Search and Discovery Statistics in HEP +Bonus Lecture: Basic Introduction to Deep Learning

Eilam Gross, Weizmann Institute of Science

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Louis Lyons, Alex Read, Bob Cousins Glen Cowan ,Kyle Cranmer Ofer Vitells & Jonathan Shlomi



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What can you expect from the Lectures

Lecture 1: Basic Concepts Histograms, PDF, Testing Hypotheses, LR as a Test Statistics, p-value, POWER, CLs Measurements Lecture 2: Wald Theorem, Asymptotic Formalism, Asimov Data Set, Feldman-Cousins, PL & CLs, Asimov Significance Lecture 3: Look Elsewhere Effect 1D LEE the non-intuitive thumb rule (upcrossings, trial $\# \sim Z$) 2D LEE (Euler Characteristic) Lecture 4: Basic Introduction to Deep Learning

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Lecture 3: Look Elsewhere Effect

1D LEE the non-intuitive thumb rule (upcrossings, trial #~Z)

2D LEE (Euler Characteristic)

Lecture 4: Basic Introduction to Deep Learning

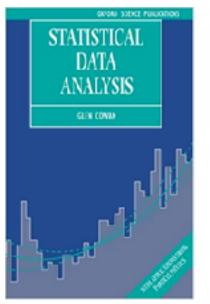
Support Material

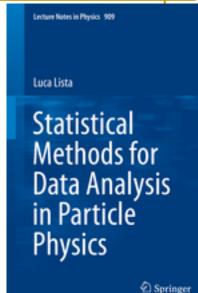
G. Cowan, Statistical Data Analysis, Clarendon Press, Oxford, 1998.

L. Lista Statistical methods for Data Analysis, 2nd Ed. Springer, 2018

G. Cowan PDG

http://pdg.lbl.gov/2017/reviews/rpp2017-rev-statistics.pdf





Preliminaries



Backgammon

What is the probability to toss exactly 3 times 6:6 in 10 rounds?





$$p = \frac{1}{6} \times \frac{1}{6} = \frac{1}{36}$$
$$q = 1 - p = \frac{35}{36}$$

The probability to toss 6:6 exactly 3 times, in 10 rounds is

$$P(k = 3: n = 10, p = \frac{1}{36}) = \begin{pmatrix} 10 \\ 3 \end{pmatrix} \left(\frac{1}{36}\right)^3 \left(1 - \frac{1}{36}\right)^7$$
$$\begin{pmatrix} 10 \\ 3 \end{pmatrix} = \frac{10!}{3!7!}$$



In a Nut Shell
The binomial distribution with parameters n and p
is
the discrete probability distribution of the k number of successes
in a sequence of n independent experiments. (Wikipedia)

$$P(k:n,p) = \binom{n}{k} p^k (1-p)^{n-k}$$
If $X \sim B(n, p)$
 $E[X] = np$

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$$\mathbf{P}(k:n,p) = \begin{pmatrix} n \\ k \end{pmatrix} p^k (1-p)^{n-k}$$

 \mathbf{i}

The Poisson distribution with parameter $\lambda = np$ can be used as an approximation to B(n, p) of the binomial distribution if n is sufficiently large and p is sufficiently small.

$$P(k:n,p) \xrightarrow{n \to \infty, np = \lambda} Poiss(k;\lambda) = \frac{\lambda^{k} e^{-k}}{k!}$$

If $X \sim Poiss(k;\lambda)$
 $E[X] = Var[X] = \lambda$



From Binomial to Poisson to Gaussian $\mathbf{P}(k:n,p) = \begin{pmatrix} n \\ k \end{pmatrix} p^{k} (1-p)^{n-k}$ $P(k:n,p) \xrightarrow{n \to \infty, np = \lambda} Poiss(k;\lambda) = \frac{\lambda^{\kappa} e^{-\kappa}}{k!}$ $\langle k \rangle = \lambda, \ \sigma_k = \sqrt{\lambda}$ $k \rightarrow \infty \Longrightarrow x = k$ Using Stirling Formula prob(x)=G(x, $\sigma = \sqrt{\lambda}$) = $\frac{1}{\sqrt{2\pi\sigma}}e^{-(x-\lambda)^2/2\sigma^2}$ U-0 $\mu + \sigma$ This is a Gaussian, or Normal distribution with mean and variance of λ

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Histograms N collisions $p(Higgs \; event) = \frac{\mathcal{L}\sigma(pp \to H) A\epsilon_{ff}}{\mathcal{L}\sigma(pp)}$ Prob to see n_{H}^{obs} in N collisions is $P(n_{H}^{obs}) = \begin{pmatrix} N \\ n_{H}^{obs} \end{pmatrix} p^{n_{H}^{obs}} (1-p)^{N-n_{H}^{obs}}$ $\ell im_{N \to \infty} P(n_H^{obs}) = Poiss(n_H^{obs}, \lambda) = \frac{e^{-\lambda} \lambda^{n_H^{obs}}}{n^{obs}!}$ 60 100 mass $\lambda = Np = \mathcal{L}\sigma(pp) \cdot \frac{\mathcal{L}\sigma(pp \to H) A\epsilon_{ff}}{\mathcal{L}\sigma(pp)} = n_{H}^{exp}$

A counting experiment

• The Higgs hypothesis is that of signal s(m_H) $s(m_H) = L\sigma_{SM} \cdot A \cdot \epsilon$ For simplicity unless otherwise noted

$$s(m_H) = L\sigma_{SM}$$

In a counting experiment

$$\mu = \frac{L\sigma_{obs}(m_H) + b}{L\sigma_{SM}(m_H)} = \frac{\sigma_{obs}(m_H)}{\sigma_{SM}(m_H)}$$

 $n - \mu(m) + h$

- μ is the strength of the signal (with respect to the expected Standard Model one)
- The hypotheses are therefore denoted by H_{μ}
- H_1 is the SM with a Higgs, H_0 is the background only model

A Tale of Two Hypotheses NULL ALTERNATE

- Test the Null hypothesis and try to reject it
- Fail to reject it OR reject it in favor of the alternative hypothesis





- Test the Null hypothesis and try to reject it
- Fail to reject it OR reject it in favor of the alternative hypothesis





We quantify rejection by p-value (later)







Reject H₁ in favor of H₀

Excluding $H_1(m_H) \rightarrow Excluding$ the Higgs with a mass m_H

We quantify rejection by p-value (later)





Likelihood

 Likelihood is the compatibility of the Hypothesis with a given data set.
 But it depends on the data

Likelihood is <u>not</u> the probability of the hypothesis given the data

$$L(H) = P(x \mid H)$$

$$P(x \mid H) \neq P(H \mid x)$$

Bayes Theorem

$$P(H \mid x) = \frac{P(x \mid H) \cdot P(H)}{\sum_{H} P(x \mid H) P(H)}$$
$$P(H \mid x) \approx P(x \mid H) \cdot \frac{P(H)}{P(H)}$$
$$P(H \mid x) \approx P(x \mid H) \cdot \frac{P(H)}{P(H)}$$

Frequentist vs Bayesian

- The Bayesian infers from the data using priors posterior $P(H | x) \approx P(x | H) \cdot P(H)$
- Priors is a science on its own.
 Are they objective? Are they subjective?
- The Frequentist calculates the probability of an hypothesis to be inferred from the data based on a large set of hypothetical repeated experiments Ideally, the frequentist does not need priors, or any degree of belief while the Baseian posterior based inference **is** a "Degree of Belief".
- However, NPs (Systematic) inject a Bayesian flavour to any Frequentist analysis

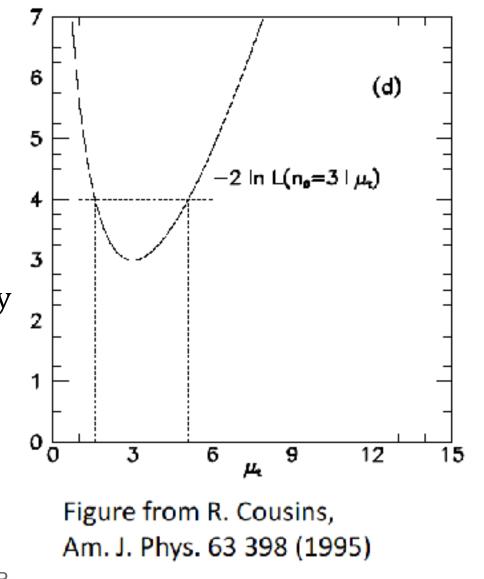


Likelihood is NOT a PDF

A Poisson distribution describes a discrete event count *n* for a real valued Mean μ .

$$Pois(n|\mu) = \mu^n \frac{e^{-\mu}}{n!}$$

Say, we observe n_o events What is the likelihood of μ ? The likelihood of μ is given by $L(\mu) = Pois(n_o | \mu)$ It is a continues function of μ but it is NOT a PDF



Testing an Hypothesis (wikipedia...)

- The first step in any hypothesis test is to state the relevant **null, say,** H_0 and **alternative hypotheses, say**, H_1
- The next step is to define a test statistic, q, under the null hypothesis
- Compute from the observations the observed value q_{obs} of the test statistic q.
- Decide (based on q_{obs}) to either
 fail to reject the null hypothesis or
 reject it in favor of an alternative hypothesis
- next: How to construct a test statistic, how to decide?

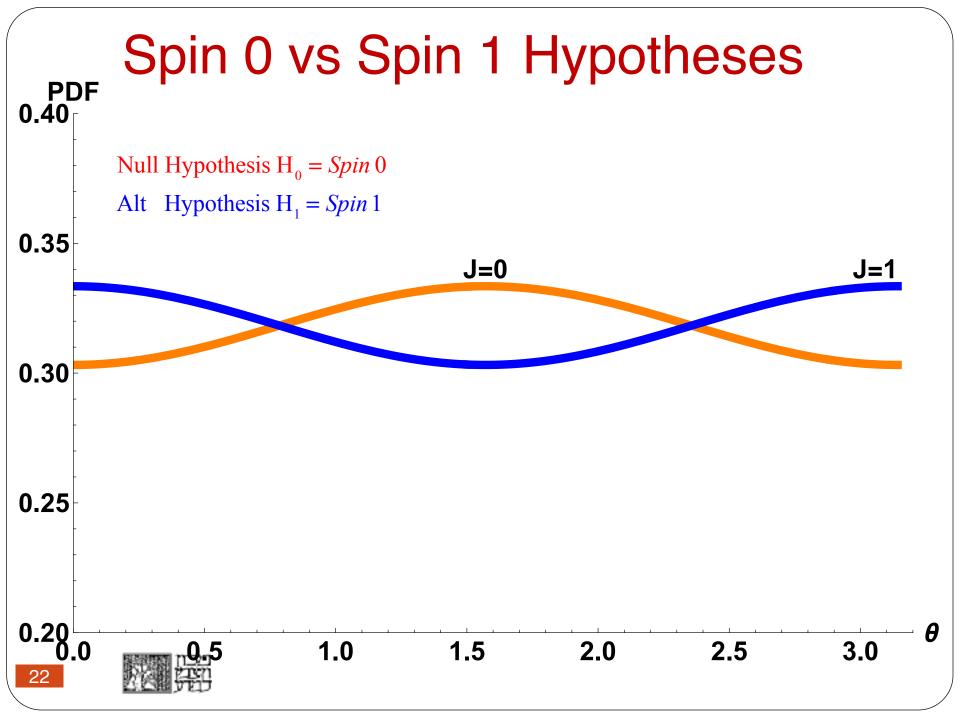


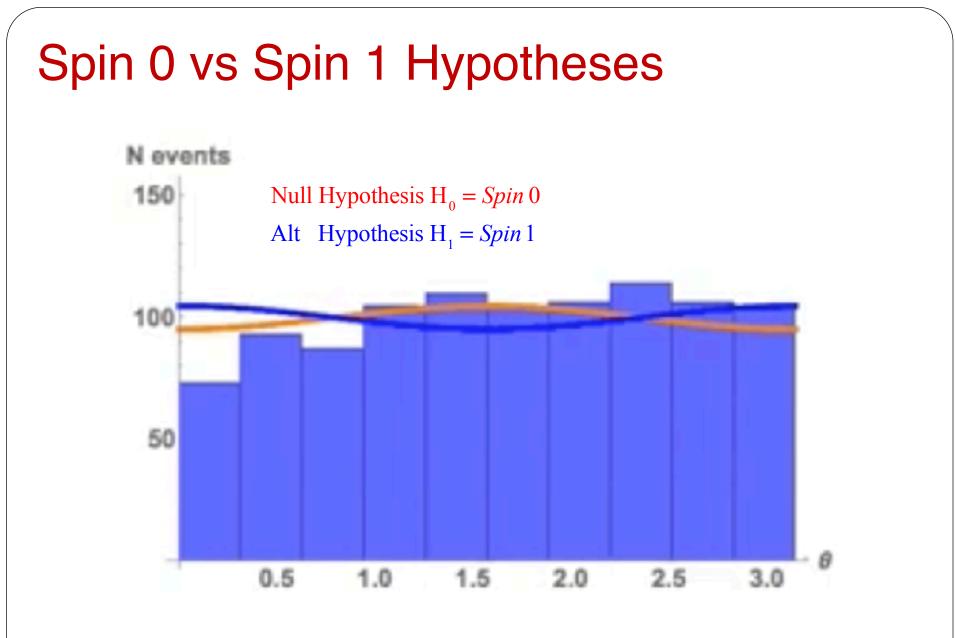
Test statistic and p-value



Case Study 1 : Spin

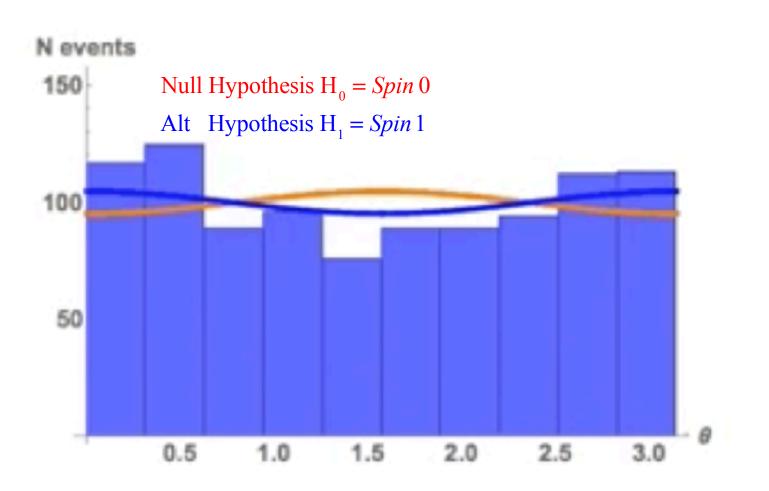




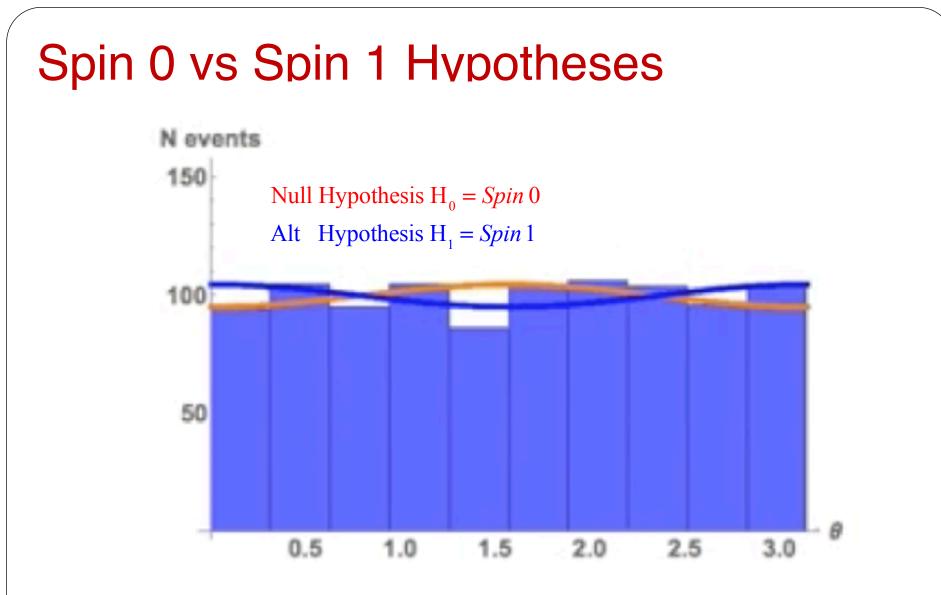




Spin 0 vs Spin 1 Hypotheses









The Neyman-Pearson Lemma

• Define a **test statistic**

$$\lambda = \frac{L(H_1)}{L(H_0)}$$

• When performing a hypothesis test between two simple hypotheses, H_0 and H_1 , **the Likelihood Ratio test**, $\lambda = \frac{L(H_1)}{L(H_0)}$

which rejects H_0 in favor of H_1 ,

is the most powerful test

for a given significance level with a threshold $\boldsymbol{\eta}$

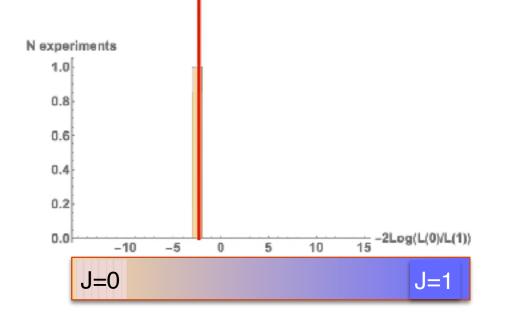
 $\alpha = prob(\lambda \leq \eta)$

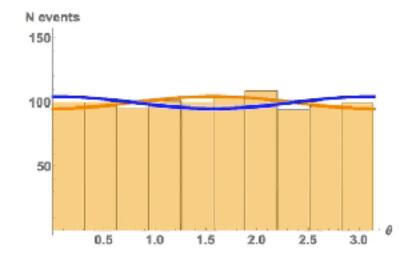


Building PDF

Build the pdf of the test statistic

$$q_{NP} = q_{NP}(x) = -2 \ln \frac{L(H_0 | x)}{L(H_1 | x)}$$





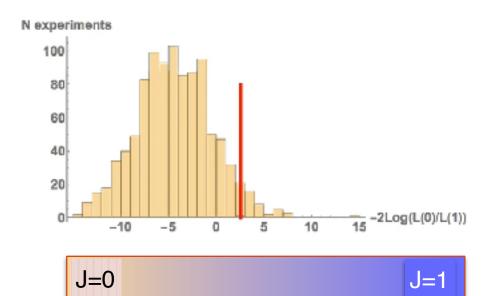


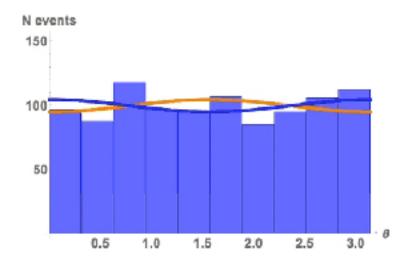


Building PDF

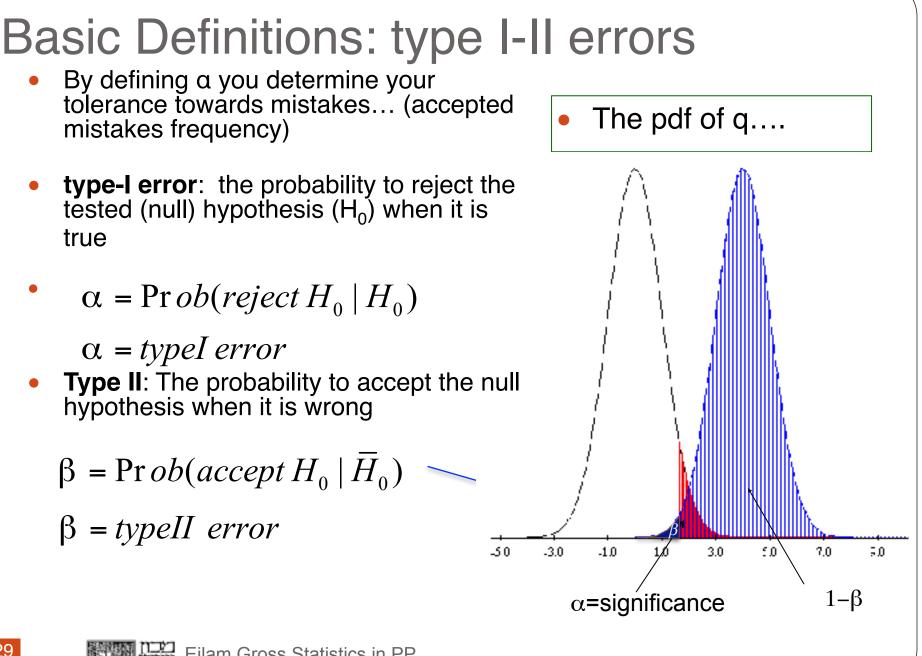
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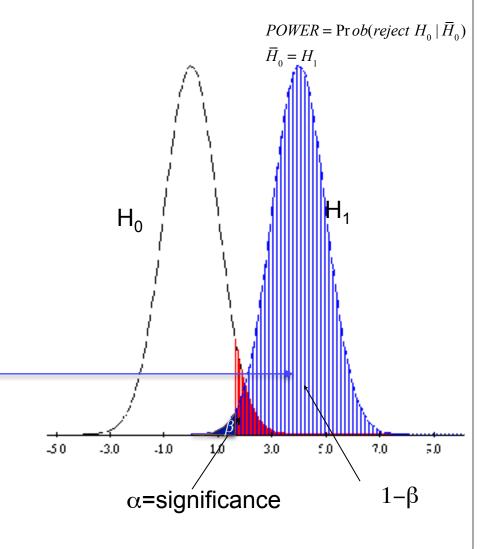






Basic Definitions: POWER

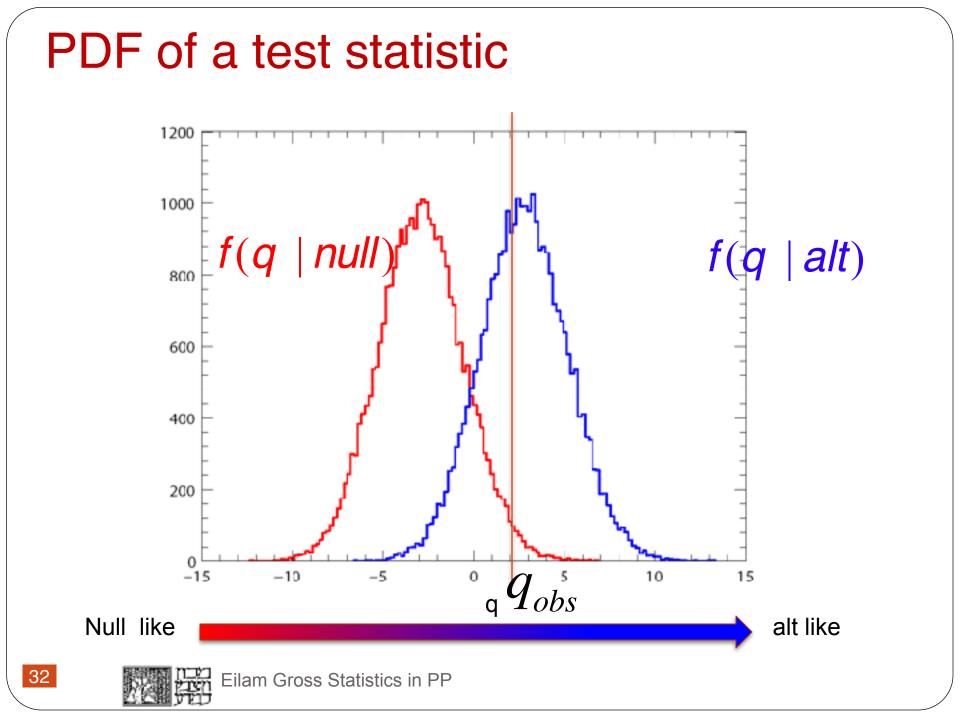
- $\alpha = \Pr{ob(reject H_0 | H_0)}$
- The POWER of an hypothesis test is the probability to reject the null hypothesis when it is indeed wrong (the alternate analysis is true)
- POWER = Pr ob(reject $H_0 | \overline{H}_0$) $\beta = Prob(accept H_0 | \overline{H}_0)$ $1 - \beta = Prob(reject H_0 | \overline{H}_0)$ $\overline{H}_0 = H_1$ $1 - \beta = Prob(reject H_0 | H_1)$
- The power of a test increases as the rate of type II error decreases

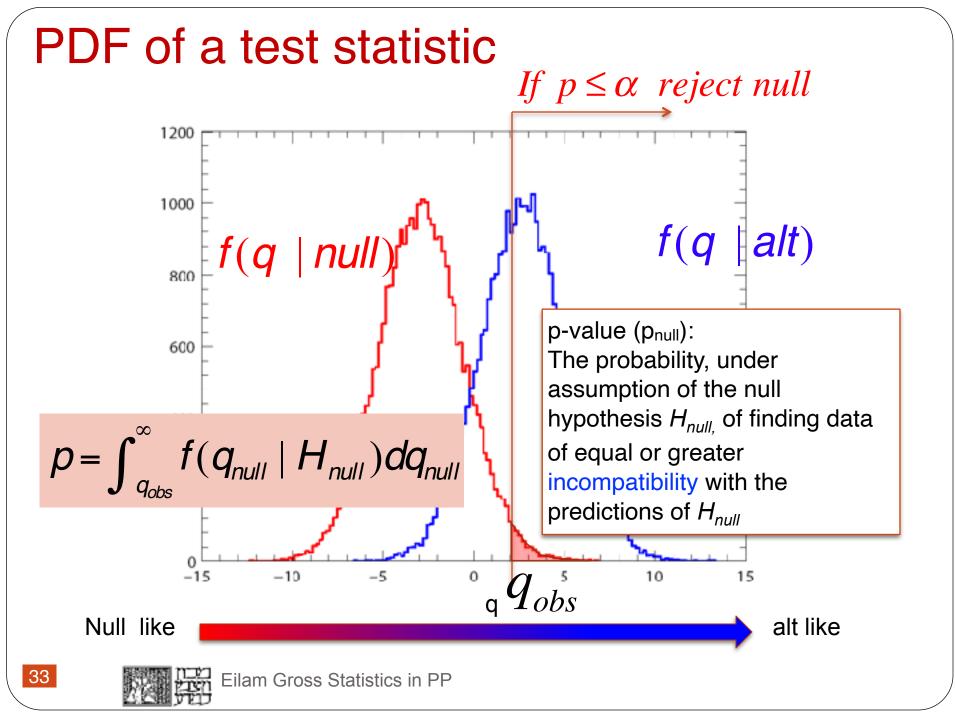


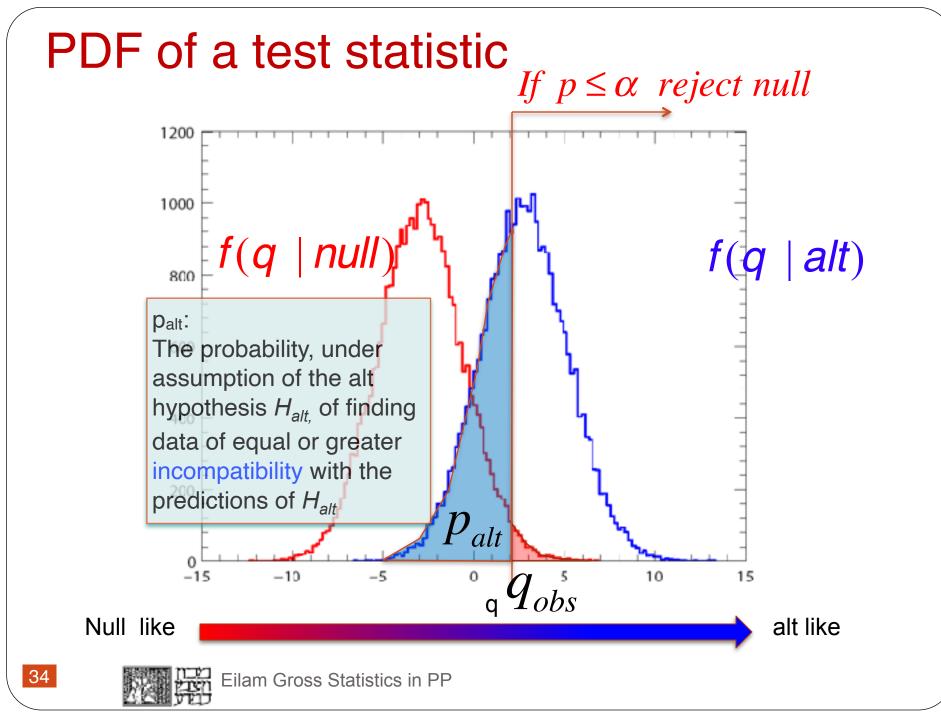
p-Value

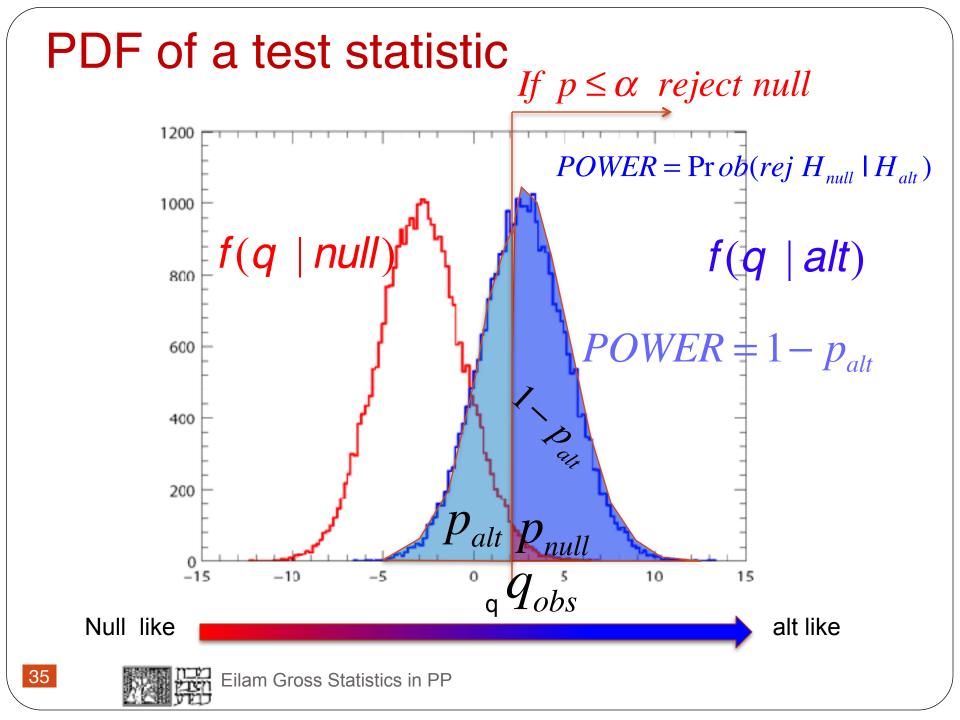
- The observed *p-value* is a measure of the compatibility of the data with the tested hypothesis.
- It is the probability, under assumption of the null hypothesis H_{null}, of finding data of equal or greater incompatibility with the predictions of H_{null}
- An important property of a test statistic is that its sampling distribution under the null hypothesis be calculable, either exactly or approximately, which allows p-values to be calculated. (Wiki)







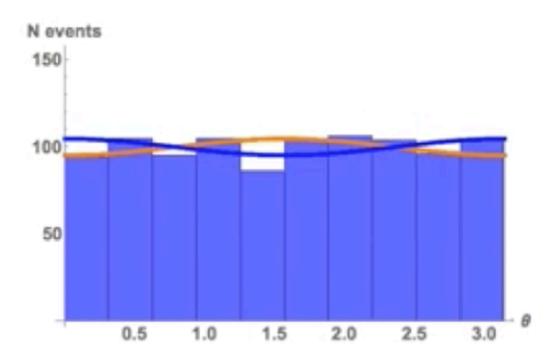




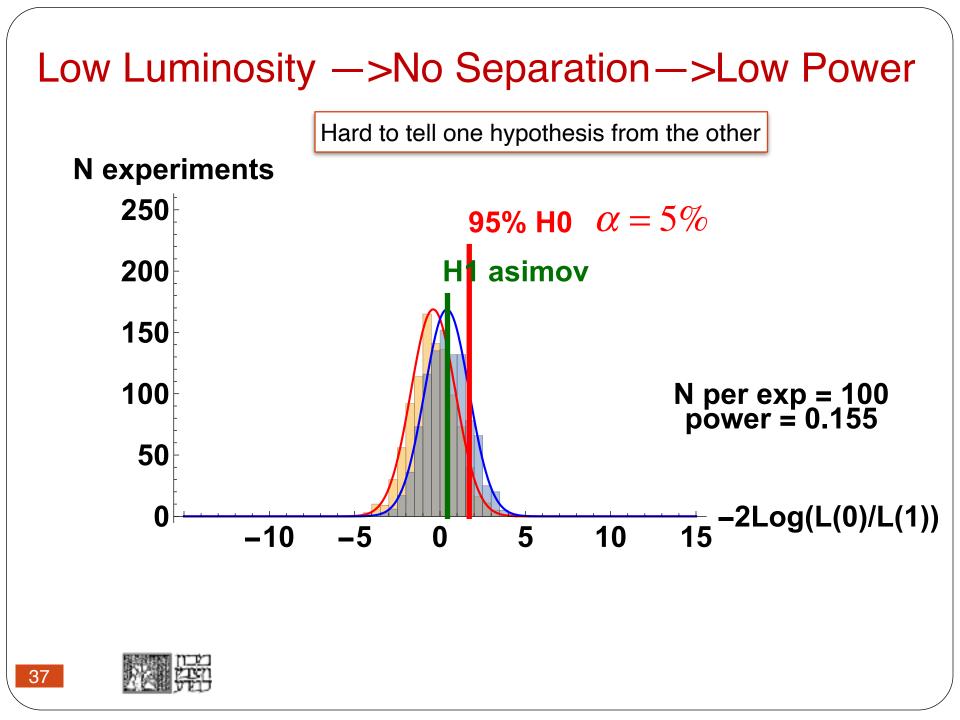
Power and Luminosity

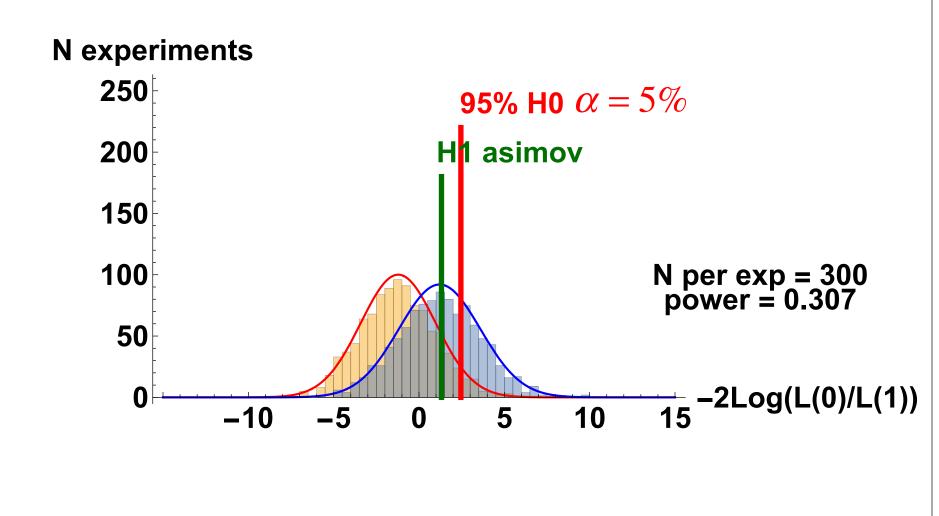
For a given significance the power increases with increased luminosity

Luminosity ~ Total number of events in an experiment

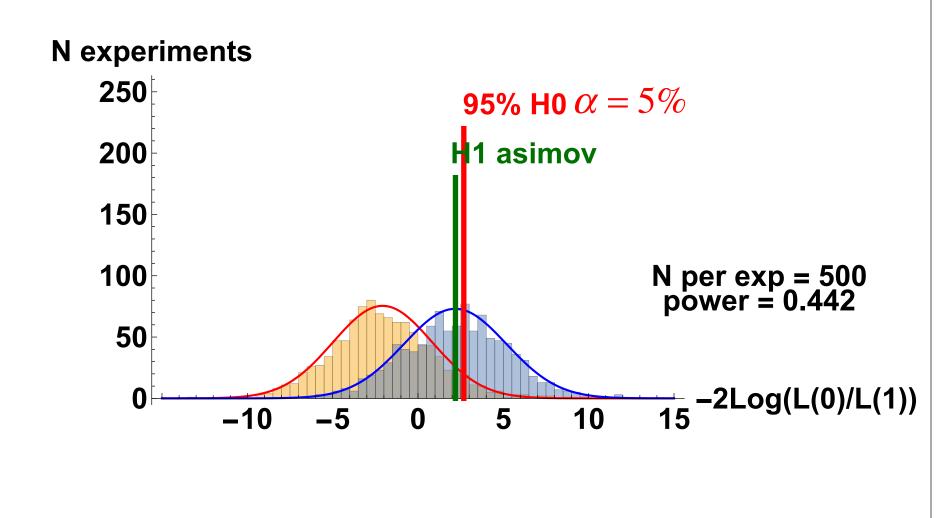




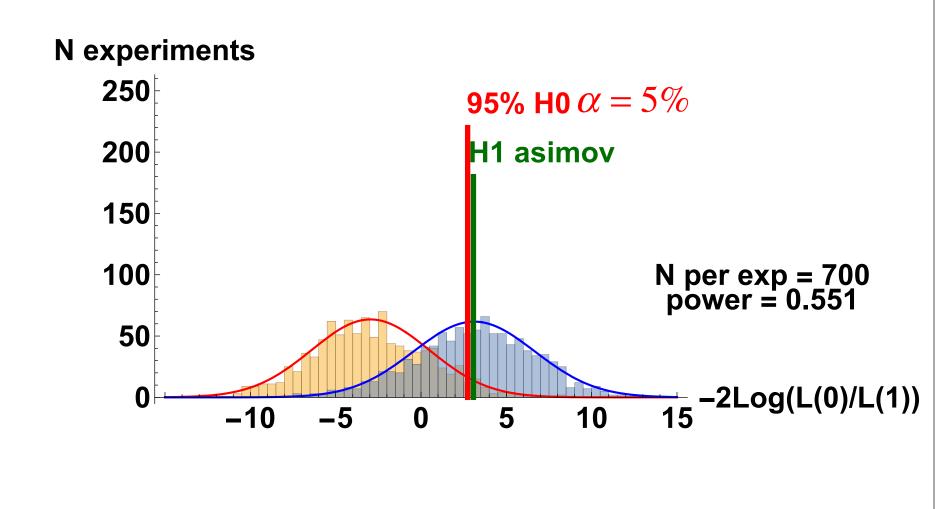




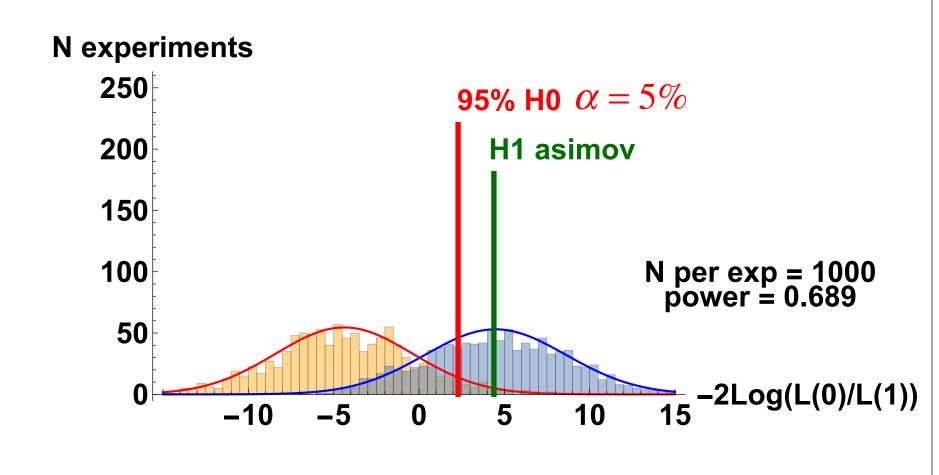






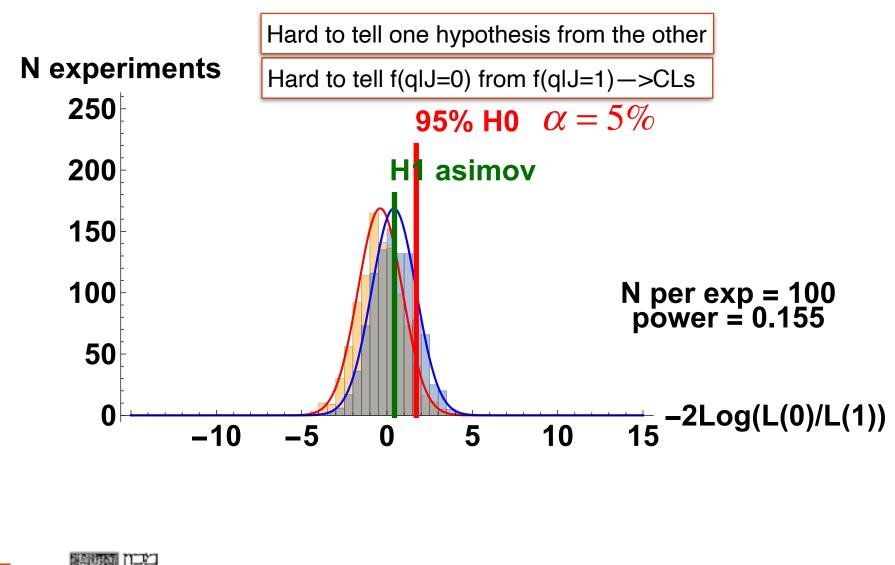








Back to Low Luminosity



Birnbaum (1977)

"A concept of statistical evidence is not plausible unless it finds 'strong evidence for H_1 as against H_0 ' with small probability (α) when H_0 is true, and with much larger probability $(1-\beta)$ when H_1 is true. "

> Birnbaum (1962) suggested that $\alpha / 1 - \beta$ (significance / power)should be used as a measure of the strength of a statistical test,rather than α alone

$$p = 5\% \rightarrow p' = 5\% / 0.155 = 32\%$$

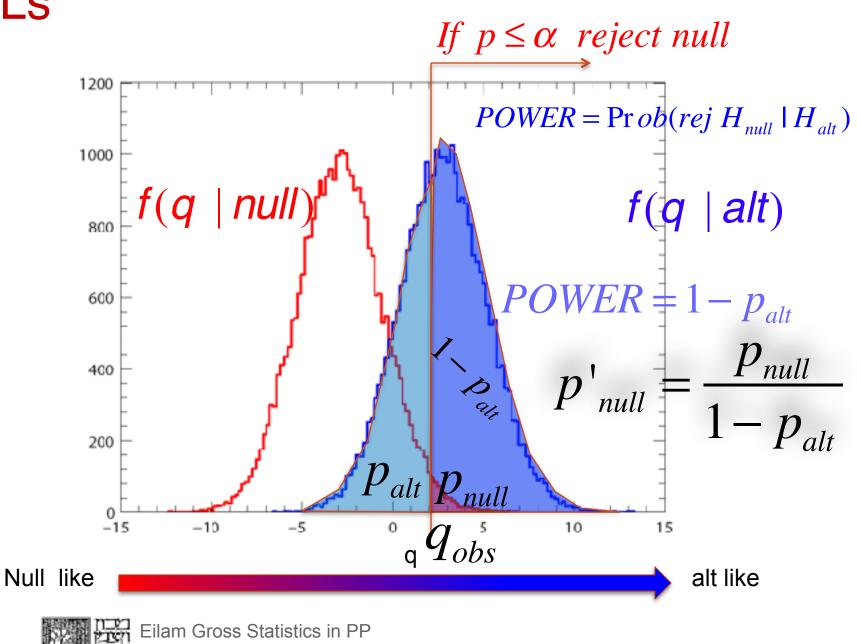
$$q = \operatorname{Prob}(rej + b) + b, \quad p' = CL_s$$

$$p'_{\mu} = \frac{p_{\mu}}{1 - p_0}$$



CLs

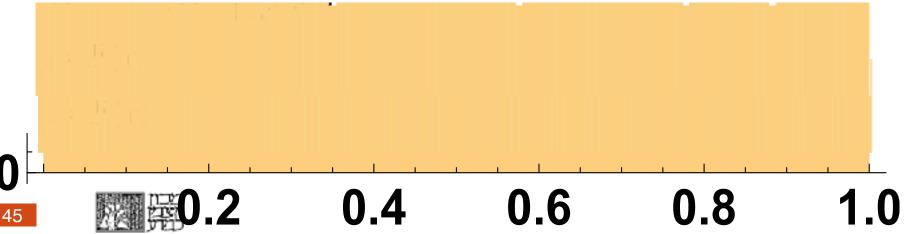
CLs



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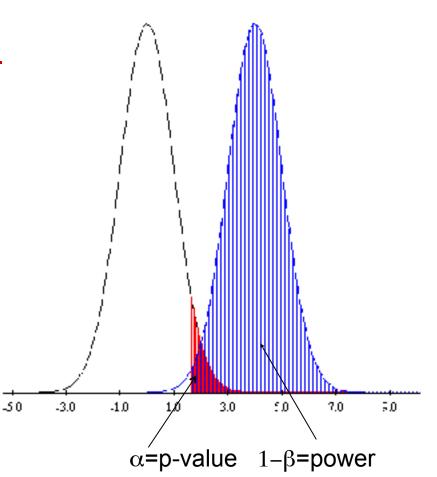
Distribution of p-value under HO f(x) PDF

cumulative $F(x) = \int_{-\infty}^{x} f(x')dx'$ let y = F(x) PDF of y $\frac{dP}{dy} = \frac{dP}{dx}\frac{dx}{dy} = \frac{f(x)}{dF} dx = \frac{f(x)}{f(x)} = 1$ F(x) distributes uniform between 0 and 1 p = 1 - F(x) distributes uniform between 0 and 1



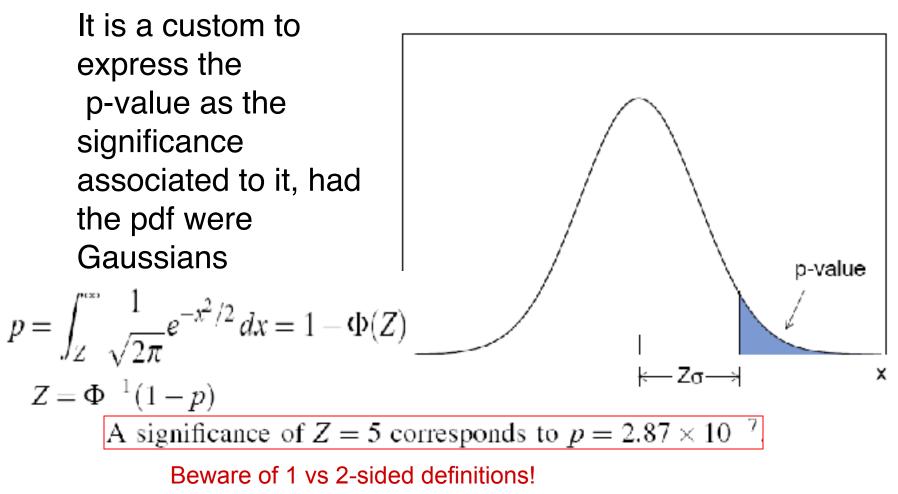
Which Statistical Method is Better

- To find out which of two methods is better plot the pvalue vs the power for each analysis method
- Given the p-value, the one with the higher power is better
- p-value~significance





From p-values to Gaussian significance



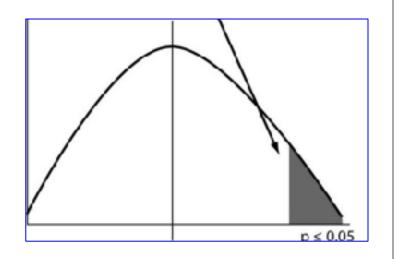
Eilam Gross Statistics in PP

1-Sided p-value

 When trying to reject an hypothesis while performing searches, one usually considers only one-sided tail probabilities.

A Sanity Requirement:

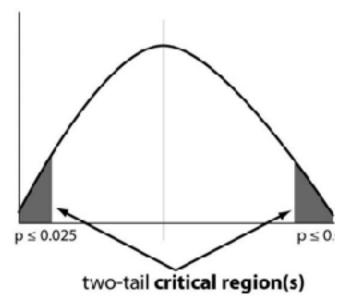
 Downward fluctuations of the background will not serve as an evidence against the background



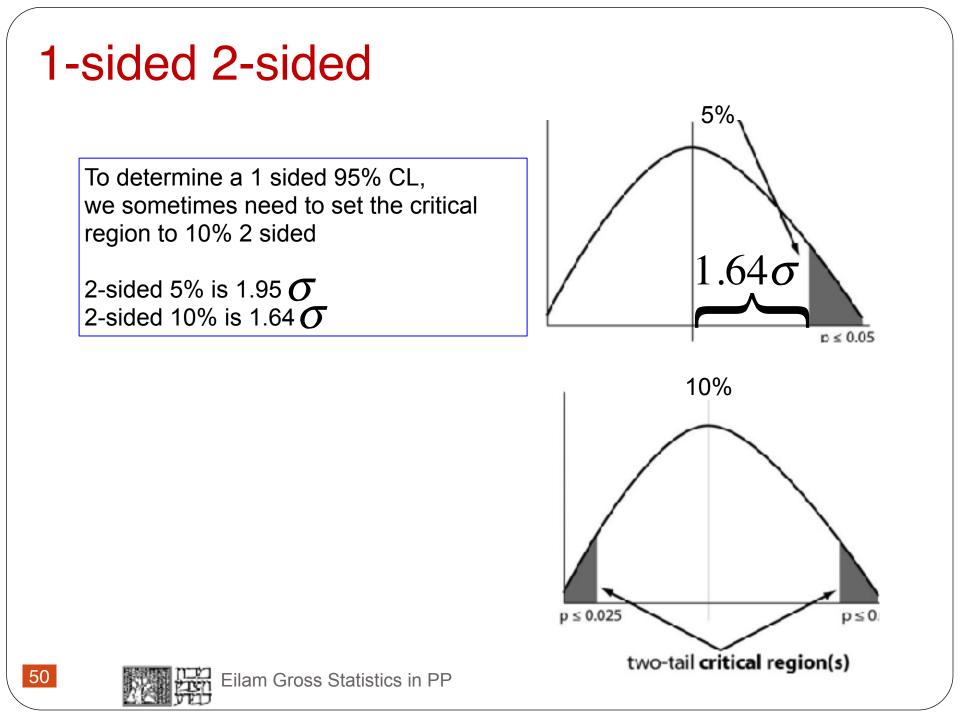
 Upward fluctuations of the signal will not be considered as an evidence against the signal

2-Sided p-value

 When performing a measurement (t_{μ}), any deviation above or below the expected null is drawing our attention and might serve an indication of some anomaly or new physics.



Here we use a 2-sided pvalue



p-value – testing the null hypothesis

When testing the b hypotheis (null=b), it is custom to set

- $\alpha = 2.9 \ 10^{-7}$
- \rightarrow if p_b<2.9 10⁻⁷ the b hypothesis is rejected

→ Discovery

When testing the s+b hypothesis (null=s+b), set $\alpha = 5\%$ if $p_{s+b} < 5\%$ the signal hypothesis is rejected at the 95% Confidence Level (CL) \rightarrow Exclusion



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Confidence Interval and Confidence Level (CL)



CL & CImeasurement $\hat{\mu} = 1.1 \pm 0.3$ $L(\mu) = G(\mu; \hat{\mu}, \sigma_{\hat{\mu}})$ $\Rightarrow CI \ of \ \mu = [0.8, 1.4] \ at \ 68\% \ CL$

- A **confidence interval** (**CI**) is a particular kind of interval estimate of a population parameter.
- Instead of estimating the parameter by a single value, an interval likely to include the parameter is given.
- How likely the interval is to contain the parameter is determined by the confidence level
- Increasing the desired confidence level will widen the confidence interval.



Confidence Interval & Coverage

•Say you have a measurement μ_{meas} of μ with μ_{true} being the unknown true value of μ

-Assume you know the probability distribution function $p(\mu_{meas} I \mu)$

 based on your statistical method you deduce that there is a 95% Confidence interval [μ₁,μ₂].
 (it is 95% likely that the μ_{true} is in the quoted interval)

The correct statement:

•In an ensemble of experiments 95% of the obtained confidence intervals will contain the true value of μ .



Confidence Interval & Coverage

•You claim, $CI_{\mu}=[\mu_1,\mu_2]$ at the 95% CL

i.e. In an ensemble of experiments CL (95%) of the obtained confidence intervals will contain the true value of μ .

- If your statement is accurate, you have full coverage
- If the true CL is>95%, your interval has an over coverage
- If the true CL is <95%, your interval has an undercoverage



Upper Limit

- Given the measurement you deduce somehow (based on your statistical method) that there is a 95% Confidence interval [0,μ_{up}].
- This means: our interval contains $\mu=0$ (no Higgs)
- We therefore deduce that $\mu < \mu_{up}$ at the 95% Confidence Level (CL)
- μ_{up} is therefore an upper limit on μ

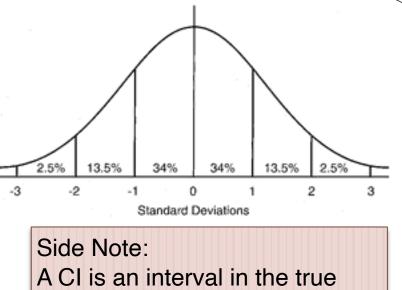
• If $\mu_{up} < 1 \rightarrow \sigma(m_H) < \sigma_{SM}(m_H) \rightarrow a SM$ Higgs with a mass m_H is excluded at the 95% CL

How to deduce a CI?

 One can show that if the data is distributed normal around the average i.e. P(datalµ)=normal

$$f(x \mid \mu, \sigma) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$$

 then one can construct a 68% CI around the estimator of μ to be



parameters phase-space

$$\hat{\mathbf{X}} \pm \mathbf{O}$$
 i.e. $x_{true} \in [\hat{x} - \sigma_{\hat{x}}, \hat{x} + \sigma_{\hat{x}}] @ 68\% CL$

- However, not all distributions are normal, many distributions are even unknown and coverage might be a real issue
 - One can guarantee a coverage with the Neyman Construction (1937)

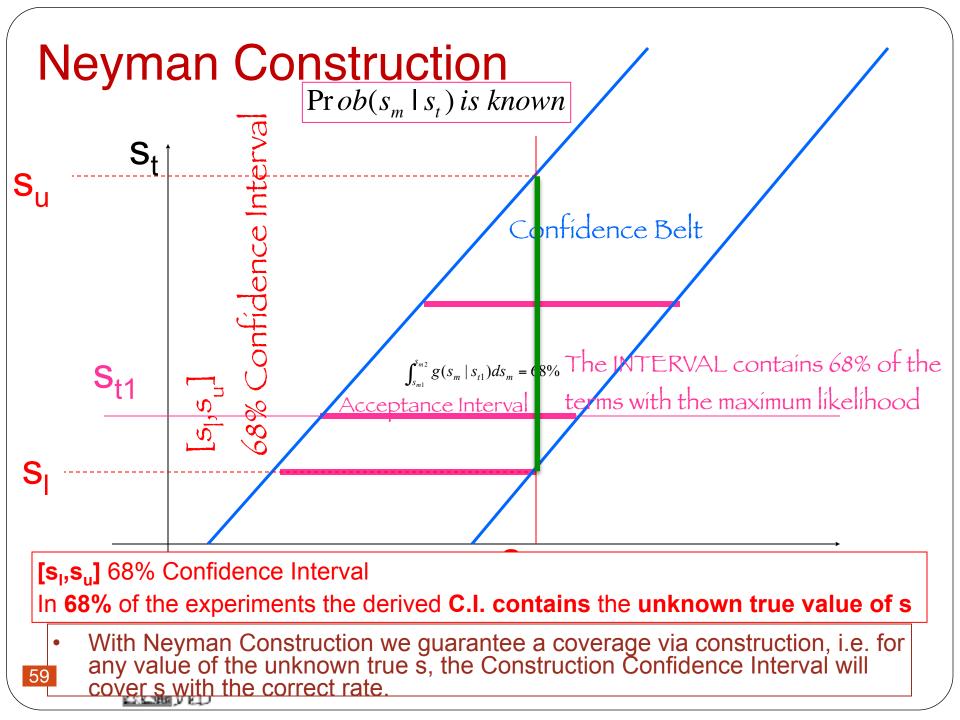
Neyman, J. (1937) <u>"Outline of a Theory of Statistical Estimation Based on the Classical Theory of Probability"</u> *Philosophical Transactions of the Royal Society of London A*, **236**, 333-380.

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The Frequentist Game a 'la Neyman

Or How to ensure a Coverage with Neyman construction





Nuisance Parameters

or Systematics



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Nuisance Parameters (Systematics)

- There are two kinds of parameters:
 - Parameters of interest (signal strength... cross section... μ)
 - Nuisance parameters (background (b), signal efficiency, resolution, energy scale,...)
- The nuisance parameters carry systematic uncertainties
- There are two related issues:
 - Classifying and estimating the systematic uncertainties
 - Implementing them in the analysis
- The physicist must make the difference between cross checks and identifying the sources of the systematic uncertainty.
 - Shifting cuts around and measure the effect on the observable... Very often the observed variation is dominated by the statistical uncertainty in the measurement.

Implementation of Nuisance Parameters

- Implement by marginalizing (Bayesian) or profiling (Frequentist)
- Hybrid: One can also use a frequentist test statistics (PL) while treating the NPs via marginalization (Hybrid, Cousins & Highland way)
- Marginalization (Integrating))
 - Integrate the Likelihood, L, over possible values of nuisance parameters (weighted by their prior belief functions -- Gaussian,gamma, others...)

•
$$L(\mu) = \int L(\mu,\theta)\pi(\theta)d\theta$$

Profile Likelihood L (S, b $L(s,bs) = \max_{h} L(s,b)$ L (ŝ,ŝ) $L(s, 5) = \max_{s, b} L(s, 5)$ 63

The Hybrid Cousins-Highland Marginalization

Cousins & Highland

$$q = \frac{L(s+b(\theta))}{L(b(\theta))} \Longrightarrow \frac{\int L(s+b(\theta))\pi(\theta)d\theta}{\int L(b(\theta))\pi(\theta)d\theta}$$

Profiling the NPs

$$q = \frac{L(s + b(\theta))}{L(b(\theta))} \Longrightarrow \frac{L(s + b(\hat{\hat{\theta}}_s))}{L(b(\hat{\hat{\theta}}_b))}$$

^

$$\hat{\theta}_s$$
 is the MLE of θ fixing s

Nuisance Parameters and Subsidiary Measurements

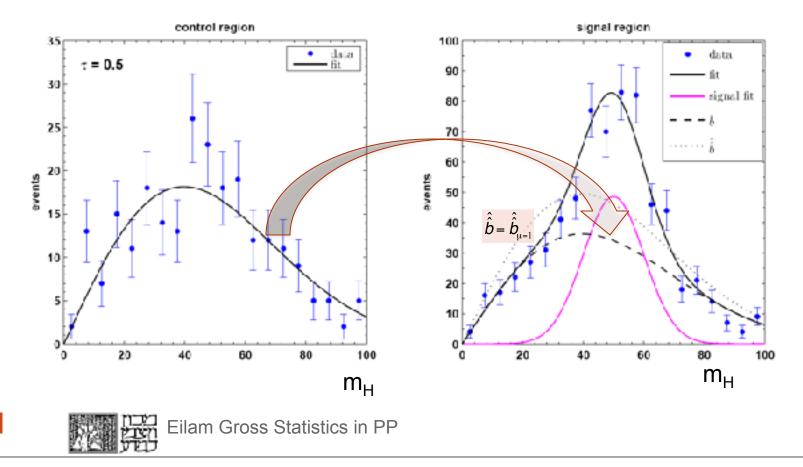
- Usually the nuisance parameters are auxiliary parameters and their values are constrained by auxiliary measurements
- Example

 $n \sim \mu s(m_H) + b$ $\langle n \rangle = \mu s + b$ $m = \tau b$

 $L(\mu \cdot s + b(\theta)) = Poisson(n; \mu \cdot s + b(\theta)) \cdot Poisson(m; \tau b(\theta))$



Mass shape as a discriminator $n \sim \mu s(m_H) + b \qquad m \sim \tau b$ $L(\mu \cdot s + b(\theta)) = \prod_{i=1}^{nbins} Poisson(n_i; \mu \cdot s_i + b_i(\theta)) \cdot Poisson(m_i; \tau b_i(\theta))$



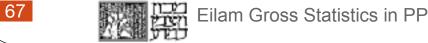
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Pulls and Ranking of NPs

The pull of
$$\theta_i$$
 is given by $\frac{\hat{\theta}_i - \theta_{0,i}}{\sigma_0}$
without constraint $\sigma\left(\frac{\hat{\theta}_i - \theta_{0,i}}{\sigma_0}\right) = 1 \quad \left\langle \frac{\hat{\theta}_i - \theta_{0,i}}{\sigma_0} \right\rangle = 0$

It's a good habit to look at the pulls of the NPs and make sure that Nothing irregular is seen

In particular one would like to guarantee that the fits do not over constrain a NP in a non sensible way



A toy case with 1 poi

$$n = \mu \epsilon A s + b$$

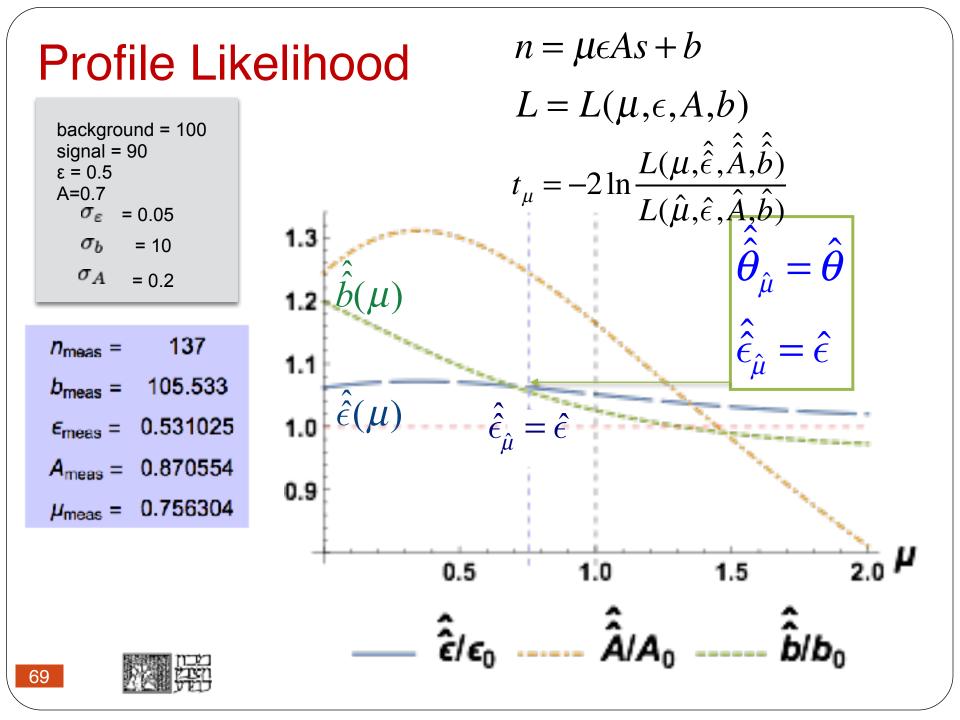
 $L = L(\mu, \epsilon, A, b)$
 $1poi: t_{\mu} = -2 \ln \frac{L(\mu, \hat{\epsilon}, \hat{A}, \hat{b})}{L(\hat{\mu}, \hat{\epsilon}, \hat{A}, \hat{b})}$

$$L(\mu,\epsilon,A) = Poiss(n \mid \mu \epsilon A + b)G(A_{meas} \mid A,\sigma_A)G(\epsilon_{meas} \mid \epsilon,\sigma_\epsilon)G(b_{meas} \mid b,\sigma_b)$$

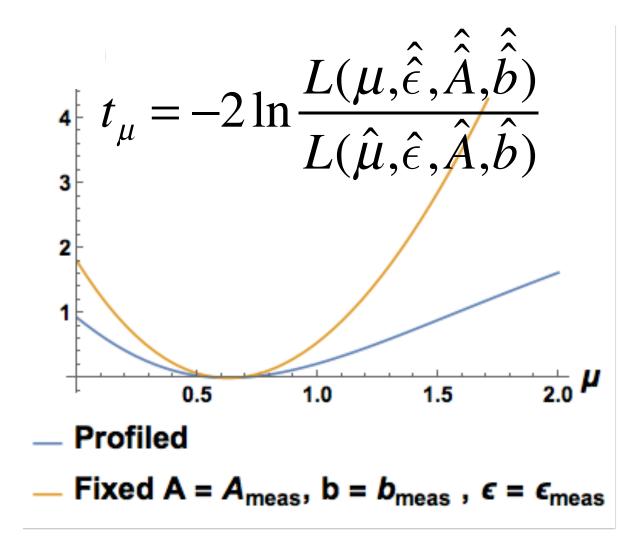
$$L(\mu,\varepsilon,A) = \frac{(\mu\varepsilon As + b)^n}{n!} e^{-(\mu\varepsilon As + b)} \frac{1}{\sigma_\varepsilon \sqrt{2\pi}} e^{-(\varepsilon_{meas} - \varepsilon)^2/2\sigma_\varepsilon^2} \frac{1}{\sigma_b \sqrt{2\pi}} e^{-(b_{meas} - b)^2/2\sigma_b^2} \frac{1}{\sigma_A \sqrt{2\pi}} e^{-(A_{meas} - A)^2/2\sigma_A^2} e^{-(A_{meas} - A)^2/2\sigma_A^2} e^{-(b_{meas} - b)^2/2\sigma_b^2} \frac{1}{\sigma_A \sqrt{2\pi}} e^{-(A_{meas} - A)^2/2\sigma_A^2} e^{-(A_{meas} - A)^2/2\sigma_A^2} e^{-(A_{meas} - b)^2/2\sigma_B^2} \frac{1}{\sigma_A \sqrt{2\pi}} e^{-(A_{meas} - A)^2/2\sigma_A^2} e^{-(A_{meas} - b)^2/2\sigma_B^2} e^{-(A_{meas} - b)^2/2\sigma_B^2} \frac{1}{\sigma_A \sqrt{2\pi}} e^{-(A_{meas} - b)^2/2\sigma_B^2} e^{-($$

Eilam Gross Statistics in PP

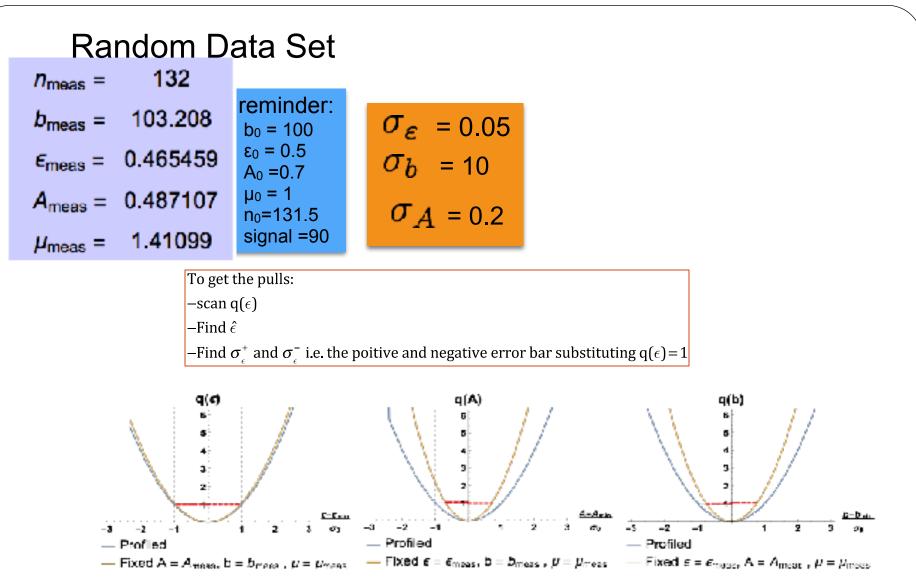
68



Profile Likelihood for Measurement

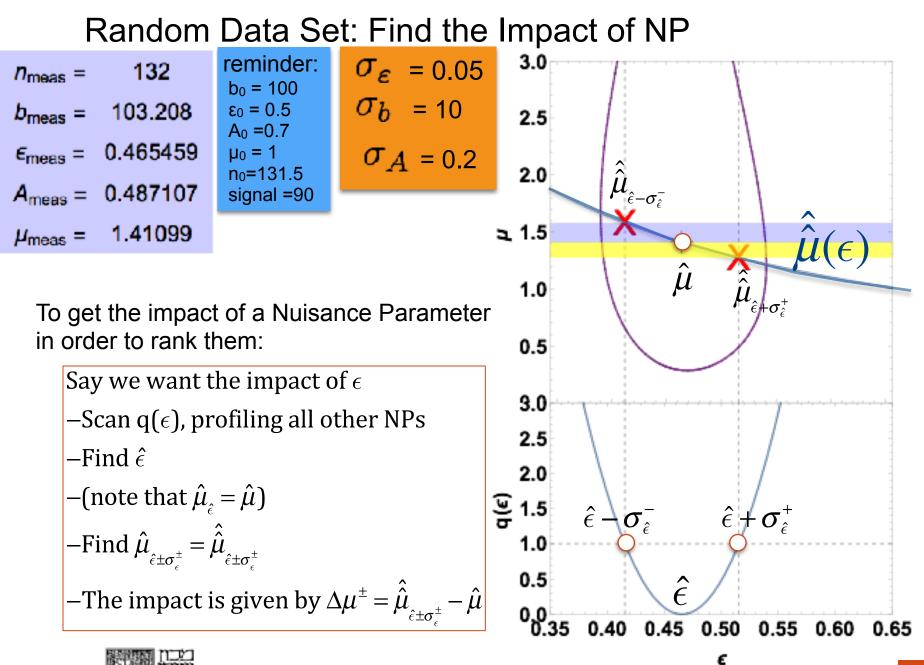




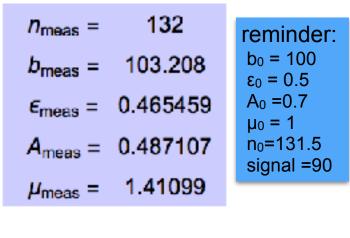


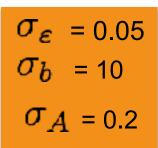
With the random data sets we find perfect pulls for the profiled scans But not for the fix scans!

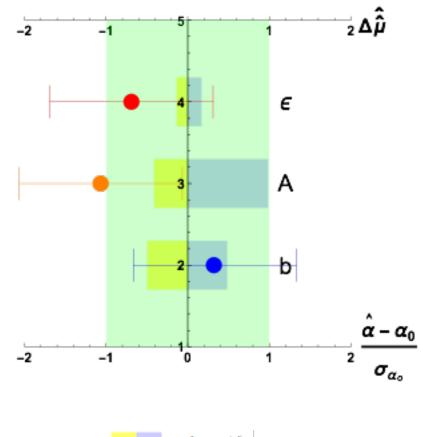


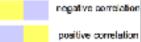


Random Data Set: SUMMARY of Pulls and Impact

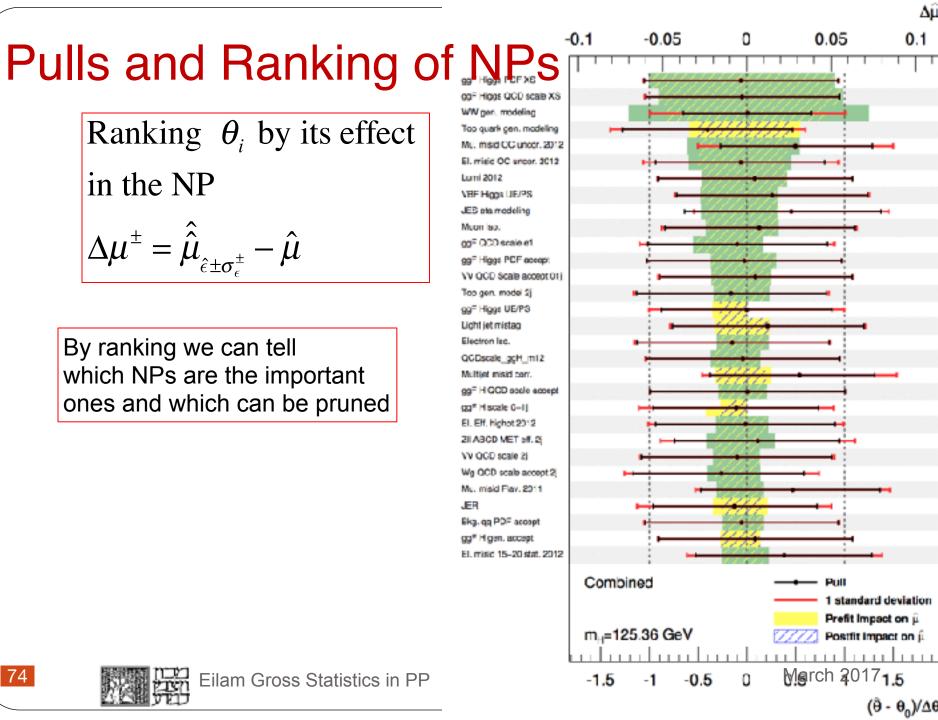












If time permits: The Feldman Cousins Unified Method



The Flip Flop Way of an Experiment

The most intuitive way to analyze the results of an experiment would be

If the significance based on q_{obs} , is less than 3 sigma, derive an upper limit (just looking at tables), if the result is >5 sigma derive a discovery central confidence interval for the measured parameter (cross section, mass....)

- This Flip Flopping policy leads to undercoverage: Is that really a problem for Physicists? Some physicists say, for each experiment quote always two results, an upper limit, and a (central?) discovery confidence interval
- Many LHC analyses report both ways.



Frequentist Paradise – F&C Unified with Full Coverage

- Frequentist Paradise is certainly made up of an interpretation by constructing a confidence interval in brute force ensuring a coverage!
- This is the Neyman confidence interval adopted by F&C....
- The motivation:

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- Ensures Coverage
- Avoid Flip-Flopping an ordering rule determines the nature of the interval

q

(1-sided or 2-sided depending on your observed data)

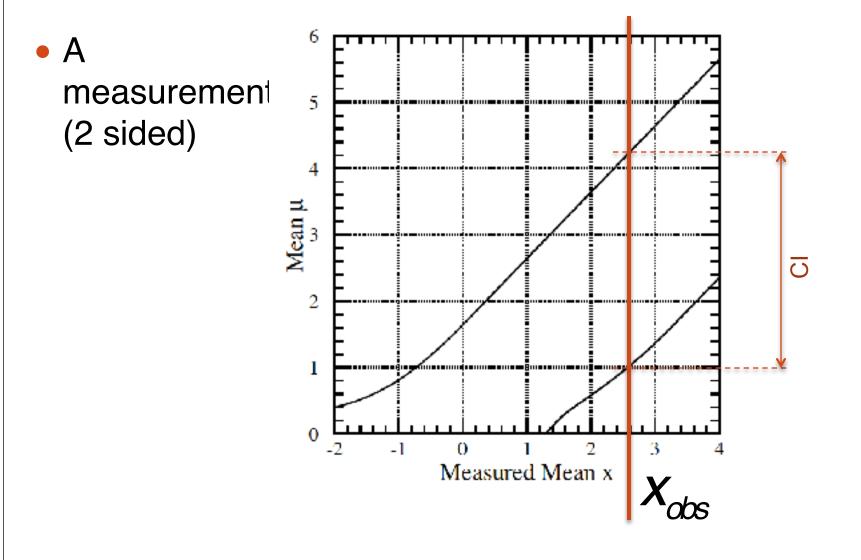
- Ensures Physical Intervals
- Let the test statistics be

$$= \begin{cases} -2\ln\frac{L(s+b)}{L(\hat{s}+b)} & \hat{s} \ge 0\\ -2\ln\frac{L(s+b)}{L(b)} & \hat{s} < 0 \end{cases}$$

where \hat{s} is the physically allowed mean s that maximizes L(\hat{s} +b) (protect a downward fluctuation of the background, n_{obs} >b ; \hat{s} >0)

• Order by taking the 68% highest q's

How to tell an Upper limit from a Measurement without Flip Flopping





 An upper limit (1 sided)

