they are inductive, they assume some prior knowledge and use Bayes' theorem

e Does the Higgs exists? What a frequentist will say about the Higgs?

e Does this Higgs exists? I expect 2 background events, if there will be a Higgs I expected 8 events, and I observe 6 events. (Consider now that instead of the Higgs is a very rare, exotic, bizarre Z' that a crazy theoretician has proposed…)

$$P(H|n) = \frac{P(n|H)P(H)}{P(n|H)P(H) + P(n|!H)P(!H)}$$

Bayesians

e An underground neutrino detector, it fails 10% of the times, and the reactor stops 30% of the time, in this moment it does not detect, what is the probability that the reactor is not running?

e An underground solar neutrino detector, it fails 10% of the times. It does not detect now, what is the probability that the Sun is off?

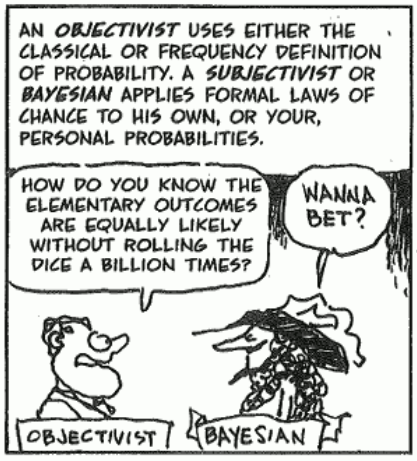
$$P(!R|!D) = \frac{P(!D|!R)P(!R)}{P(!D|!R)P(!R) + P(!D|R)P(R)}$$

as $P(!D|!R) = 1$, we have:

$$P(!R|!D) = \frac{0.3}{0.3 + 0.7 \times 0.1} = 0.81$$

Frequentist vs Bayesians

- The impossible divide (*L. Lyons* quote?):
  - **Frequentists:** use impecable logic to answers questions that nobody cares about!
  - **Bayesians** address the questions everyone is interested on using assumptions that nobody believes



- Finally it is not so dramatic: enough data speaks by itself!

Bayesian posterior probability

- Bayesians obtain a *posterior* probability from data and a *prior* probability

$$P(h|x) = \frac{P(x|h)\pi(h)}{\int P(x|h)\pi(h)\mathrm{d}h}$$

e

Consider dices of 4, 6, 12, 24 sides. Take one of them, rolling it 6 times we get: 3,5,6,1,2,2, what is the probability that has 4, 6 12 or 24 sides? What is the dependence with your priors?

1. hypothesis: n = 4,6,12 and 24 sides
2. probability P(i|n) = 1/n (if i<n), 0 otherwise
3. start with prior probabilities, suggestion: π(n)=1/4
4. change the priors: π(4)=1/2, π(6)=1/8, π(12)=1/8, π(24)=1/4

PDFs

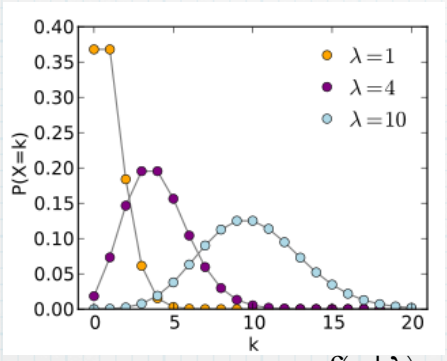
- Probability (mass) density functions and random variables (rvs)

$$\int_{-\infty}^{\infty} f(x)\,\mathrm{d}x = 1$$

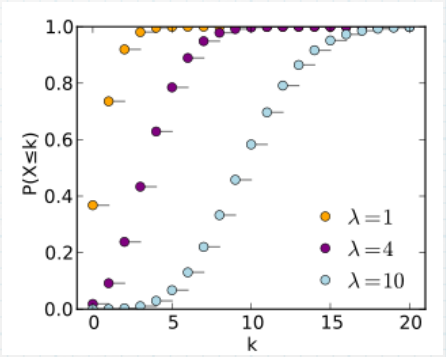
- Cumulative (mass) density functions

$$F(x) = \int_{-\infty}^{x} f(x)\,\mathrm{d}x$$

e Generate n-large number of poisson rvs with λ=10 and get is cumulative distribution



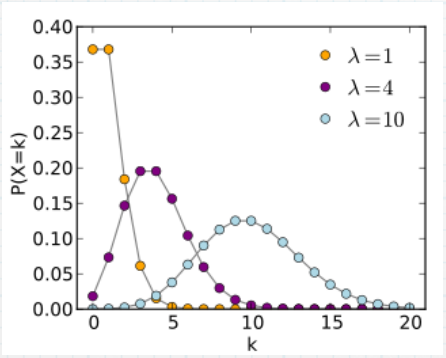
f(x | λ)

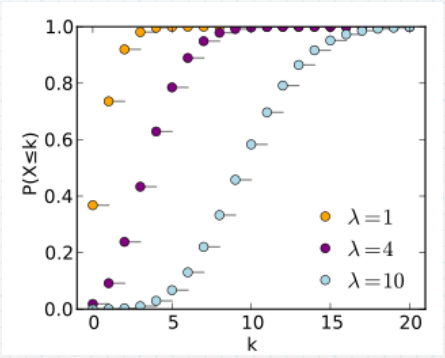


F(x | λ)

PDFs

- cumulative distributions of a pdf are flat!
  - Use it to generate random numbers
  - u random uniform [0,1], x = $cdf^{-1}(u)$





PDFs

- Expectation values:

$$E[g(x)] \equiv \int g(x)\, f(x)\, \mathrm{d}x$$

The *mean* (or average value), is the expected value of x:

$$E[x] = \mu \equiv \int x\, f(x)\, \mathrm{d}x$$

The *variance*, the expected value of $(x-\mu)^2$:

$$V[x] = \sigma^2 = E[(x-\mu)^2] = E[x^2] - \mu^2 \equiv \int (x-\mu)^2\, f(x)\, \mathrm{d}x$$

We call *standard deviation* to:

$$\sigma = \sqrt{V[x]}$$

Finally, the *expected value* is the x value with the higher $f(x)$, and the *median*, is the x value that devices the PDF distribution in half, $\int_0^x f(x)\,\mathrm{d}x = 0.5$. For the symmetric PDFs, the mean and median are the same, this is the case of the Gaussian PDF.

e Compute the mean and standard deviation of a uniform distribution between 0. and d. What is the "resolution" of a digital detector with pitch = d?

PDFs

- The common HEP PDFs

name	PDF	example
Binomial	$f(n\|N,p) = \frac{N!}{n!(N-n)!}p^n(1-p)^{N-n}$	Branching ratio
Multinomial	$f(\mathbf{n}\|N,\mathbf{p}) = \frac{N!}{\Pi_{i=1}^m n_i!}\Pi_{i=1}^m p_i^{n_i}$	Histogram with N fixed entries
Poisson	$f(n\|\nu) = \frac{\nu^n}{n!}e^{-\nu}$	Number of events observed
Uniform	$f(x\|a,b) = \frac{1}{(b-a)}$	Monte Carlo method
Exponential	$f(x\|\tau) = \frac{1}{\tau}e^{-x/\tau}$	Decay time
Gaussian	$f(x\|\mu,\sigma) = \frac{1}{\sqrt{2\pi}\sigma}e^{-\frac{(x-\mu)^2}{2\sigma^2}}$	Measurement error
χ^2_n	$f(x\|n) = \frac{1}{2^{n/2}\Gamma(n/2)}x^{n/2-1}e^{-x/2}$	Goodness of fit
Breit-Wigner	$f(x\|\Gamma,x_0) = \frac{1}{\pi}\frac{\Gamma/2}{\Gamma^2/4+(x-x_0)^2}$	Mass of a resonance
Landau	$f(\Delta E\|\beta)$	Ionization energy loss

- Their mean and variances

name	average	variance
Binomial	Np	$Np(1-p)$
Multinomial	Np_i	$Np_i(1-p_i)$
Poisson	ν	ν
Uniform	$\frac{b-a}{2}$	$\frac{(b-a)^2}{12}$
Exponental	τ	τ^2
Gaussian	μ	σ^2
χ^2_n	n	$2n$
Breit-Wigner		∞
Landau	∞	∞

PDFs

- Central Limit Theorem: adding rvs with given pdfs, the addition follows a gaussian pdf

e Generate n=100 rvs following a uniform distribution in [0.,1.] and take the addition, repeat m-large times, and get the distribution.

e Generate n-large events with a binomial pmt with p=0.01 and N=100, what is the distribution of the *yes* events?

e Generate n-large events with a poison pmf with $\lambda=10$

e Generate n-large (100) events with a gaussian pdf (μ,σ), compute for each one: $(x-\mu)^2/\sigma^2$, what is the distribution that you get?

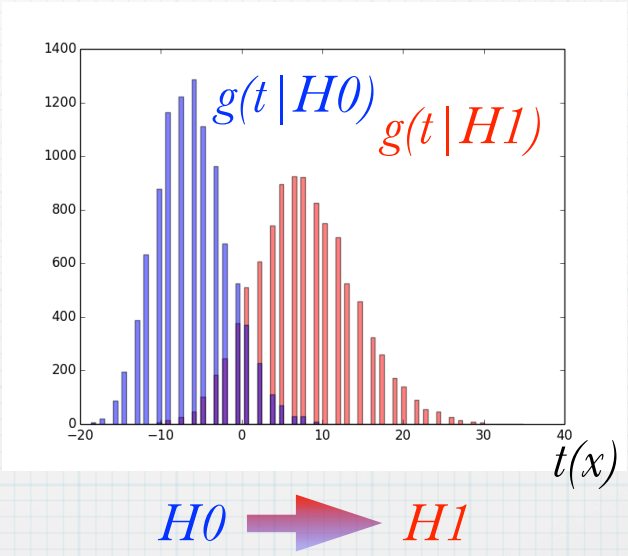
Hypothesis testing

- Hypothesis testing: Comparing a well known hypothesis (null) H0 with respect an hypothetical hypothesis (H1), with one observation, when to exclude the H1 and to reject H0?

Hypothesis testing

- hypothesis pdfs: $f(x|H0)$, $f(x|H1)$,
- test-statistics $t(x)$ escalar with ordering of events (i.e $H0<H1$)
  - $g(t|H0)$ and $g(t|H1)$, the pdfs of t for H0 and H1
  - Likelihood Ratio, $\Lambda(x)$, is the "optimal" $t(x)$

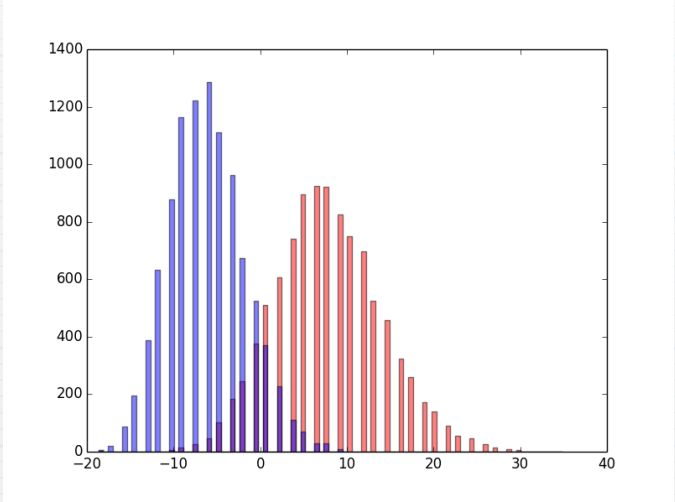
$$\Lambda = \frac{\mathcal{L}(H_1)}{\mathcal{L}(H_0)} = \frac{f(x|H_1)}{f(x|H_0)}$$



Hypothesis testing

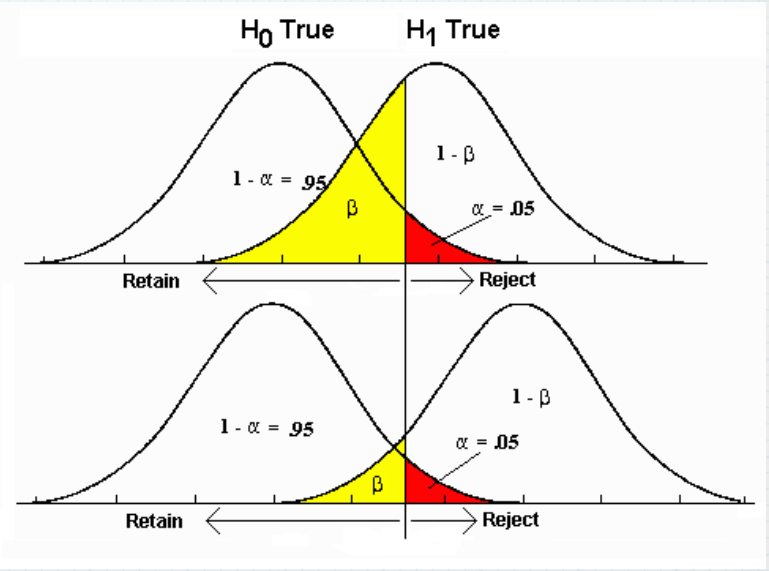
Consider H0, a poisson distribution ν = 10, and H1, a poisson ν = 20, construct the test-statistics as the likelihood ratio, Λ

Consider n-bins, each one independent, H0, follows a poisson with ν = [2,1,0.5], and H1, a poisson ν = [1,3,1], construct a test-statistics from the likelihood ratio, Λ (suggestion use $-2\log\Lambda$)



Hypothesis testing

- Data ***x***, observation ***$t_0(x)$***
- Errors:
  - Type I, **α**, false positives
  - Type II, **β**, false negatives
- Power **1-β**



$$\alpha = \int_{t_c}^{\infty} t(x|H_0)\,\mathrm{d}x,$$

$$\beta = \int_{-\infty}^{t_c} t(x|H_1)\,\mathrm{d}x.$$

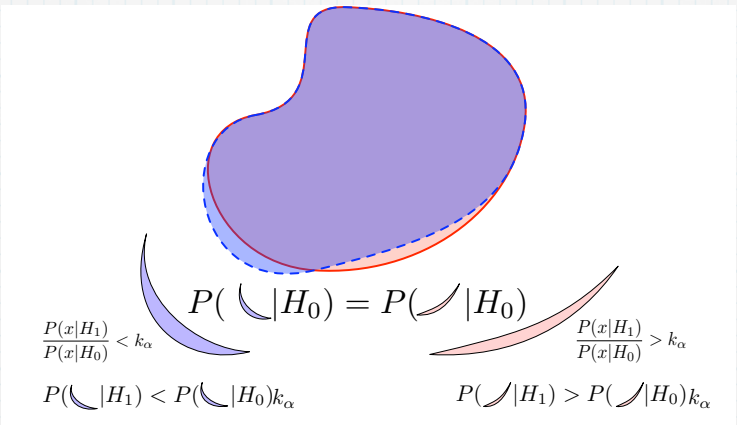
- *p-value*: fraction of events of *H* equal or less similar to *H* that the observation $t_0(x)$
  - **α**, *p-value* of *H0*, **β**, *p-value* of *H1*

Hypothesis testing

- Neyman-Pearson Lema:
  - For a fix **α**, called size of the test, the likelihood ratio, ***Λ***, is the test-statistics that maximizes the power, ***1-β***, that is it is optimal, fulfills:

$$\Lambda = \frac{\mathcal{L}(H_1)}{\mathcal{L}(H_0)} = \frac{f(\mathbf{x}|H_1)}{f(\mathbf{x}|H_0)} > k_\alpha$$

  - The power is the the efficiency on *H1* of the cut k

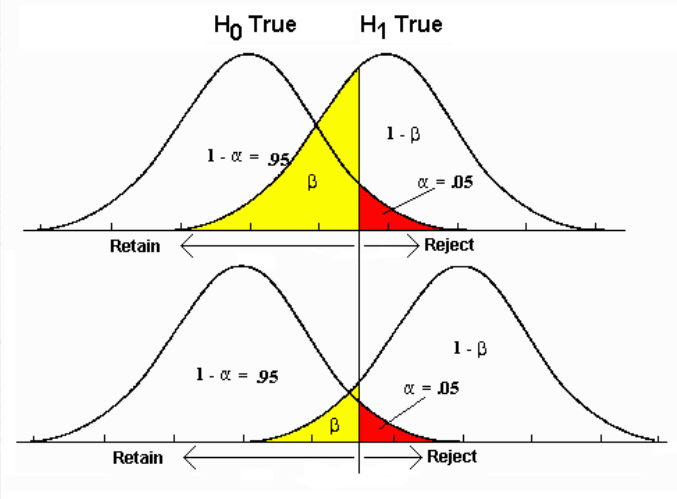


Hypothesis testing

- Tradition in HEP:
  - **discovery** of *H1*, if **α**, *p-value* of *H0*, is smaller $2.87\ 10^{-7}$,"5-σ"
  - **exclusion** of *H1* at 90 (95)% Confidence Leve (CL), if **β**, *p-value* of *H1*, is smaller than 0.1 (0.05)
  - **sensitivity** of the experiment: the ROC (**1-β** vs **α**) curve

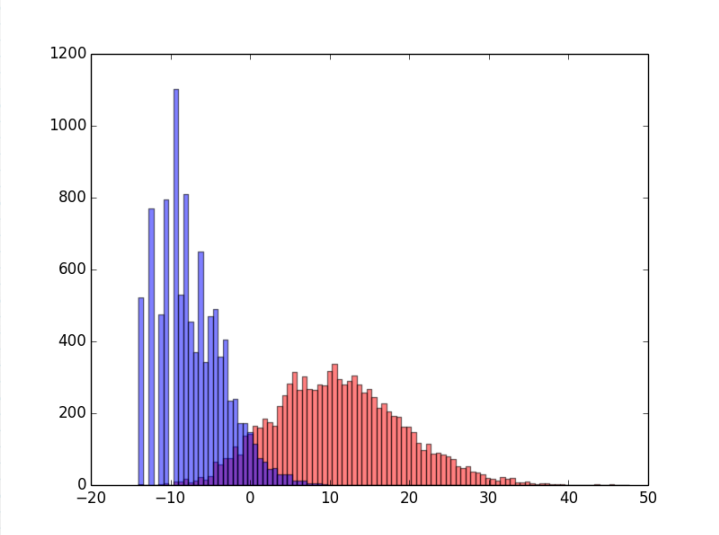
$$\alpha < 2.87 \times 10^{-7},$$

$$\beta < 0.1\ (0.05)$$



Hypothesis testing

Consider n-bins, each one independent, H0, follows a poisson with ν = [1.5,1,0.5], and H1, a poisson ν = [3.5,4,2.5], construct a test-statistics from the likelihood ratio (suggestion -2 *log Λ*), we observe [2,1,1], what is the *p-value* for H1? at what confidence level H1 is excluded? what is the *p-value* of H0?



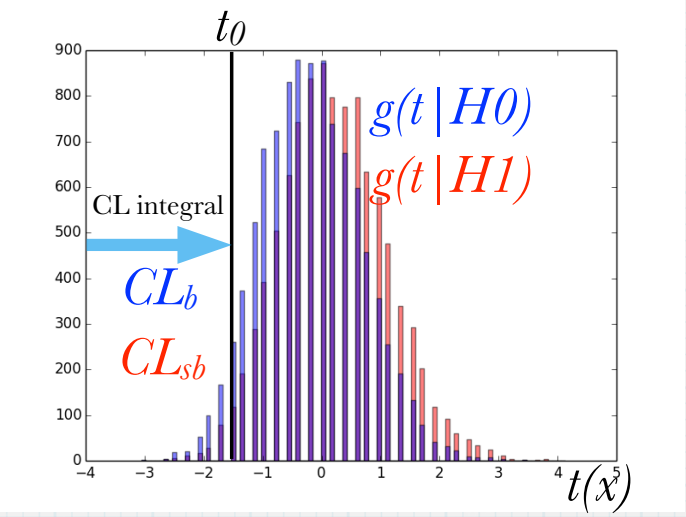
Compute the ROC curve (1-**β** vs **α**)

Hypothesis testing - CLs

- CLs method
  - Can we exclude when there is no sensitivity?
  - Use *CLs = CLsb/CLb* not proper coverage, but commonly used)

$$CLs = \frac{CL_{s+b}}{CL_b} = \frac{p_{s+b}}{1-p_b} = \frac{\beta}{1-\alpha}.$$

notice $CL_b\,(1\text{-}\alpha) > CL_{sb}\,(\beta)$

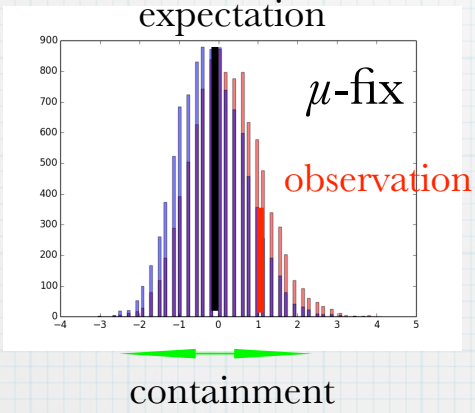


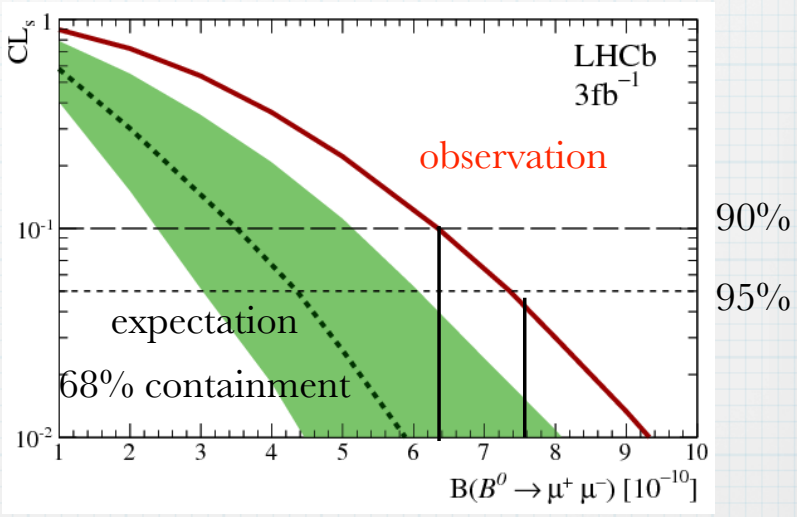
e Consider n-bins, each one independent, H0, follows a poisson with ν = [10,5], and H1, a poisson ν = [12,6], the observation is [6,1], what is the *p-value* for H1? what is the 1-**α**? What is the CLs?

Hypothesis testing - CLs

- Composite hypothesis
  - *H1* can depends on certain parameters:
    - ***μ*** strength of the signal *H1 = B + μ S*, *H0 = B*, *B* is background, *S* is signal
    - scan on *μ*!
  - The B→μ⁺μ⁻ case (we did not know the Br!)

CLs

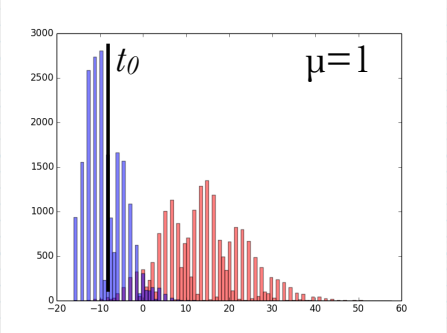


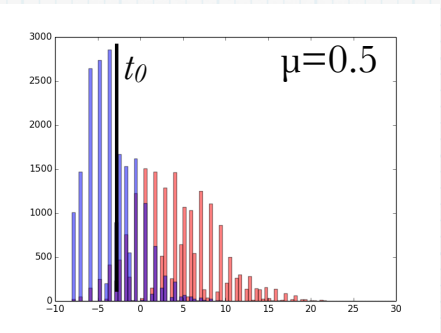


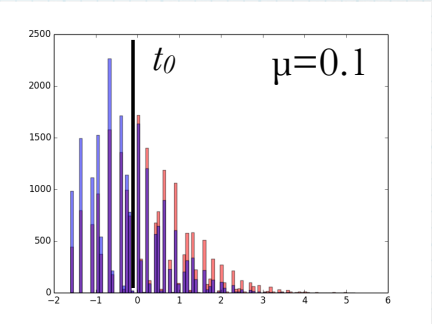
$\mu = \mathrm{Br}/\mathrm{Br}^{\mathrm{SM}}$

Hypothesis testing - CLs

- Scan on μ
  - From the $g(t|B)$, *pdf* of t for $H0=B$, get the median (expectation) and a containment (i.e. 68%) t-region
  - Get the $t_0(\mu)$ and compute $CLs(\mu)$
- Exclude μ values at given confidence level (CL) [see confidence intervals]





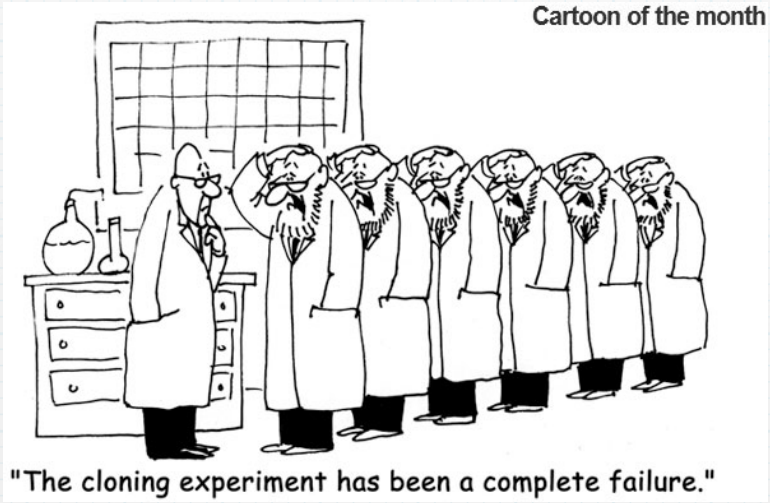


e

Consider n-bins, each one independent, H0=B, follows a poisson with B = [1.5,1,0.5], and H1=B+μS, a poisson S = [2,4,2], the observation is [1,1,1], compute the expectation vs μ? What is excluded μ region at 90 % CL with CLs?

Goodness of the fit

- How good does the hypothesis fits the data?
- When two data samples are identical?



Goodness of the fit

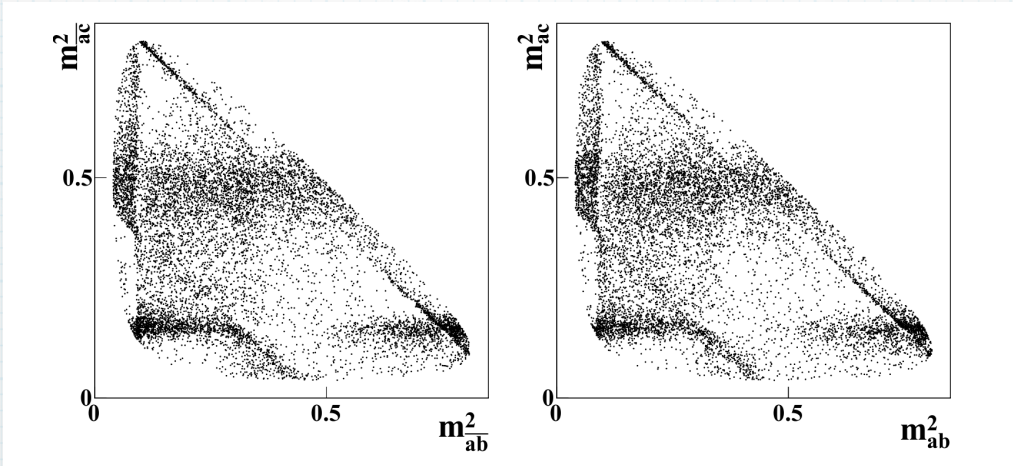
Flipping n=20 coins, m=10 times, we got 12,10,9,6,11,10,9,10,12,11 heads, is this fear? Flipping a coin m=10 times, we got 9 heads, is this fear?

Do a text to a physics student class in Quantum Physics, now repeat the text to a group of spanish literature students, how you compare both samples?

- Goodness of the fit test
  - Several tests: Chi2, Kolmogorov, Energy, k-nearest neighbor, etc…
  - use the p-value
    - Define a test-statistics *t(x)*, get the *pdf*, *g(t)*, and the cumulative *cdf*, *G(t)*
      - a suggestion: $t(x) = -\log(f(x))$
    - Compute the *p-value* of t_0, if $p<0.05$ reject agreement at 95 %CL

Goodness of the fit

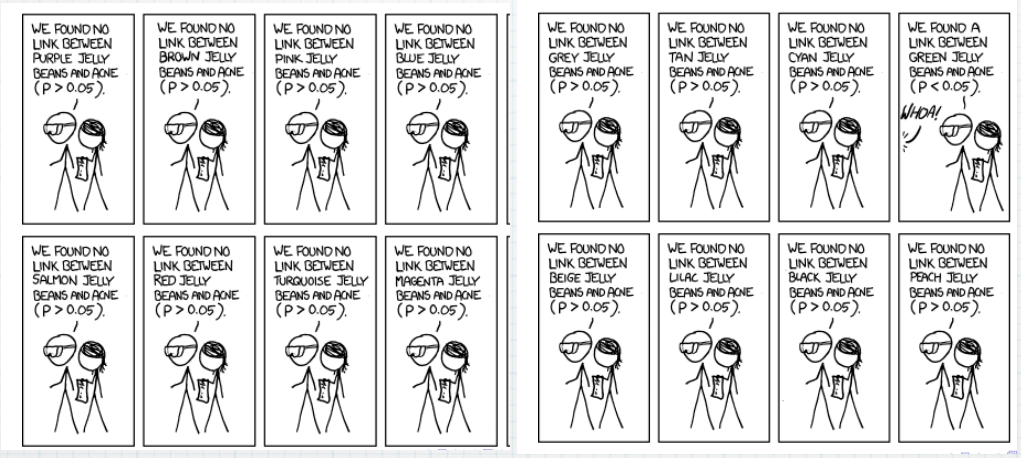
- Are this sample equal?
  - If not, there is CP-violation!

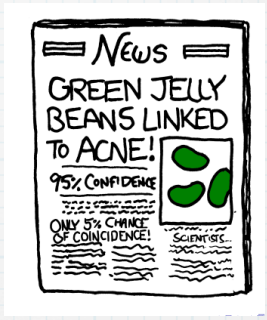


B-bar *B*

Goodness of the fit - *p-value*

- Look Elsewhere effect
  - Looking for a rare (small *p-value*) event in a m-large number of places could result in a discovery, how to "normalize" the search?
  - move from *local* to *global p-value*





Confidence Intervals

- Confidence Intervals:
  - Looking for a phenomena, if not found, put limits at a given confidence level (CL) on the strength parameter μ
  - Or to set an interval of a CL for a parameter μ

Confidence Intervals

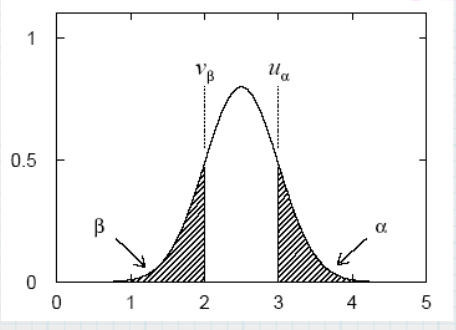
- What does it means a CL interval?
  - **Frequentist**: the interval *covers* the true parameter μ a CL (i.e 95%) of the cases.
    - If you will perform m-large number of experiments and get m-intervals, in a CL (i.e 95%) fraction of the experiments, the interval covers the true μ.
  - **Bayesians**: talk about *credible* intervals, the probability that the true μ is inside the interval is CL (i.e. 95%)
    - P(μ ∈ Interval) = CL
- Construction of frequentist intervals:
  - Classical or **Feldman-Cousins** construction

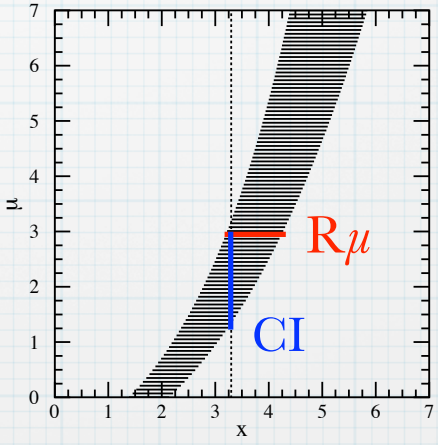
Confidence Intervals

- Classical - Neyman's construction
  - For a given value of μ, find the region Rμ of x at a given CL
    - ambiguity: select central, upper, lower interval
  - For a given $x0$ measurement, find the interval of μ, where x in in the Rμ

$$\alpha = \int_{x_l}^{\infty} f(x)\,dx, \quad \beta = \int_{-\infty}^{x_u} f(x)\,dx;$$

upper	$\alpha = 1 - CL$	$\beta = 0$
lower	$\alpha = 0$	$\beta = 1 - CL$
central	$\alpha = (1 - CL)/2$	$\beta = (1 - CL)/2$

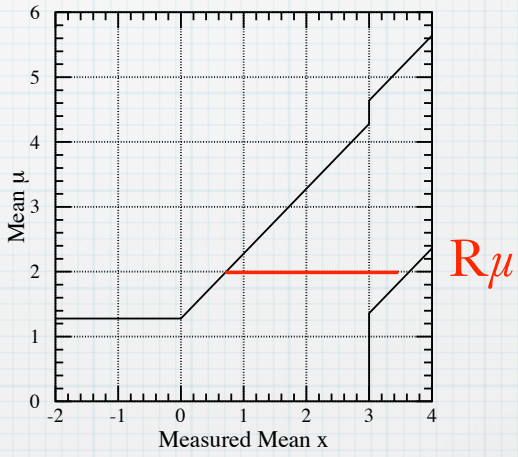




Confidence Intervals

- Flip-flopping problem of naive physicist before searching for a new phenomena:
  - "If I get a negative result, I publish as if I got nothing; if I do not "observe" (<3σ), I publish an CL upper limit; If I "observe" something (>3σ) I publish a central CL interval!
  - The publication depend on the result! worrisome… it does not have the correct coverage either…

e Is the coverage Rμ correct for μ=2?



Confidence Intervals

- Alternative test-statistic ML-μ (à la Feldman-Cousins):
  - Use likelihood ratio with respect the **maximum likelihood** ML (**physical**) μ estimate (hat μ)

$$q(\mu) = \begin{cases} -2\log\frac{\mathcal{L}(\mu)}{\mathcal{L}(\hat{\mu})} & \text{if } \hat{\mu} > 0 \\ -2\log\frac{\mathcal{L}(\mu)}{\mathcal{L}(\mu=0)} & \text{if } \hat{\mu} \leq 0 \end{cases}$$

q-ordering is:
$q(\mu) < q(\text{ML-}\mu)$

  - Remember that the likelihood is:

$$\mathcal{L}(\mu) = \mathcal{L}(B + \mu S) = f(x|B + \mu S), \quad \mathcal{L}(\mu = 0) = \mathcal{L}(B) = f(x|B)$$

  - ML-μ must be physical, $S<0$ is not allowed!
    - Will you publish a negative signal search after building your experiment?

Confidence Intervals

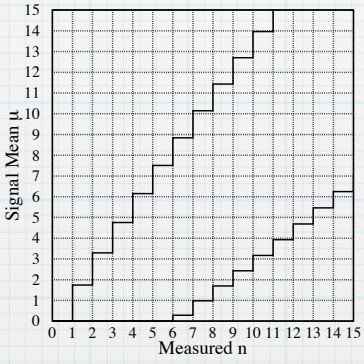
- Feldman-Cousins construction:
  - Use $q(\mu)$ ordering to define Rμ!
    - unambiguous! not needed to decide upper, lower, central, no flip-flopping dilema! and correct (or conservative) coverage

e In a single experiment, you expect $b=3$ background events, and you look for an unknown signal, s, you observe n, what is the classical and FC confidence intervals? What happens if you measure $n=0$? compare the classical vs FC methods in that case.

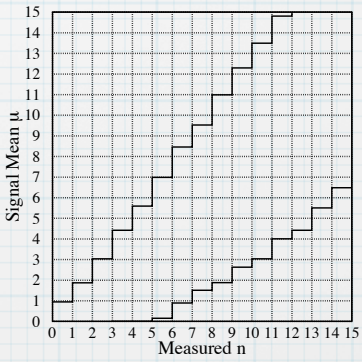
n	0	1	2	3	4	5	6	7	8
$f(n\|s=0.5)$	0.03	0.106	0.185	0.216	0.189	0.132	0.077	0.038	0.017
classical order		5	3	1	2	4	6	7	
$\hat{s}$	0	0	0	0	1	2	3	4	5
$f(n\|\hat{s})$	0.050	0.149	0.224	0.224	0.195	0.175	0.161	0.149	140
$\frac{L(n\|s=0.5)}{f(n\|\hat{s})}$	0.607	0.708	0.826	0.963	0.966	0.753	0.480	0.259	
FC order	6	5	3	2	1	4	7		

$s=0.5$

classical



FC

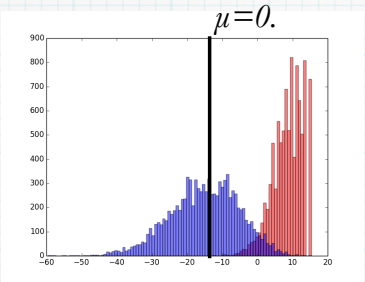


Confidence Intervals

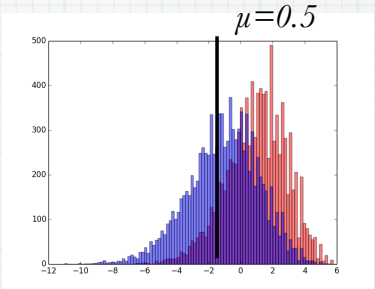
e Consider a n-bins independent experiment, with background expectation b=[1.5,1,0.5] and signal s=[2,6,2] for strength μ=1, the observation is n=[3,6,2], what is the ML-μ? Obtain the FC interval at 90 % CL for μ. Plot the CLs value vs μ.

$ML\text{-}\mu=0.8$

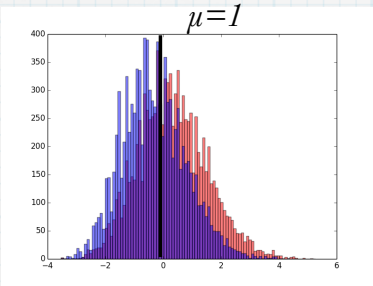
$\mu=0.$



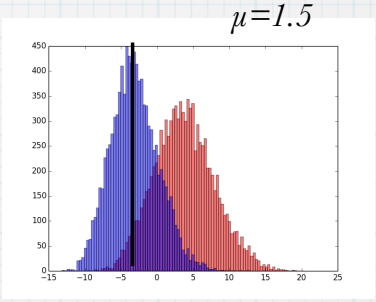
$\mu=0.5$



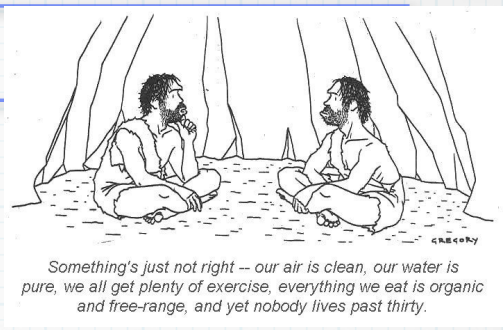
$\mu=1$



$\mu=1.5$

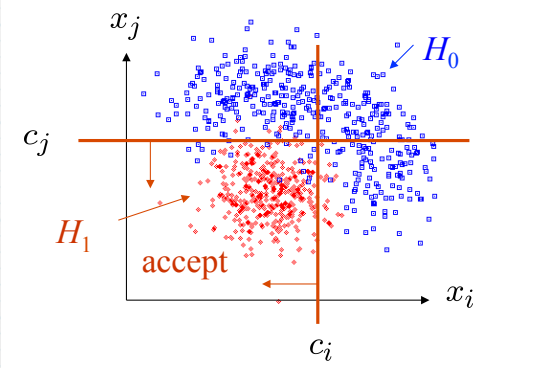


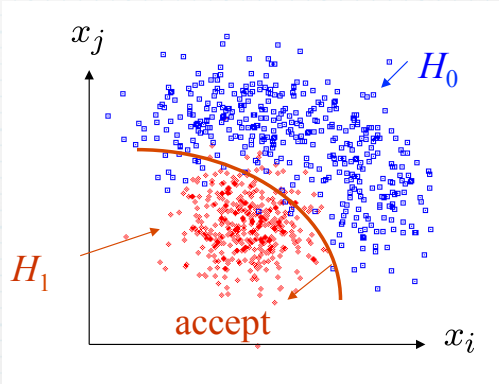
MVA



Something's just not right -- our air is clean, our water is pure, we all get plenty of exercise, everything we eat is organic and free-range, and yet nobody lives past thirty.

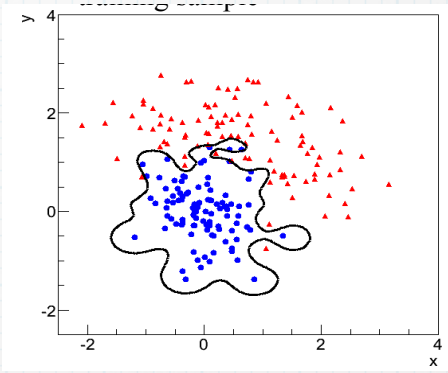
- Context:
  - In hypothesis testings: how to get a test-statistics *t(x)* when we do not know the pdfs *f(x)*? Specially if we **x** is n-dim!
  - How to separate different populations in a n-dim space?





MVA

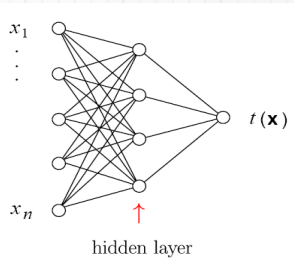
- Multi Variate Analysis (MVA)
  - Provide a test-statistics t(x) to separate population or hypothesis
  - Most of them are learning machine methods: they are trained with samples with known populations
    - Be careful to not overtrain!
    - Divide training sample in (at least) two!
      - Use for train and test
  - Performance via the ROC curve



- Non exhaustive list:
  - Fished Discriminant
  - Neural Network (NN): similar to nervous system neurons
  - (Boosted) Decision Trees: classification into branches
  - Probability Density Estimation (based on non-parametric pdfs)

MVA-NN

- Neural Networks
  - They are training machines
  - They have neurons (nodes) and synapses
  - As many entries and input variables, ***x***
  - One final node that provides *t(x)*
  - Several hidden layers



$$h_i(\vec{x}) = s\left(w_{i0} + \sum_{j=1}^{n} w_{ij}x_j\right)$$

$$t(\vec{x}) = s\left(a_0 + \sum_{i=1}^{n} a_i h_i(\vec{x})\right) .$$

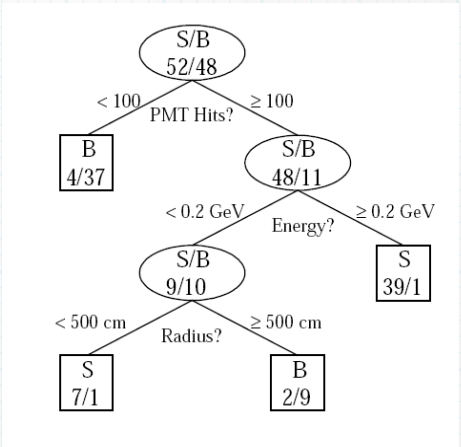
- Training based on minimization of an error function

event data	$\mathbf{x}_i$
class label	$y_i = +1, -1$
weigth	w_i

$$E[\sum_i w_i \, (t(\mathbf{x_i}) - y_i)^2]$$

MVA-BDT

- Decision trees
  - Classify data in branches
    - using a cut on a variable
    - optimizing the purity



$$\eta_S = \frac{\sum_{i\in S} w_i}{\sum_{i\in S} w_i + \sum_{i\in B} w_i},$$

- Boost
  - Create K-classifiers $h_k(\mathbf{x})$ in a iterative process
    - re-weigth events that were badly classified
    - obtain a new tree
  - Add them with different weights

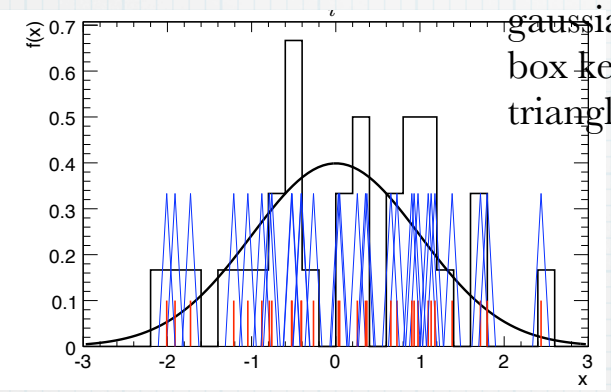
$$t(\mathbf{x}) = \sum_{k=1}^{K} \alpha_k h_k(\mathbf{x})$$

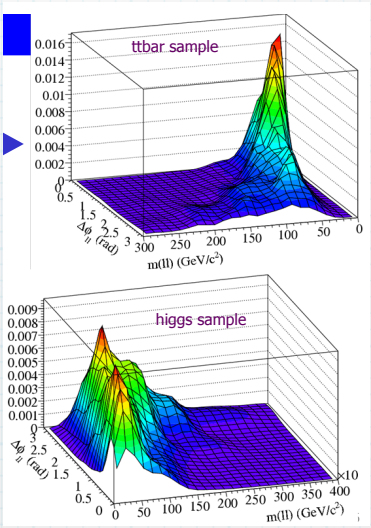
MVA-PDE

- PDE
  - define non-parametric PDFs
    - use kernel functions:
      - box, triangle, gaussian
  - methods to smooth the n-dim

$$\hat{f}(\mathbf{x}) = \frac{1}{Mw^d} \sum_{i=1}^{M} k\left(\frac{\mathbf{x} - \mathbf{x}_i}{w}\right)$$

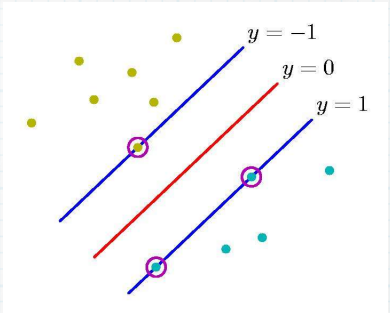
$$k(\mathbf{u}) = \frac{1}{(2\pi)^{n/2}} e^{-\mathbf{u}^2/2}$$





MVA

- SV
  - transform **x** n-dim into **y** m-dim space (m>n)
    - "kernel" transformation
  - define a *hyper-plane* (frontier) in m-dim



e

Use the data file that contains several variables for signal and background categories and generate a test-statistics using different MVA methods. Suggestion: use the TMVA package in ROOT. Compute the ROC curves.