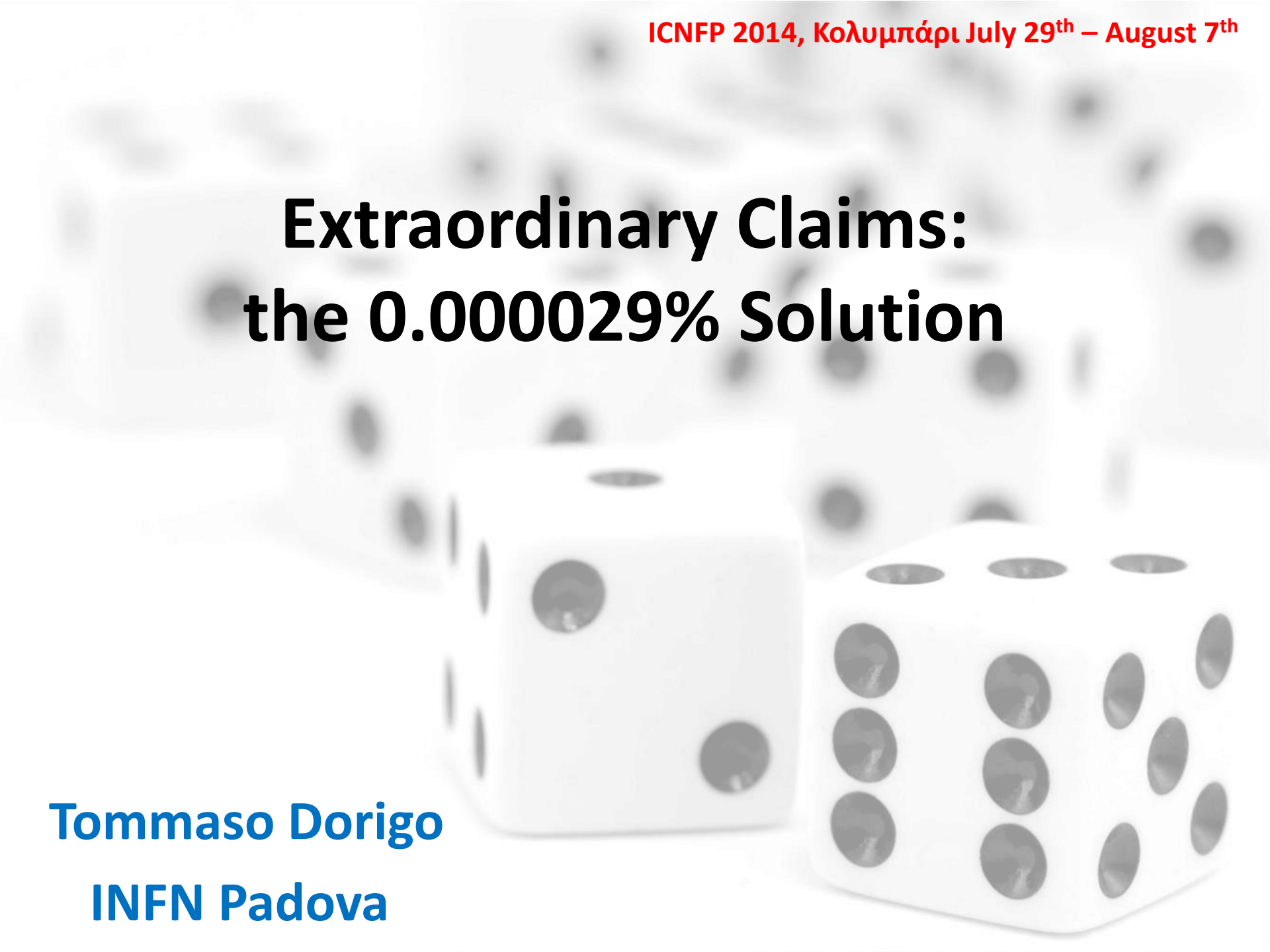
ICNFP 2014, Κολυμπάρι July 29th – August 7th

Extraordinary Claims: the 0.000029% Solution



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Why this talk

- Driven by the Higgs search and discovery hype, in the last few years science popularization magazines, physics blogs, and other outreach agents have been very busy, and in general successful, explaining to the public the idea that a scientific discovery in physics research requires that an effect be found with a statistical significance exceeding five standard deviations.

- Personally, I regret it. Science outreach has succeeded at explaining and making well known a convention which **is entirely arbitrary**, and one which should be used with caution, or substituted with something smarter

- It is the purpose of this talk to refresh our memory about where the five-sigma criterion comes from, what it was designed to address, where it may fail, and to consider its limitations and the **need for good judgement when taking the decision to claim a discovery**

Contents

- A few basic definitions
  - p-value, significance, type-I and type-II error rates
- History of the five-sigma criterion in HEP
  - Rosenfeld on exotic baryons
  - Lynch and the GAME program
  - Successful and failed applications in recent times
- The trouble with it
  - Ill-quantifiable LEE
  - Subconscious Bayes factors
  - Systematics
  - The Jeffrey-Lindley paradox
- How to fix it ?
  - Lyons' table
  - Agreeing on flexible thresholds

Statistical significance: What it is

- Statistical significance is a way to report the probability that an experiment obtains data at least as discrepant as those actually observed, under a given "null hypothesis“ H_0
- In physics H_0 usually describes the currently accepted and established theory (but there are exceptions).
- One starts with the **p**-value, i.e. the probability of obtaining a test statistic (a function of the data) at least as extreme as the one observed, if H_0 is true.

  p can be converted into the corresponding number of "sigma," i.e. standard deviation units from a Gaussian mean. This is done by finding **x** such that the integral from **x** to infinity of a unit Gaussian G(0,1) equals **p**:

$$\frac{1}{\sqrt{2\pi}} \int_x^\infty e^{-\frac{t^2}{2}} dt = p$$

- According to the above recipe, a **15.9%** probability is a one-standard-deviation effect; a **0.135%** probability is a three-standard-deviation effect; and a **0.0000285%** probability corresponds to five standard deviations - "**five sigma**" for insiders.

Notes

The alert observer will no doubt notice a few facts:

- the convention is to use a "one-tailed" Gaussian: we do not consider departures of x from the mean in the uninteresting direction
  - Hence "negative significances" are mathematically well defined, but not interesting

- the conversion of p into σ is fixed and independent of experimental detail. As such, using Nσ rather than p is **just a shortcut** to avoid handling numbers with many digits: we prefer to say "5σ" than "0.00000029" just as we prefer to say "a nanometer" instead than "0.000000001 meters" or "a Petabyte" instead than "1000000000000 bytes"

- The whole construction rests on a proper definition of the p-value. Any shortcoming of the properties of p (e.g. a tiny non-flatness of its PDF under the null hypothesis) totally invalidates the meaning of the derived Nσ
  - In particular, using "sigma" units does in no way mean we are espousing some kind of Gaussian approximation for our test statistic or in other parts of our problem.

    Beware – this has led many to confusion

- The "*probability of the data*" has no bearing on the concept, and is not used. What is used is the probability of a subset of the possible outcomes of the experiment, defined by the outcome actually observed (as much or more extreme)

Type-I and type-II error rates

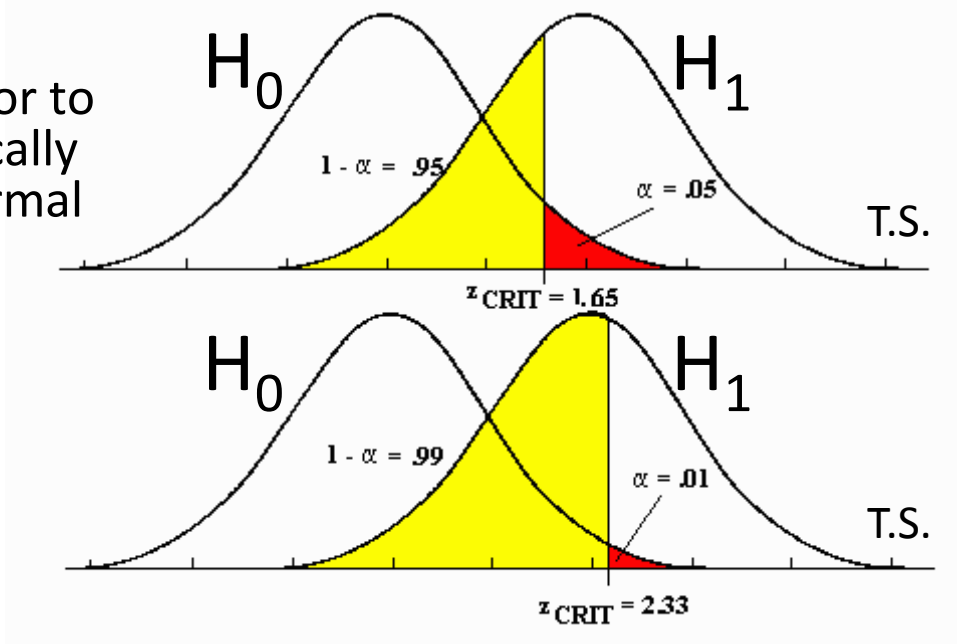
In the context of hypothesis testing the type-I error rate α is the probability of rejecting the null hypothesis when it is true.

Testing a simple null hypothesis versus a composite alternative (eg. m=0 versus m>0) at significance level α is **dual** to asking whether 0 is in the confidence interval for m at confidence level 1-α.

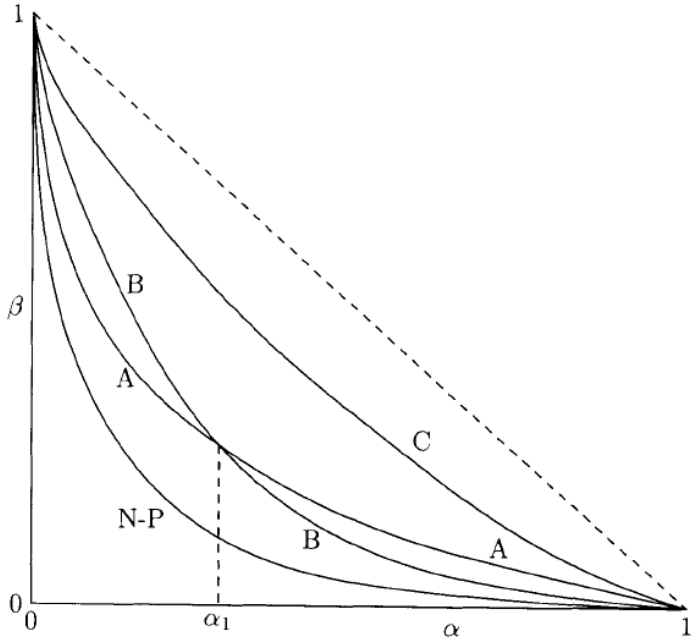
Strictly connected to α is the concept of "power" (1-β), where β is the type-2 error rate, defined as the probability of accepting the null, even if the alternative is instead true.

By choosing α for an experiment (eg. to decide a criterion for a discovery claim, or to set a confidence interval) one automatically also chooses β. In general there is no formal recipe for the decision.

As shown in the graph, the choice of a stricter requirement for α (i.e. a smaller type-I error rate) implies a higher chance of accepting a false null (yellow region), i.e. smaller power.

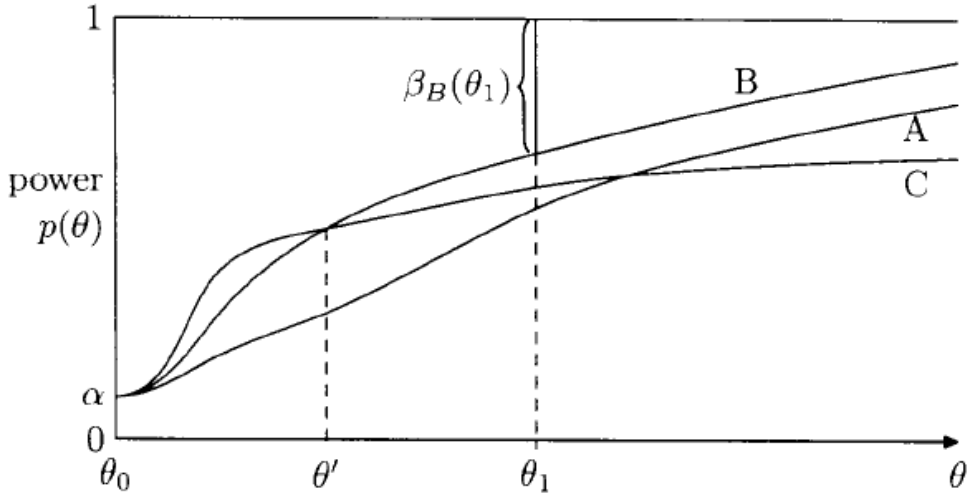


Alpha vs Beta and power graphs



- Choices of α and β are conflicting: where to stay in the curve provided by your analysis method highly depends on **habits in your field**
- What makes a difference is the test statistic: note on the right how the N-P likelihood-ratio test outperforms others for simple-vs-simple HT, as dictated by the Neyman-Pearsons lemma

As data size increases, the power curve (shown below) becomes closer to a step function



The power 1-β of a test usually also depends on the parameter of interest: different methods may have best performance in different parameter space points

Some history of 5σ

- In 1968 Arthur Rosenfeld wrote a paper titled "*Are There Any Far-out Mesons or Baryons?*“ [1]. In it, he demonstrated that the number of claims of discovery of such exotic particles published in scientific magazines agreed reasonably well with the **number of statistical fluctuations** that one would expect in the analyzed datasets.

  (“Far-out hadrons” are hypothetical particles which can be defined as ones that do not fit in SU(3) multiplets. In 1968 quarks were not yet fully accepted as real entities, and the question of the existence of exotic hadrons was important.)

- Rosenfeld examined the literature and pointed his finger at large trial factors coming into play due to the massive use of combinations of observed particles to derive mass spectra containing potential discoveries:

  > "[...] This reasoning on multiplicities, extended to all combinations of all outgoing particles and to all countries, leads to an estimate of 35 million mass combinations calculated per year. How many histograms are plotted from these 35 million combinations? A glance through the journals shows that a typical mass histogram has about 2,500 entries, so the number we were looking for, h is then 15,000 histograms per year (Our annual surveys also tells you that the U.S. measurement rate tends to double every two years, so things will get worse)."

More Rosenfeld

> "[...] Our typical 2,500 entry histogram seems to average 40 bins. This means that therein a physicist could observe 40 different fluctuations one bin wide, 39 two bins wide, 38 three bins wide... This arithmetic is made worse by the fact that when a physicist sees 'something', he then tries to enhance it by making cuts..."

(I will get back to the last issue later)

> "In summary of all the discussion above, I conclude that each of our 150,000 annual histograms is capable of generating somewhere between 10 and 100 deceptive upward fluctuations [...]".

That was indeed a problem! A comparison with the literature in fact showed a correspondence of his eyeballed estimate with the number of unconfirmed new particle claims.

Rosenfeld concluded:

> "To the theorist or phenomenologist the moral is simple: **wait for nearly 5σ effects**. For the experimental group who has spent a year of their time and perhaps a million dollars, the problem is harder... go ahead and publish... but they should realize that any bump less than about 5σ **calls for a repeat of the experiment.**"

Gerry Lynch and GAME

- Rosenfeld's article also cites the half-joking, half-didactical effort of his colleague Gerry Lynch at Berkeley:

> "My colleague Gerry Lynch has instead tried to study this problem 'experimentally' using a 'Las Vegas' computer program called Game. Game is played as follows. You wait until a unsuspecting friend comes to show you his latest 4-sigma peak. You draw a smooth curve through his data (based on the hypothesis that the peak is just a fluctuation), and punch this smooth curve as one of the inputs for Game. The other input is his actual data. If you then call for 100 Las Vegas histograms, Game will generate them, with the actual data reproduced for comparison at some random page. You and your friend then go around the halls, asking physicists to pick out the most surprising histogram in the printout. Often it is one of the 100 phoneys, rather than the real "4-sigma" peak. "

- Obviously particle physicists in the '60s were more "bump-happy" than we are today. The proposal to raise to 5-sigma of the threshold above which a signal could be claimed was an earnest attempt at reducing the flow of claimed discoveries, which distracted theorists and caused confusion.

Let's play GAME

It is instructive even for a hard-boiled sceptical physicist raised in the years of Standard Model Precision Tests Boredom to play with GAME.

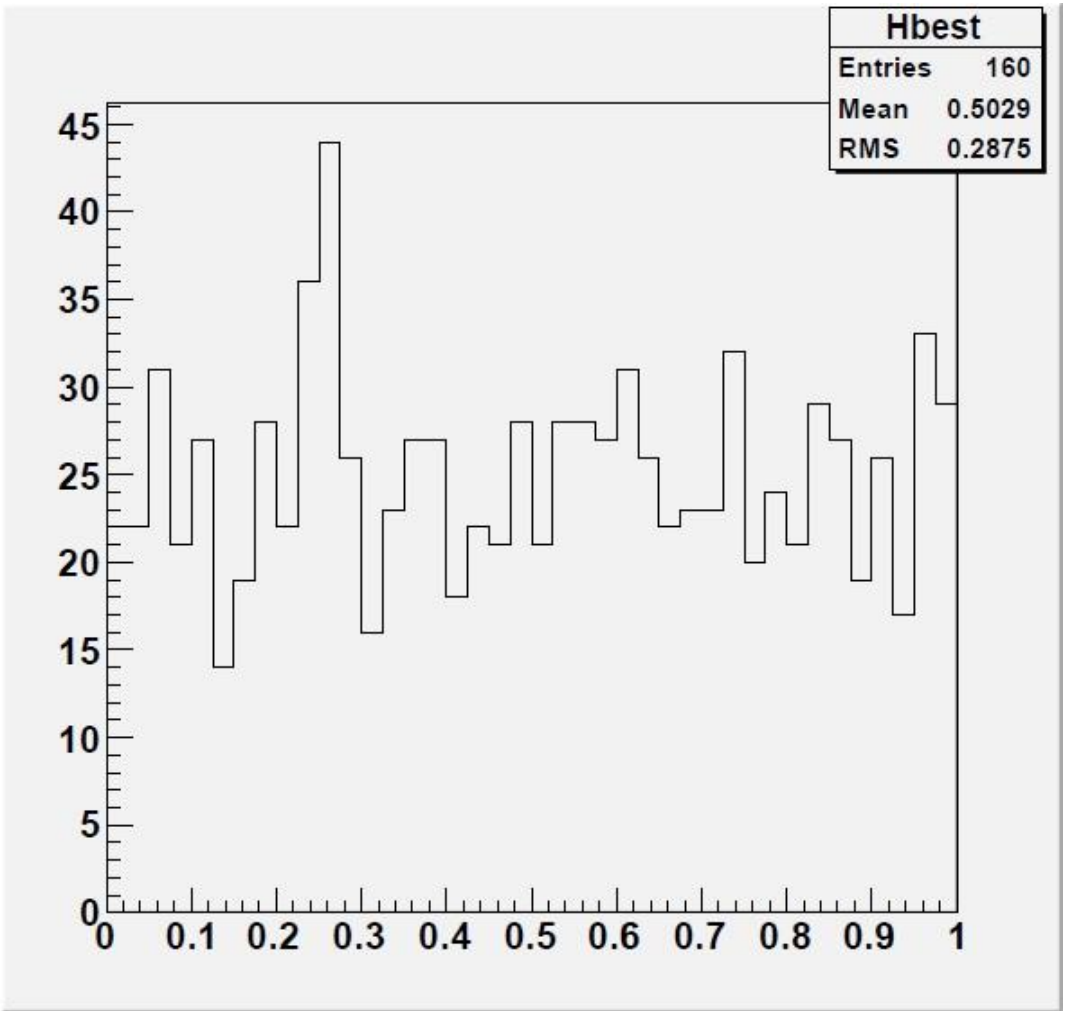
In the following slides are shown a few histograms, each selected by an automated procedure as the one containing "the most striking" peak among a set of 100, all drawn from a smooth distribution.

> Details: 1000 entries; 40 bins; the "best" histogram in each set of 100 is the one with most populated adjacent pair of bins (in the first five slides) or triplets of bins (in the second set of five slides)

You are asked to consider **what you would tell your student if she came to your office with such a histogram**, claiming it is the result of an optimized selection for some doubly charmed baryon, say, that she has been looking for in her research project.

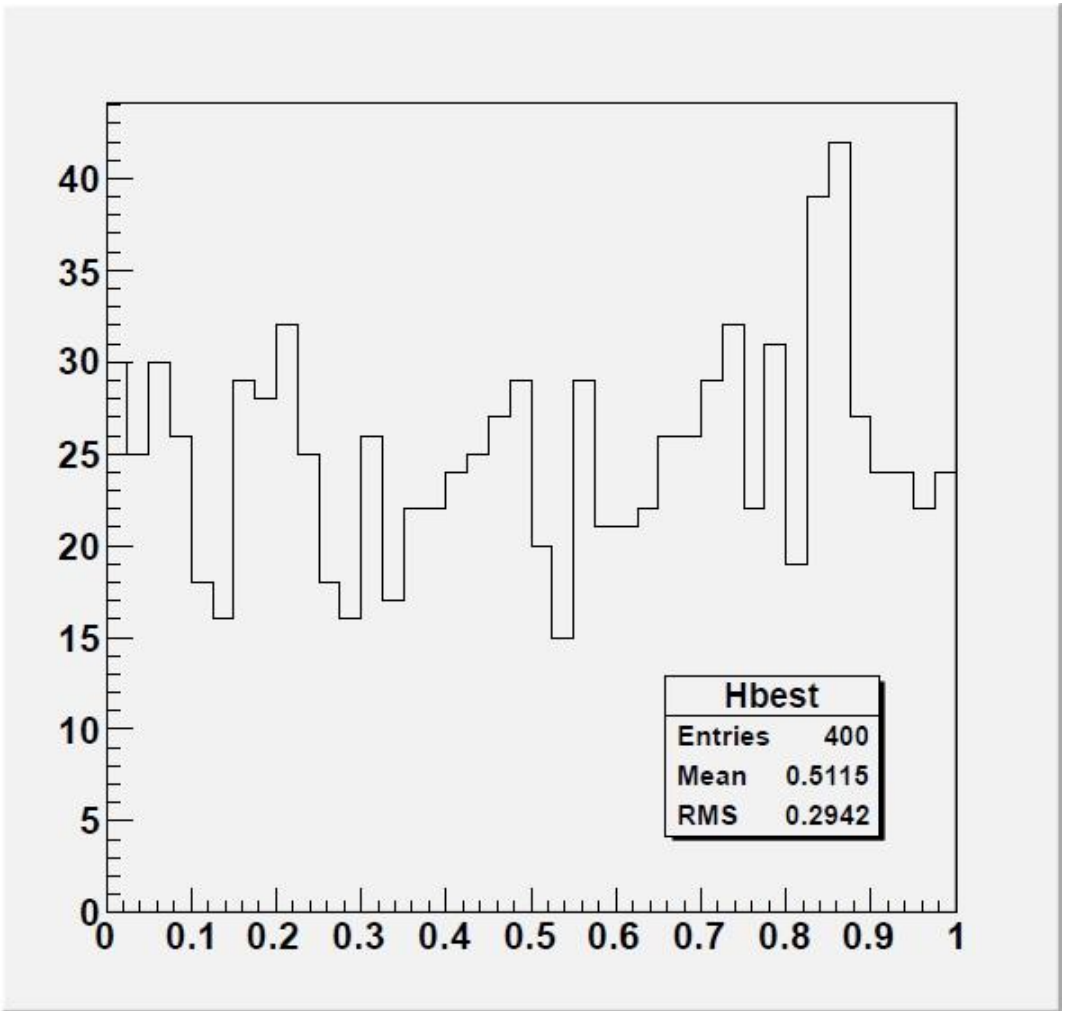
2-bin bumps

- Here are the outputs of the most significant 2-bin bumps in five 100-histogram sets: #1



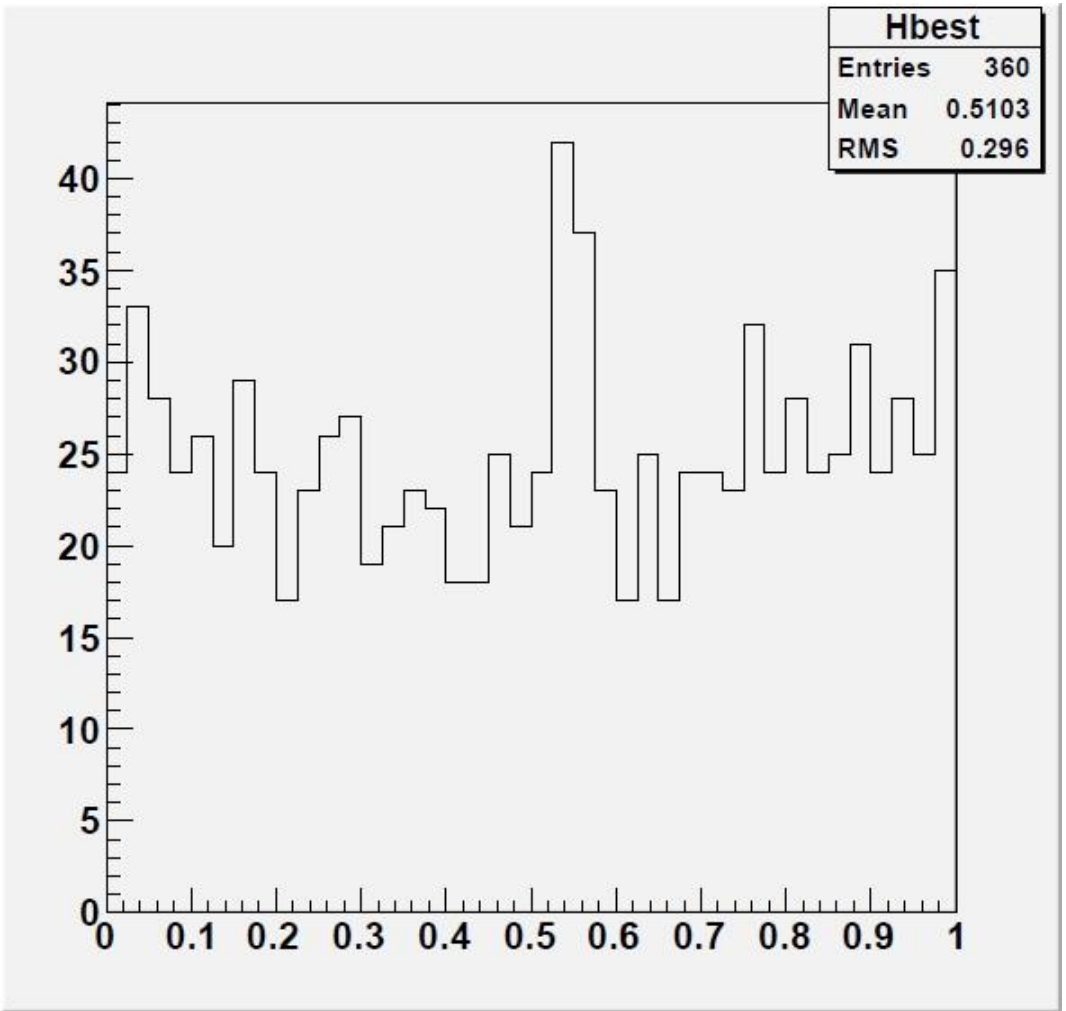
2-bin bumps

- Here are the outputs of the most significant 2-bin bumps in five 100-histogram sets: #2



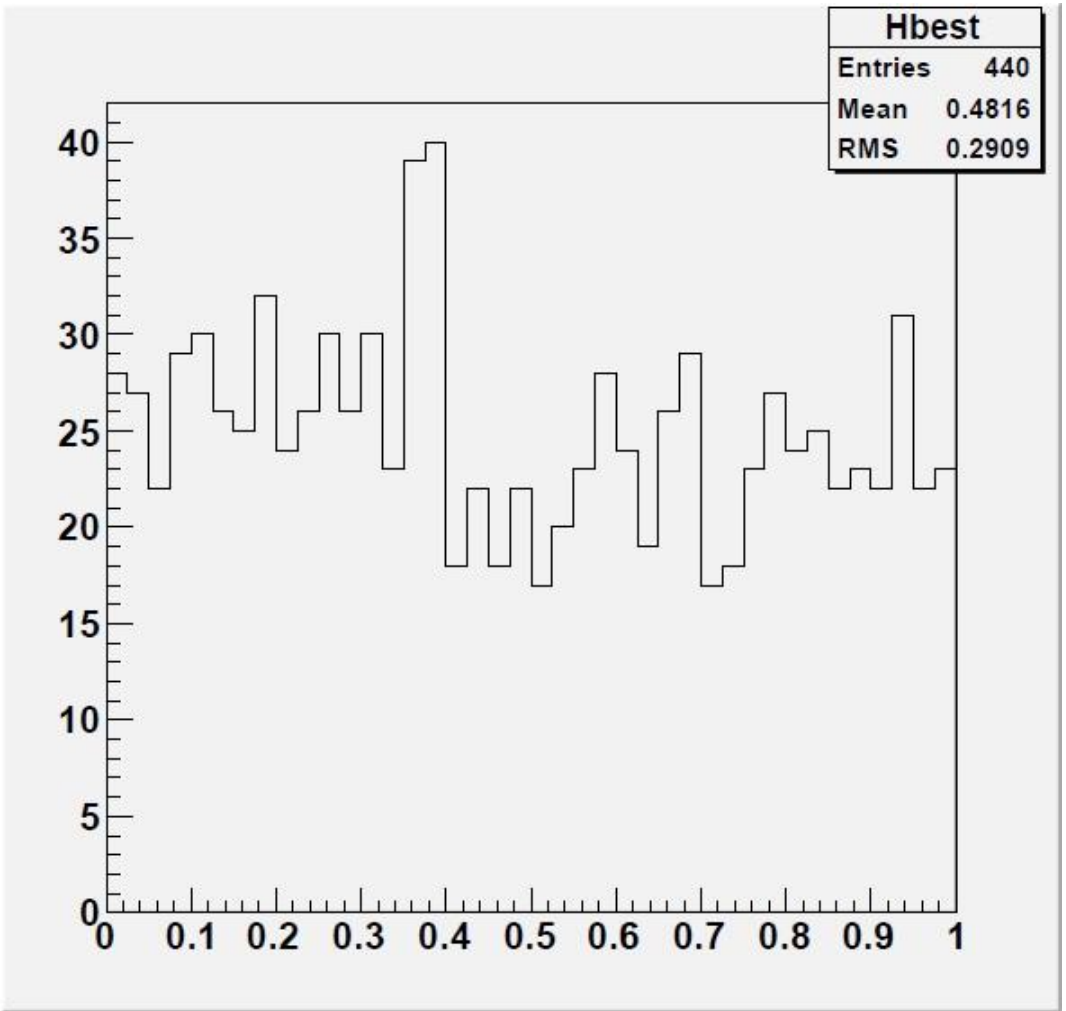
2-bin bumps

- Here are the outputs of the most significant 2-bin bumps in five 100-histogram sets: #3



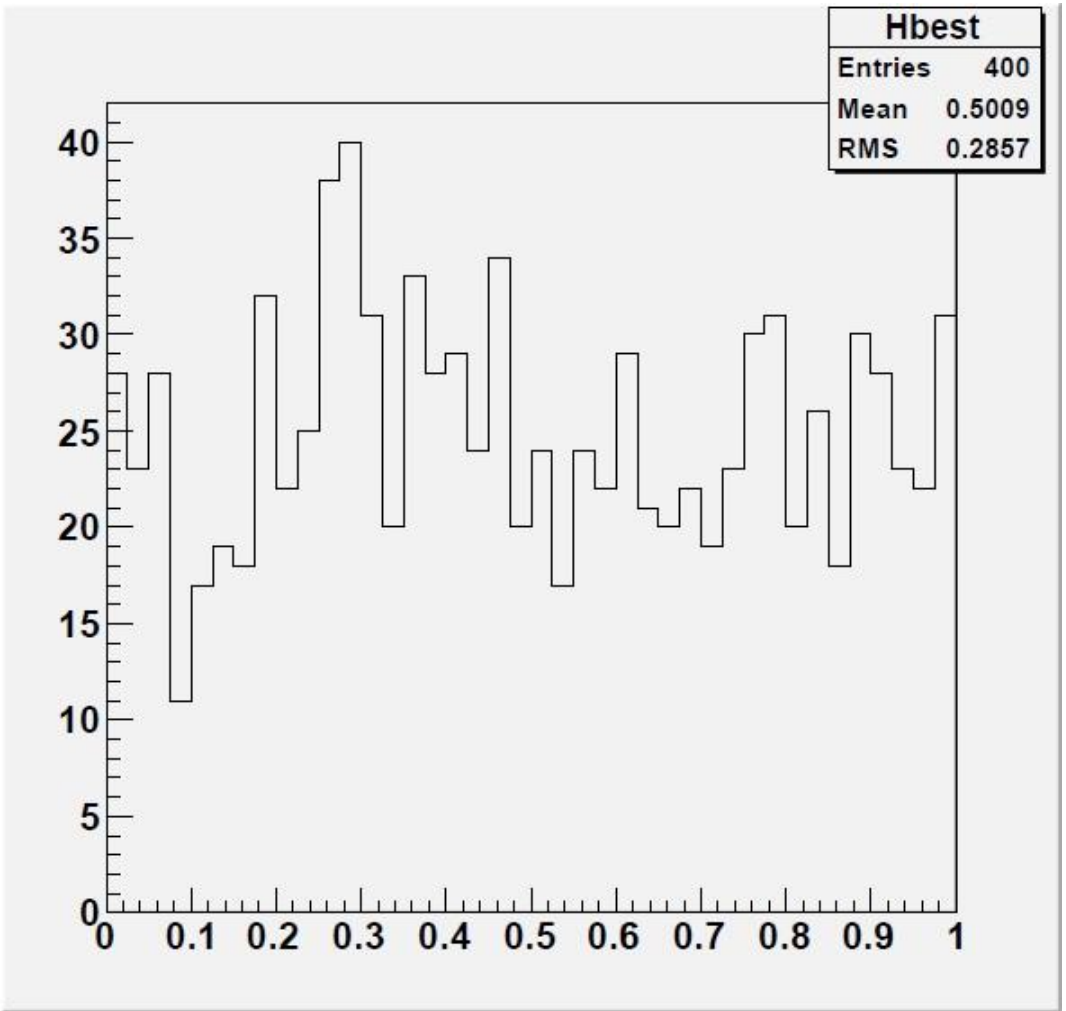
2-bin bumps

- Here are the outputs of the most significant 2-bin bumps in five 100-histogram sets: #4



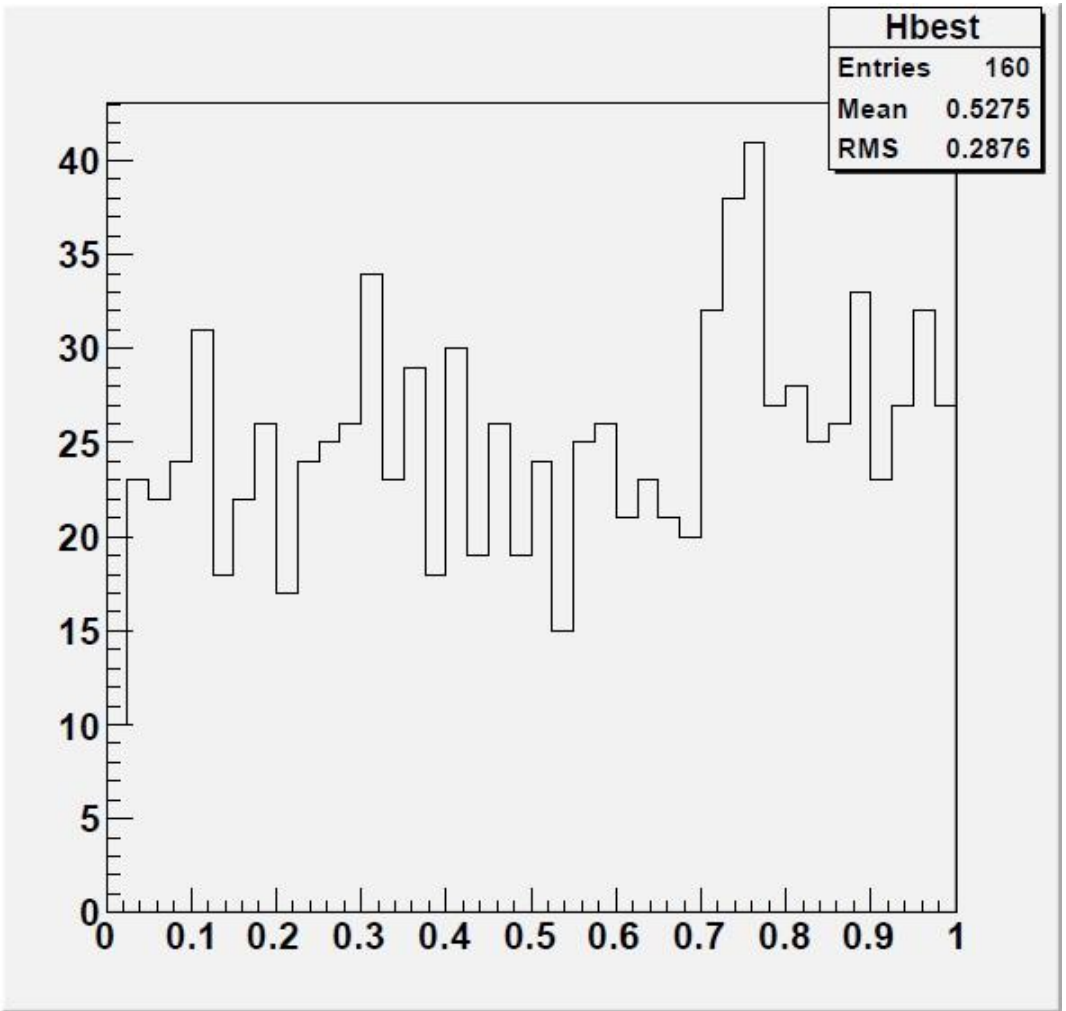
2-bin bumps

- Here are the outputs of the most significant 2-bin bumps in five 100-histogram sets: #5



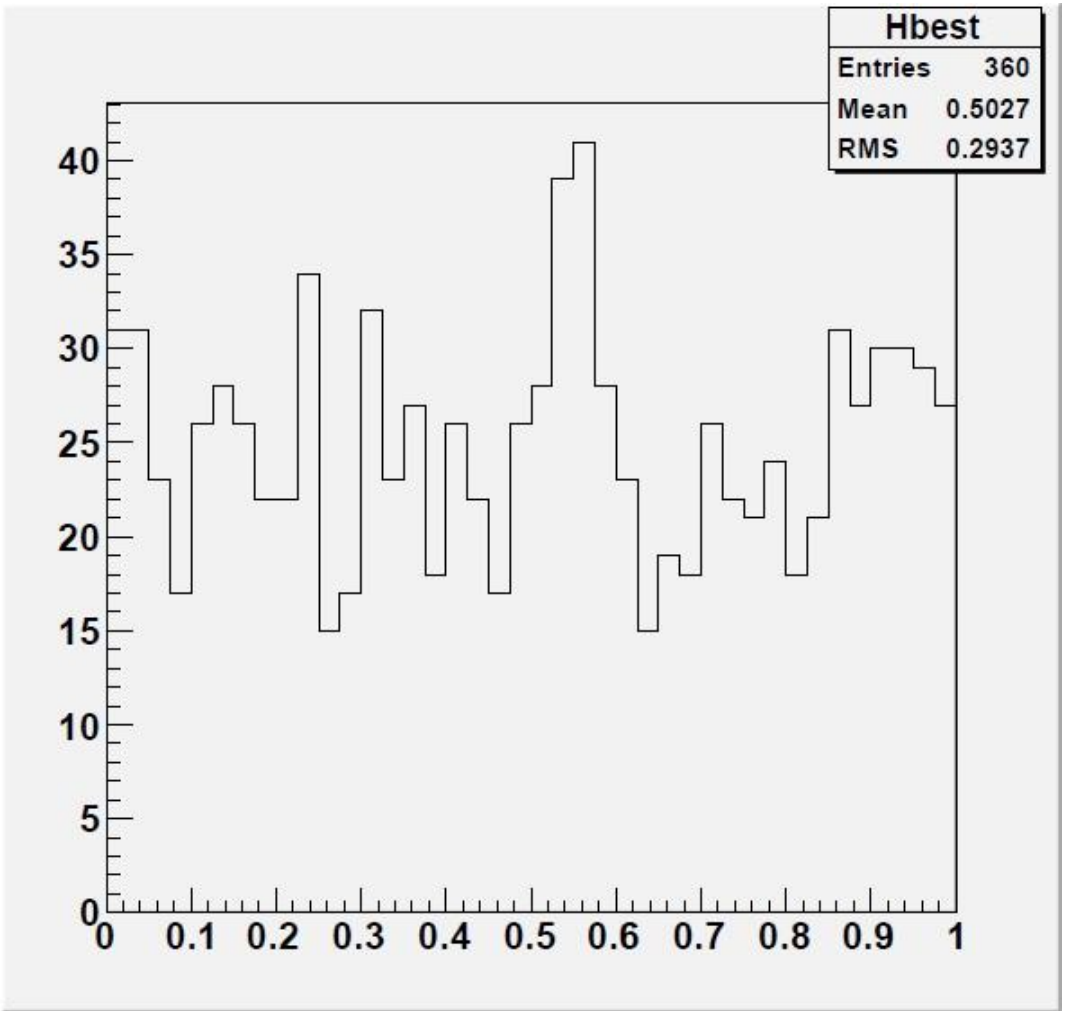
3-bin bumps

- Here are the outputs of the most significant 3-bin bumps in five 100-histogram sets: #1



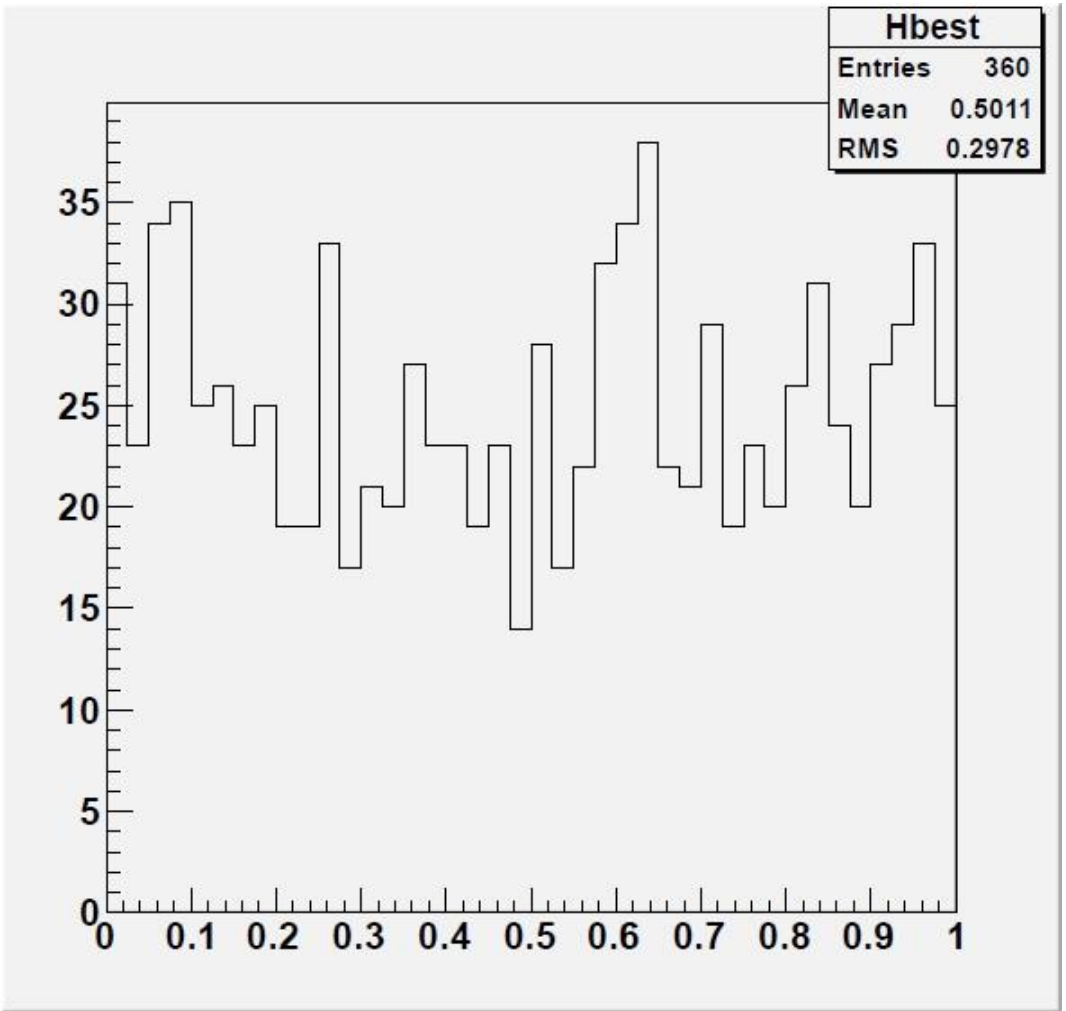
3-bin bumps

- Here are the outputs of the most significant 3-bin bumps in five 100-histogram sets: #2



3-bin bumps

- Here are the outputs of the most significant 3-bin bumps in five 100-histogram sets: #3



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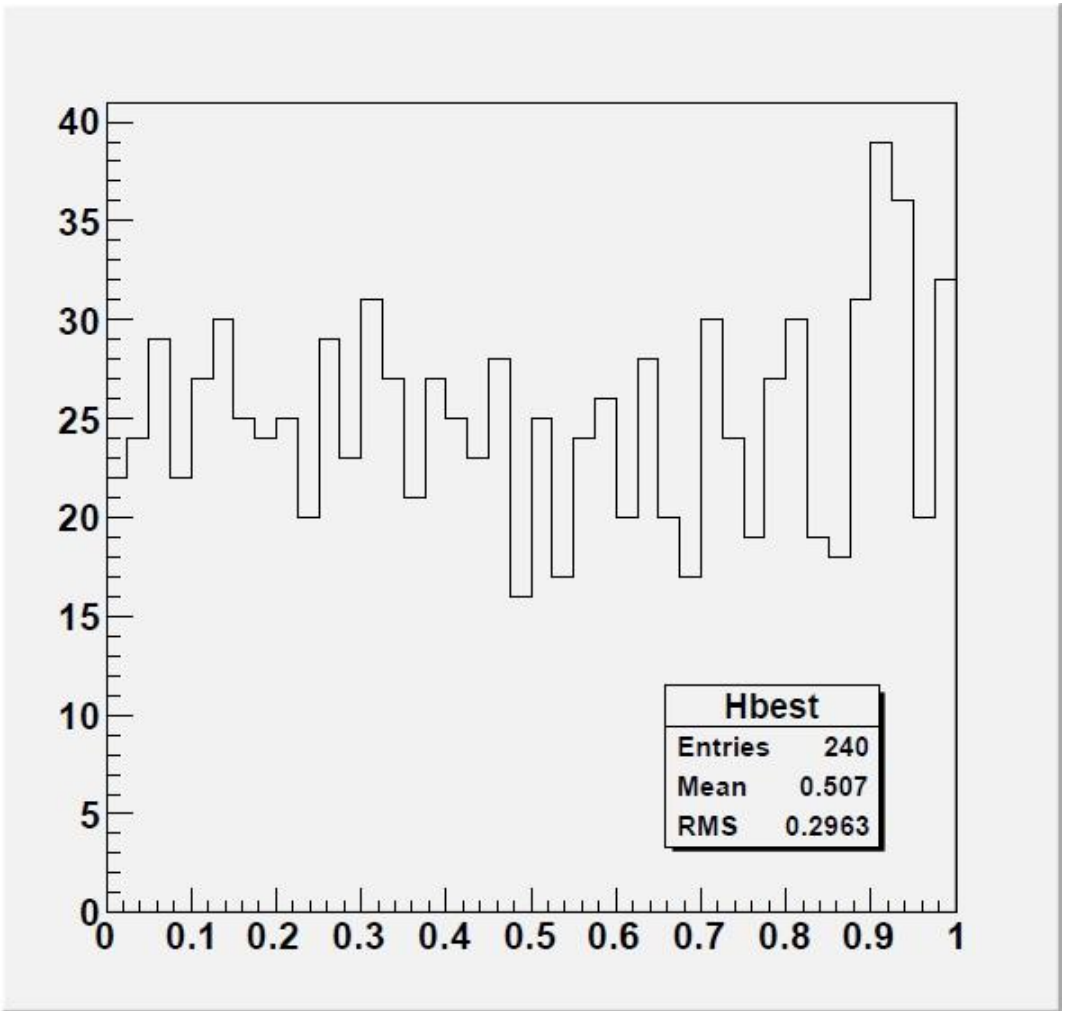

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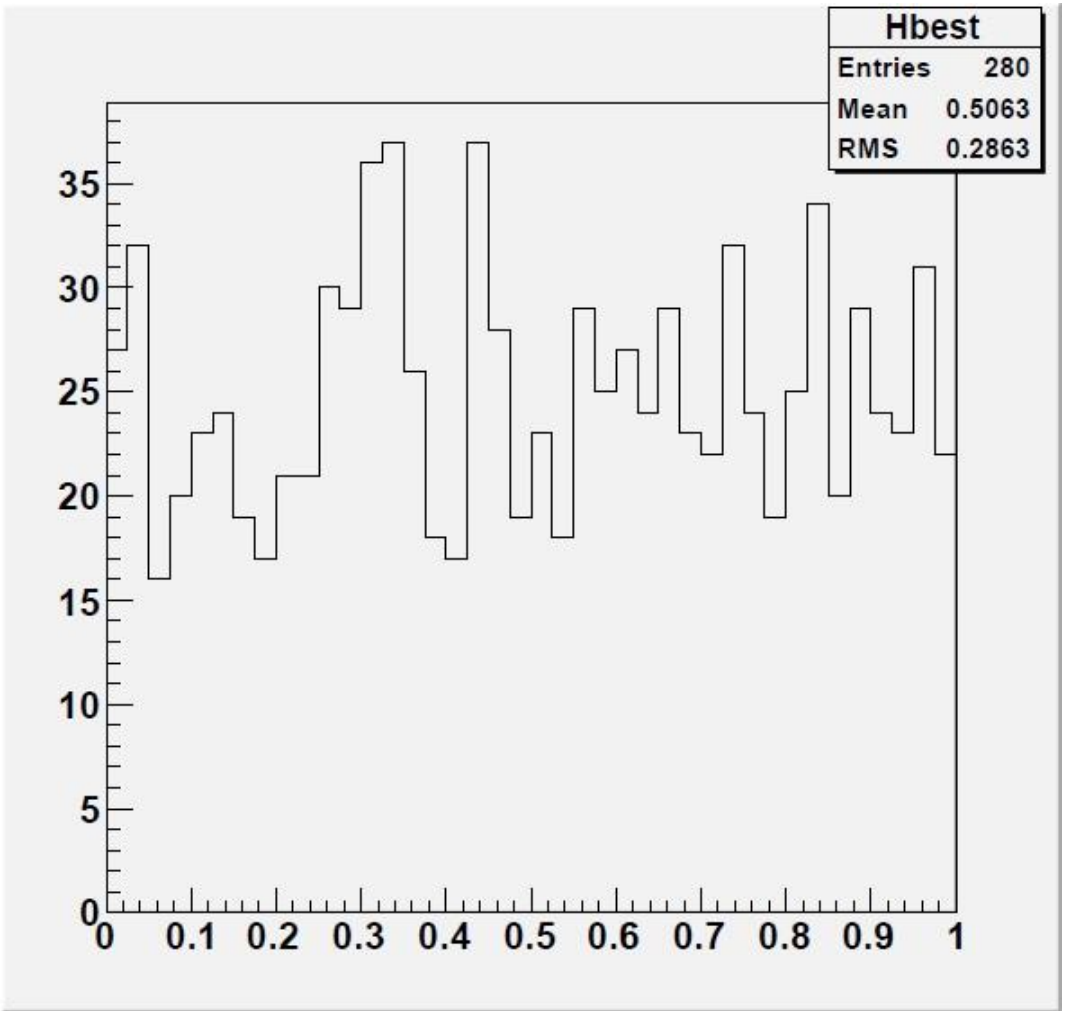


Notes on GAME

Each of the histograms in the previous slides is the best one in a set of a hundred; yet the isolated signals have p-values corresponding to 3.5σ - 4σ effects

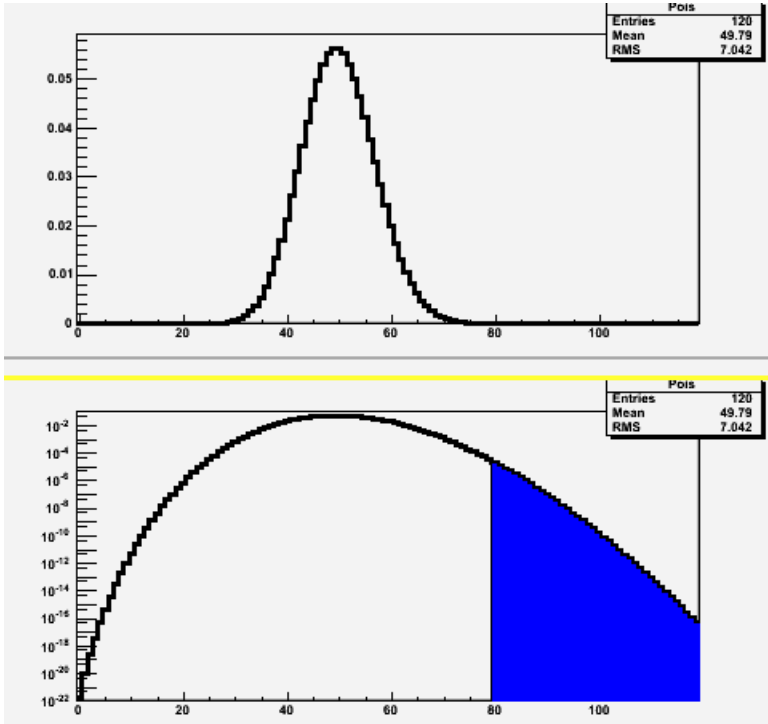
E.g. some of the 2-bin bumps contain 80 evts with an expectation of 2*1000/40=50, and

$$p_{Poisson}(\mu=50;N>=80)=5.66*10^{-5} \rightarrow N=3.86\sigma$$

Why?

Because the bump can appear anywhere (x39) in the spectrum – we did not specify beforehand where we would look because we admit 2- as well as 3-bin bumps as "interesting" (also, we could extend the search to wider structures without penalty)

One should also ponder on the often overlooked fact that **researchers finding a promising "bump" will usually modify the selection a posteriori, voluntarily or involuntarily enhancing it**. This makes the trials factor quite hard to estimate a priori



P(N|μ=50) in linear (top) and semi-log scale (bottom)

What 5σ may do for you

- Setting the bar at 5σ for a discovery claim undoubtedly removes the large majority of spurious signals due to statistical fluctuations
  - The trials factor required to reach 10^{-7} probabilities is of course very large, but the large number of searches being performed in today's experiments makes up for that
  - Nowadays we call this "**LEE**", for "look-elsewhere effect".
  - 50 years after Rosenfeld, we do not need to compute the trials factor by hand: we can estimate a "global" as well as a "local" p-value using brute force computing, or advanced tricks (**more later**).

- The other reason at the roots of the establishment of a high threshold for significance has been the ubiquitous presence in our measurements of unknown, or ill-modeled, systematic uncertainties
  - To some extent, a 5σ threshold protects systematics-dominated results from being published as discoveries

Protection from trials factor and unknown or ill-modeled systematics are the rationale behind the 5σ criterion

It is to be noted that the criterion has no basis in professional statistics literature, and is considered **totally arbitrary** by statisticians, no less than the 5% threshold often used for the type-I error rate of research in medicine, biology, cognitive sciences, etcetera. As shown before, the type-1 error rate is an arbitrary choice.

How 5σ became a standard 1: the Seventies

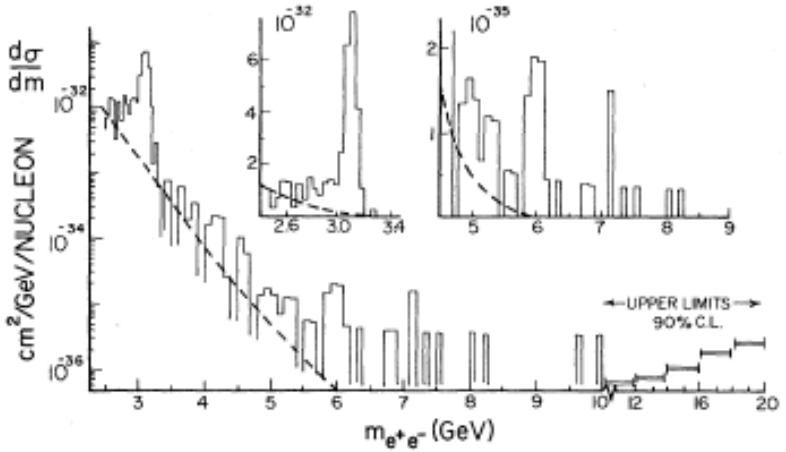
A lot has happened in HEP since 1968. In the seventies, the gradual consolidation of the SM shifted the focus of particle hunts from random bump hunting to more targeted searches

Let's have a look at a few important searches to understand how the 5σ criterion gradually became a standard

- **The J/ψ discovery** (1974): no question of significance – the bumps were too big for anybody to bother fiddling with statistical tests
- **The τ discovery** (1975-1977): no mention of significances for the excesses of (eμ) events; rather a very long debate on hadron backgrounds.

- **The Oops-Leon(1976)**: "Clusters of events as observed occurring anywhere from 5.5 to 10.0 GeV appeared less than 2% of the time[8]. Thus the statistical case for a narrow (<100 MeV) resonance is strong although we are aware of the need for a confirmation."[2]

In footnote 8 they add: "An equivalent but cruder check is made by noting that the "continuum" background near 6 GeV and within the cluster width is 4 events. The probability of observing 12 events is again <=2%"
... But P(μ=4;N>=12) is 0.00091... so this seems to include a x20 trials factor. Daniel Kaplan may confirm ?



The real Upsilon

The Upsilon discovery (1977): burned by the Oopsleon, the E288 scientists waited more patiently for more data after seeing a promising 3σ peak at 9.5 GeV

- They did statistical tests to account for the trials factor (comparing MC probability to Poisson probability)
- Even after obtaining a peak with very large significance (>8σ) they continued to investigate systematical effects
- Final announcement claims discovery but does not quote significance, noting however that the signal is "statistically significant"[3]

Nov 19th 1976

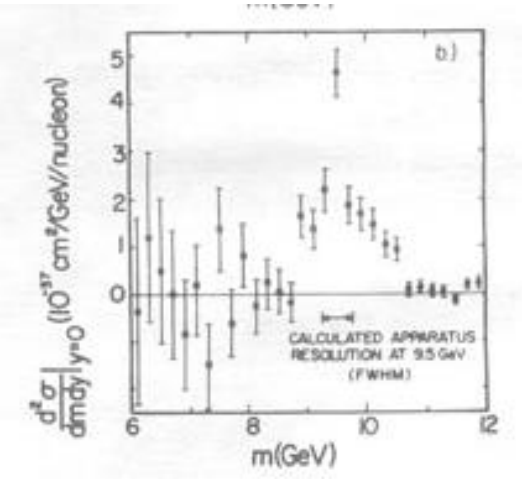
I determined this factor by monte carlo. I threw 30 events over 100 bins (expectation is 2 for 6 bins) and searched for clusters of 10 in 6 bins. I found 15 successes in 40000 trys or $CL = 3.75 \times 10^{-4}$. The poisson probability for ≥10 for an expectation of 2 is 1.94×10^{-5}. This bin counting factor is 19.3. JKY assumption would say 94 and 100/6 would say 17.

Nov 21st 1976

CONCLUSION : μμ I data is consistent with a narrow resonance.

So, to reiterate : ① PROBABILITY THAT THE 9.6 fits SMOOTH CONTINUUM ~ 1 in 1-2000 – i.e. ~ 3σ

② μμ I DATA CONSISTANT WITH APPARATUS RESOLUTION.



June 6th 1977

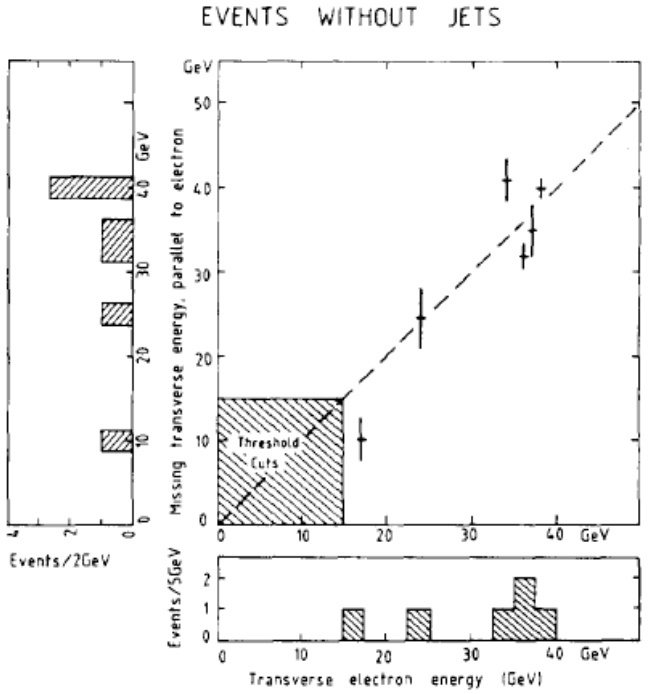
Now that the signal (>8σ) is no longer questionable from statistical objections, systematics must be considered.

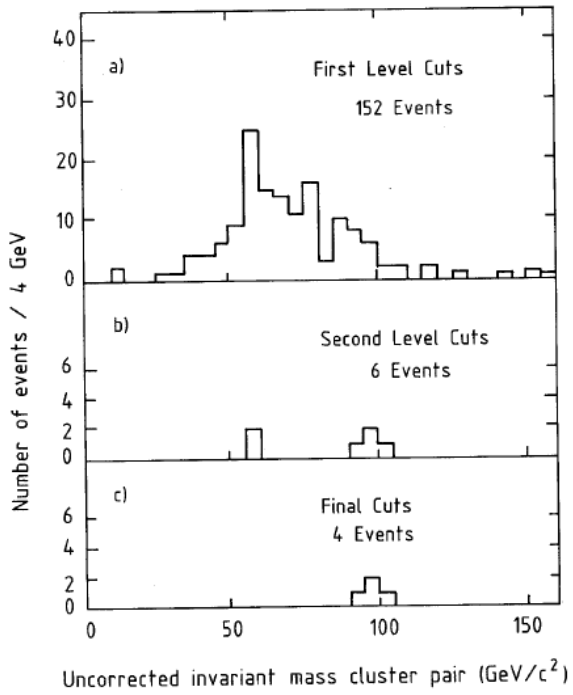
① Programming error, double counting, etc. – will be studied by

The W and Z bosons

- The W discovery was announced on January 25th 1983 based on 6 electron events with missing energy and no jets. No statistical analysis is discussed in the discovery paper[4], which however tidily rules out backgrounds as a source of the signal
  - Note that in the W search there was no trials factor to account for, as the signature was unique and predetermined; further, the theory prediction for the mass (82+-2 GeV) was matched well by the measurement (81+-5 GeV).

- The Z was "discovered" shortly thereafter, with an official CERN announcement made in May 1983 based on 4 events.
  - Also for the Z no trials factor was applicable
  - No mention of statistical checks in the paper[5], except notes that the various background sources were negligible.





The top quark discovery

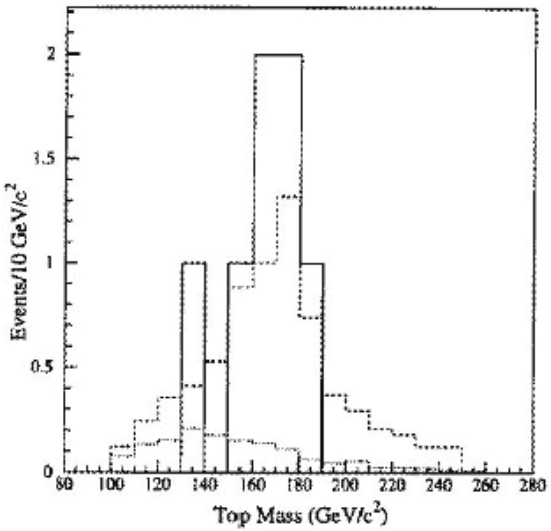
- In 1994 the CDF experiment had a serious counting excess (2.7σ) in b-tagged single-lepton and dilepton datasets, plus a towering mass peak at a value not far from where indirect EW constraints placed their bets
  - the mass peak, or corresponding kinematic evidence, was over 3σ by itself;

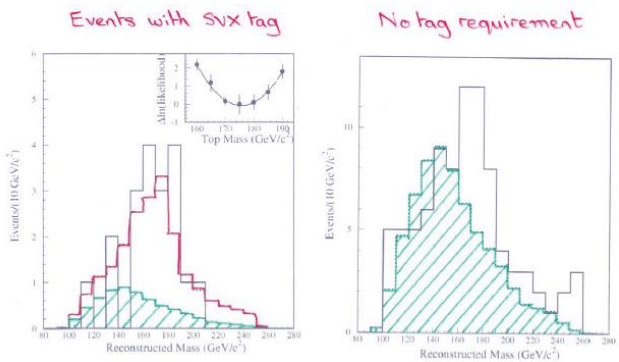
    $M=174+-10^{+13}_{-12}$ GeV (now it's 173+-0.5!)

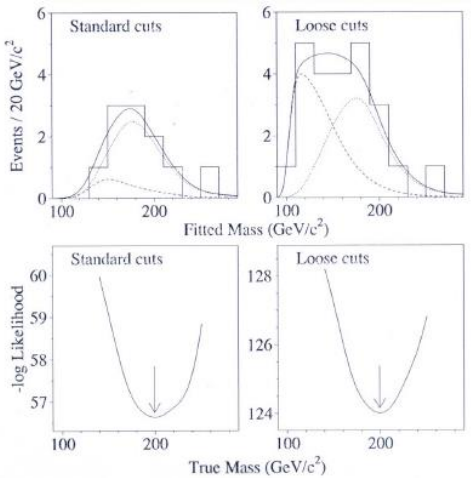
  Nonetheless the paper describing the analysis (120-pages long) spoke of "evidence" for top quark production[6]

- One year later CDF and DZERO[7] both presented 5σ significances based on their counting experiments, obtained by analyzing 3x more data

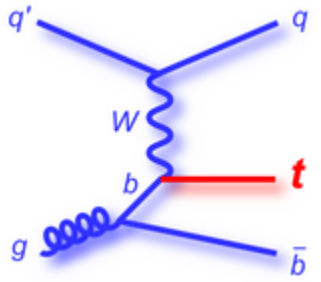
The top quark was thus the first particle discovered by a willful application of the "5σ" criterion





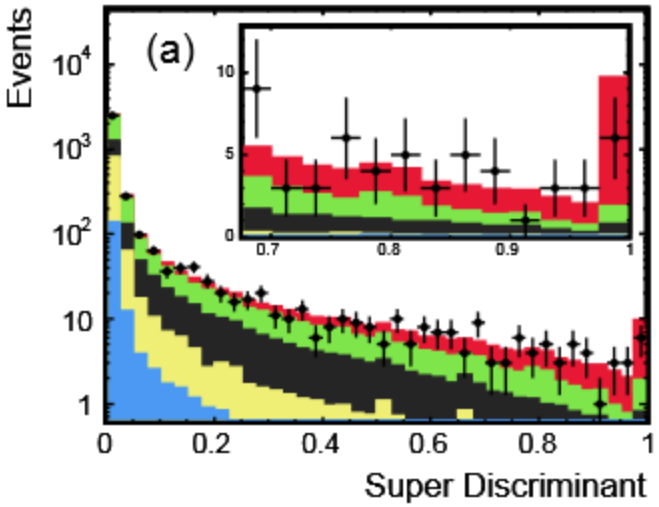


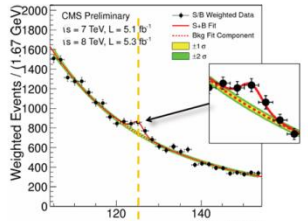
Following the top quark...

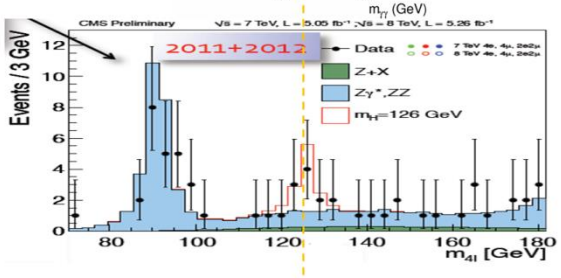


- Since 1995, the requirement of a p-value below $3*10^{-7}$ slowly but steadily became a standard. Two striking examples of searches that diligently waited for a 5-sigma effect before claiming discovery are:
  - **Single top quark production**: the top produced by electroweak processes in hadron-hadron collisions is harder to detect, and took 14 more years from the discovery of top pair production. The CDF and DZERO collaborations competed for almost a decade in the attempt to claim to have observed the process, obtaining 2-sigma, then 3- and 4-sigma effects, and only resolving to claim observation in 2009 [8], when clear 5-sigma effects had been observed.
  - In 2012 the **Higgs boson** was claimed by ATLAS and CMS[9]. Note that the two experiments had mass-coincident >3σ evidence in their data 6 months earlier, but the 5σ recipe was followed diligently.

    It is precisely the Higgs discovery what brought to the media attention the five-sigma criterion.





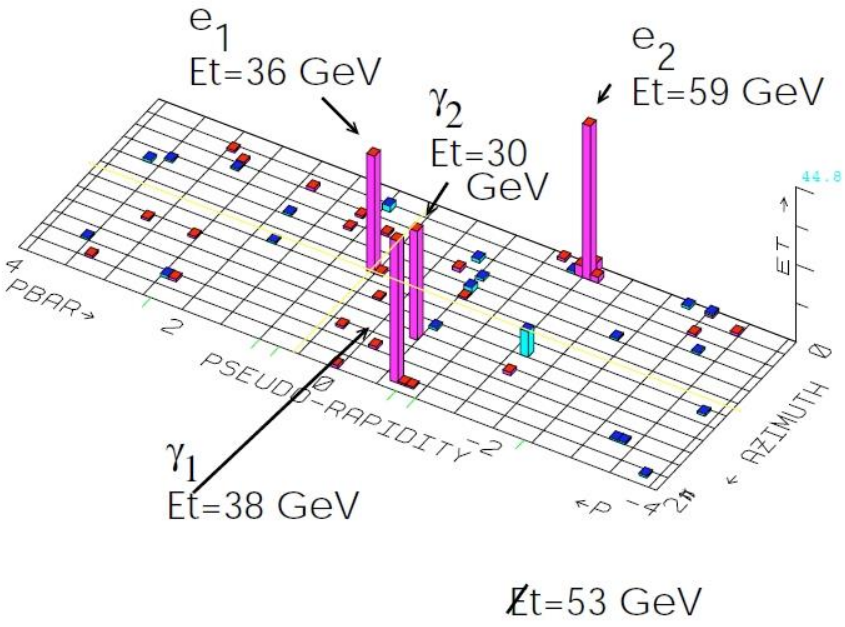


Discoveries that petered out - 1

In April 1995 CDF collected an event that fired four distinct “alarm bells” by the online trigger, Physmon. It featured two clean electrons, two clean photons, large missing transverse energy, and nothing else

It could be nothing! No SM process appeared to come close to explain its presence Possible backgrounds were estimated below 10^{-7}, a 6-sigma find

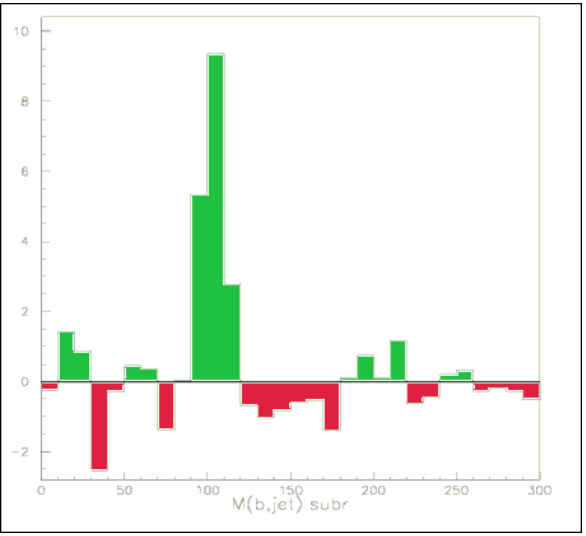
- The observation[10] caused a whole institution to dive in a 10-year-long campaign to find “cousins” and search for an exotic explanation; it also caused dozens of theoretical papers and revamping or development of SUSY models
- In Run 2 no similar events were found; DZERO did not see anything similar



Discoveries that petered out - 2

In 1996 CDF found a clear resonance structure of b-quark jet pairs at 110 GeV, produced in association with photons

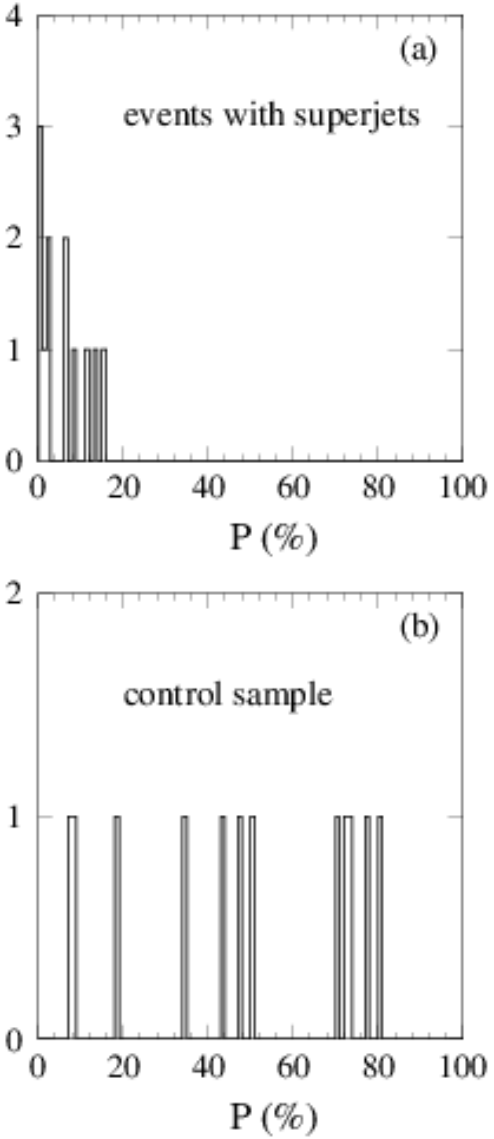
- The signal [11] had almost 4σ significance and looked quite good – but there was no compelling theoretical support for the state, no additional evidence in orthogonal samples, and the significance did not pass the threshold for discovery → archived.



In 1998 CDF observed 13 "superjet" events in the W+2,3-jet sample; a 3σ excess from background expectations (4+-1 events) but weird kinematics

Checking a "complete set" of kinematical variables yielded a significance in the 6σ ballpark

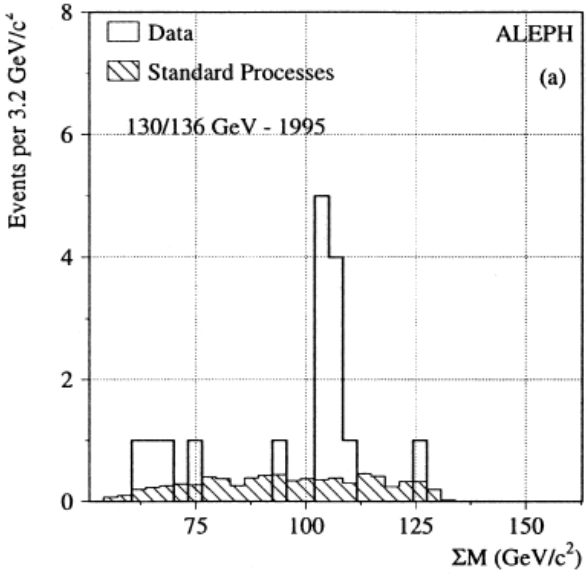
The analysis was published [12]only after a fierce, three-year-long fight within the collaboration; no similar events appeared in the x100 statistics of Run II.



Discoveries that petered out - 3

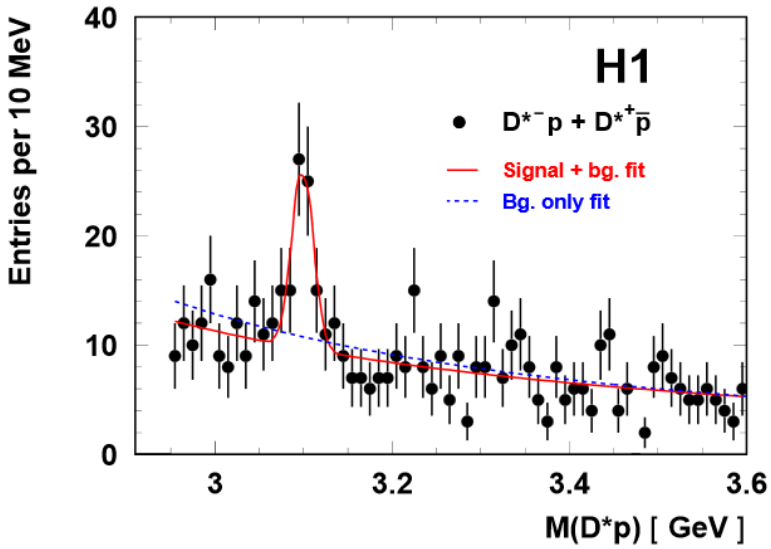
1996 was a prolific year for particle ghosts in the 100-110 GeV region. ALEPH also observed a 4σ-ish excess of Higgs-like events at 105 GeV in the 4-jet final state of electron-positron collisions at 130-136 GeV. They published the search[13], which found 9 events in a narrow mass region with a background of 0.7, estimating the effect at the 0.01% level

- the paper reports a large number of different statistical tests based on the event numbers and their characteristics. Of course a sort of LEE is at work also when one makes many different tests...



In 2004 H1 published a pentaquark signal at 6 sigma significance[14]. The prominent peak at 3.1 GeV was indeed suggestive, however it was not confirmed by later searches.

In the paper they write that "From the change in maximum log-likelihood when the full distribution is fitted under the null and signal hypotheses, corresponding to the two curves shown in figure 7, the statistical significance is estimated to **be p=6.2σ**"



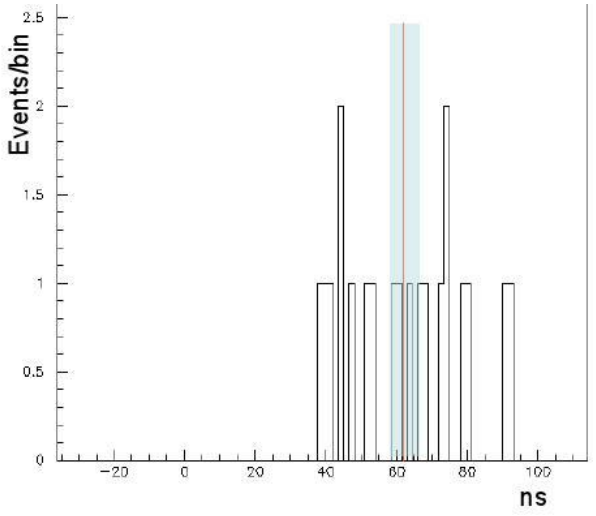
Note: H1 worded it "Evidence" in the title !! A wise departure from blind application of the 5-sigma rule...

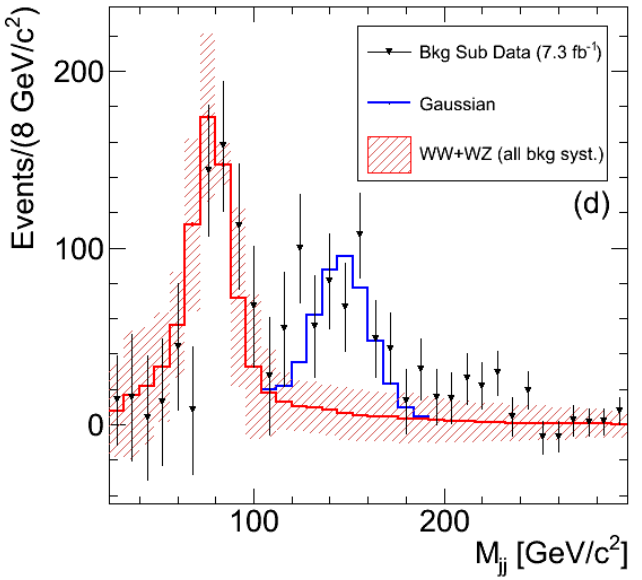
Discoveries that petered out - 4

A mention has also to be made of two more recent, striking examples:

- In 2011 the OPERA collaboration produced a measurement of neutrino travel times from CERN to Gran Sasso which appeared smaller by 6σ than the travel time of light in vacuum[15]. The effect spurred lively debates, media coverage, checks by the ICARUS experiment and dedicated beam runs. It was finally understood to be due to a large source of systematic uncertainty – a loose cable[16]

- Also in 2011 the CDF collaboration showed a large, 4σ signal at 145 GeV in the dijet mass distribution of proton-antiproton collision events producing an associated leptonic W boson decay[17]. The effect grew with data size and was systematical in nature; indeed it was later understood to be due to the combination of two nasty background contaminations[18].





An almost serious table

Given the above information, an intriguing pattern emerges...

Claim	Claimed Significance				Verified or Spurious
Top quark evidence	3				True
Top quark observation			5		True
CDF bbγ signal		4			False
CDF eeggMEt event				6	False
CDF superjets				6	False
Bs oscillations			5		True
Single top observation			5		True
HERA pentaquark				6	False
ALEPH 4-jets		4			False
LHC Higgs evidence	3				True
LHC Higgs observation			5		True
OPERA v>c neutrinos				6	False
CDF Wjj bump		4			False

A look into the Look-Elsewhere Effect

- From the discussion above, we learned that a compelling reason for enforcing a small test size as a prerequisite for discovery claims is the presence of large trials factors, aka LEE

- LEE was a concern 50 years ago, but nowadays we have enormously more CPU power. Nevertheless, the complexity of our analyses has also grown considerably
  - Take the Higgs discovery: CMS combined dozens of final states with hundreds of nuisance parameters, partly correlated, partly constrained by external datasets, often non-Normal.

    → we still sometimes cannot compute the trials factor satisfactorily by brute force!
  - A further complication is that in reality **the trials factor also depends on the significance of the local fluctuation,** adding dimensionality to the problem.

- A study by E. Gross and O. Vitells[19] demonstrated how it is possible to estimate the trials factor in most experimental situations

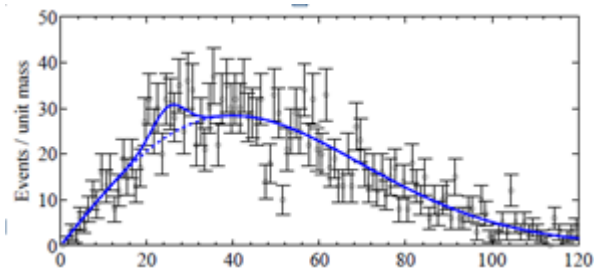
Trials factors

In statistics literature the situation in which one speaks of a trials factor is one of a hypothesis test when a nuisance parameter is present only under the alternative hypothesis. The regularity conditions under which Wilks' theorem applies are then not satisfied.

Let us consider a particle search when the mass is unknown. The null hypothesis is that the data follow the background-only model **b(m)**, and the alternative hypothesis is that they follow the model **b(m)+ μs(m|M)**, with **μ** a signal strength parameter and **M** the particle's true mass, which here acts as a nuisance only present in the alternative. μ=0 corresponds to the null, μ>0 to the alternative.

One then defines a test statistic encompassing all possible particle mass values,

$$q_0(\hat{m}_H) = \max_{m_H} q_0(m_H)$$



This is the maximum of the test statistic defined above for the bgr-only, across the many tests performed at the various possible masses being sought. The problem consists in assigning a p-value to the maximum of q(m) in the entire search range.

One can use an asymptotic "regularity" of the distribution of the above q to get a global p-value by using the technique of Gross and Vitells.

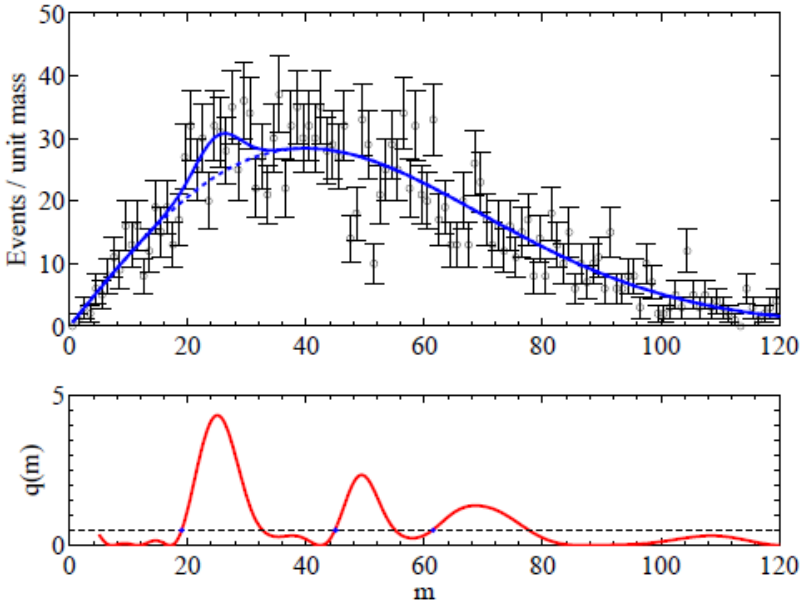
Local minima and upcrossings

One counts the number of "upcrossings" of the distribution of the test statistic, as a function of mass. Its wiggling tells how many independent places one has been searching in.

The number of local minima in the fit to a distribution is closely connected to the freedom of the fit to pick signal-like fluctuations in the investigated range

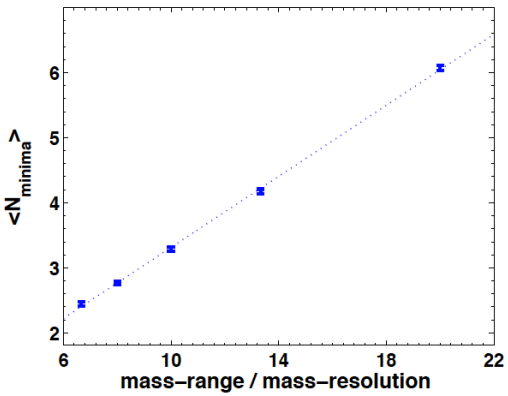
The number of times that the test statistic (below, the likelihood ratio between H_1 and H_0) crosses some reference line can be used to estimate the trials factor. One estimates the global p-value with the number N_0 of upcrossings from a minimal value of the q_0 test statistic (for which $p=p_0$) by the formula

$$p_b^{global} = P(q_0(\hat{m}_H) > u) \leq \langle N_u \rangle + \frac{1}{2} P_{\chi_1^2}(u)$$



The number of upcrossings can be best estimated using the data themselves at a low value of significance, as it has been shown that the dependence on Z is a simple negative exponential:

$$\langle N_u \rangle = \langle N_{u_o} \rangle e^{-(u-u_o)/2}$$



Notes about the LEE estimation

Even if we can usually compute the trials factor by brute force or estimate with asymptotic approximations, there is a degree of uncertainty in how to define it

If I look at a mass histogram and I do not know where I try to fit a bump, I may consider:

1. the location parameter and its freedom to be anywhere in the spectrum
2. the width of the peak
3. the fact that I may have tried different selections before settling on the one I actually end up presenting
4. the fact that I may be looking at several possible final states
5. My colleagues in the experiment can be doing similar things with different datasets; should I count that in ?
6. There is ambiguity on the LEE depending who you are (grad student, exp spokesperson, lab director...)

Also note that Rosenfeld considered the whole world's database of bubble chamber images in deriving a trials factor)

The bottomline is that while we can always compute a local significance, it may not always be clear what the true global significance is.

Systematic uncertainties

- Systematic uncertainties affect any physical measurement and it is sometimes quite hard to correctly assess their impact.

  Often one sizes up the typical range of variation of an observable due to the imprecise knowledge of a nuisance parameter at the 1-sigma level; then one stops there and assumes that the probability density function of the nuisance be Gaussian.

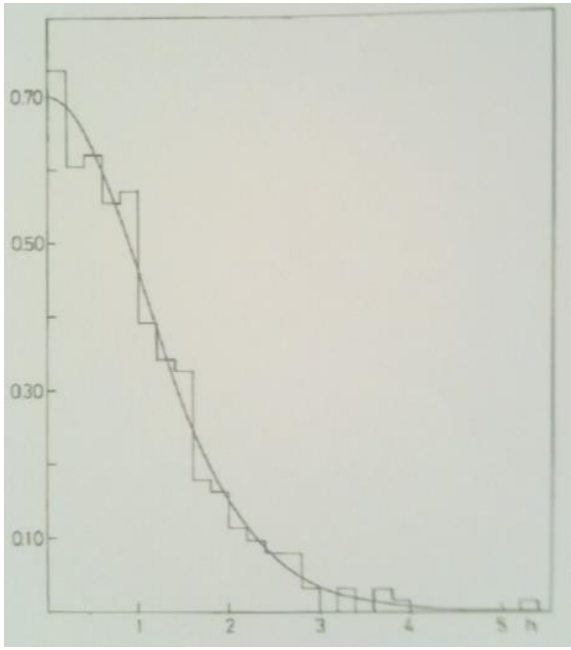
  → if however the PDF has larger tails, it makes the odd large bias much more frequent than estimated

- Indeed, the potential harm of large non-Gaussian tails of systematic effects is one arguable reason for sticking to a 5σ significance level even when we can somehow cope with the LEE. However, the "coverage" that the criterion provides to mistaken systematics is not always sufficient.

- One quick example: if a 5σ effect has uncertainty dominated by systematics, and the latter is underestimated by a factor of 2, the 5σ effect is actually a 2.5σ one (a p=0.006 effect): in p-value terms this means that the size of the effect is overestimated by a factor 20,000!

A study of residuals

The distribution of residuals of 306 measurements in [20]



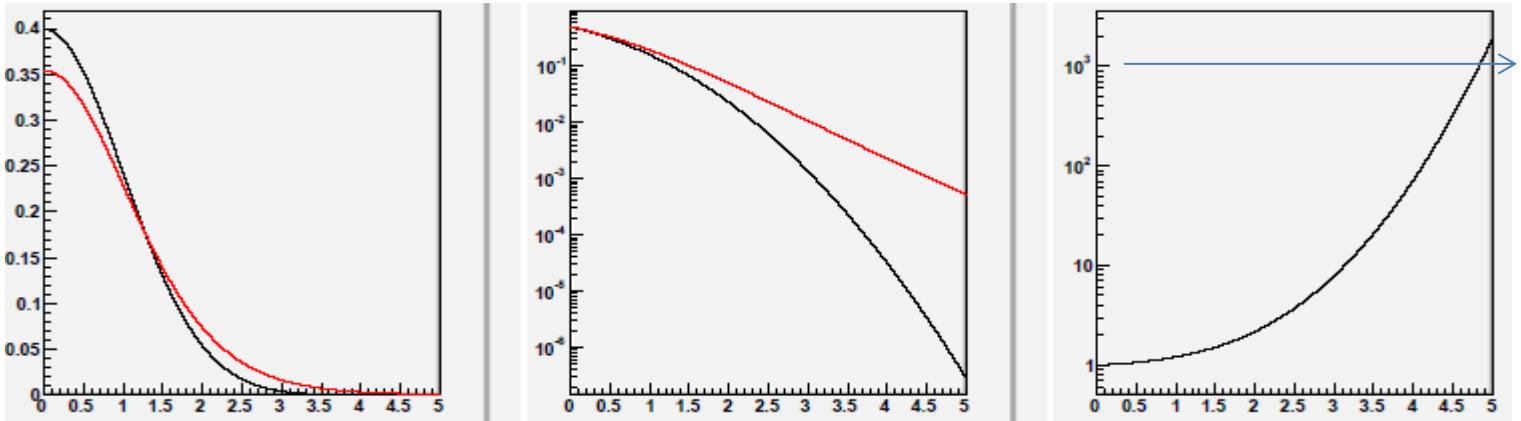
A study of the residuals of particle properties in the RPP in 1975 revealed that they were **not Gaussian in fact**. Matts Roos et al. [20] considered residuals in kaon and hyperon mean life and mass measurements, and concluded that these seem to all have a similar shape, well described by a Student distribution $S_{10}(h/1.11)$:

$$S_{10}\left(\frac{x}{1.11}\right)=\frac{315}{256\sqrt{10}}\left(1+\frac{x^2}{12.1}\right)^{-5.5}$$

Of course, one cannot extrapolate to 5-sigma the behaviour observed by Roos and collaborators in the bulk of the distribution; however, one may consider this as evidence that the uncertainties evaluated in experimental HEP may have a significant non-Gaussian component

Black: a unit Gaussian;
red: the $S_{10}(x/1.11)$ function

Left: 1-integral distributions of the two functions.
Right: ratio of the 1-integral values as a function of z



x1000!

The "subconscious Bayes factor"

Louis Lyons [21] calls this way the ratio of prior probabilities we subconsciously assign to the two hypotheses

When comparing a "background-only" H_0 hypothesis with a "background+signal" one H_1 one often uses the likelihood ratio $\lambda=L_1/L_0$ as a test statistic

- The $p<0.000027\%$ criterion is applied to the distribution of λ under H_0 to claim a discovery

However, what would be more relevant to the claim would be the ratio of the probabilities:

$$\frac{P(H_1 \mid data)}{P(H_0 \mid data)} = \frac{p(data \mid H_1)}{p(data \mid H_0)} \times \frac{\pi_1}{\pi_0} = \lambda \frac{\pi_1}{\pi_0}$$

where p(data|H) are the likelihoods, and π are the priors of the hypotheses

In that case, if our prior belief in the alternative, π_1, were low, we would still favor the null even with a large evidence λ against it.

- The above is a Bayesian application of Bayes' theorem, while HEP physicists prefer to remain in Frequentist territory. Lyons however notes that "*this type of reasoning does and should play a role in requiring a high standard of evidence before we reject well-established theories: there is sense to the oft-quoted maxim 'extraordinary claims require extraordinary evidence' "*.

A diversion: the "point null" and the Jeffreys-Lindley paradox

All what we have discussed so far makes sense strictly in the context of classical (aka Frequentist) statistics. One might well ask what is the Bayesian view of the problem

The issue revolves around the existence of a null hypothesis, H_0, on which we base a strong belief. It is quite special to physics that **we do believe in our "point null"** – a theory which works for a specific value of a parameter, known with arbitrary accuracy; in other sciences a true "point null" hardly exists

The fact that we must often compare a null hypothesis (for which a parameter has a very specific value) to an alternative (which has a continuous support for the parameter under test) bears on the definition of a prior belief for the parameter. Bayesians speak of a "probability mass" at $\theta=\theta_0$.

The use of probability masses in priors in a simple-vs-composite test throws a monkey wrench in the Bayesian calculation, as it can be proven that no matter how large and precise is the data, Bayesian inference **strongly depends** on the scale over which the prior is non-null – that is, on the **prior belief** of the experimenter.

The Jeffreys-Lindley paradox [22] may bring Frequentists and Bayesians to draw **opposite conclusions** on some data when comparing a point null to a composite alternative. This fact bears relevance to the kind of tests we are discussing, so let us give it a look.

The paradox

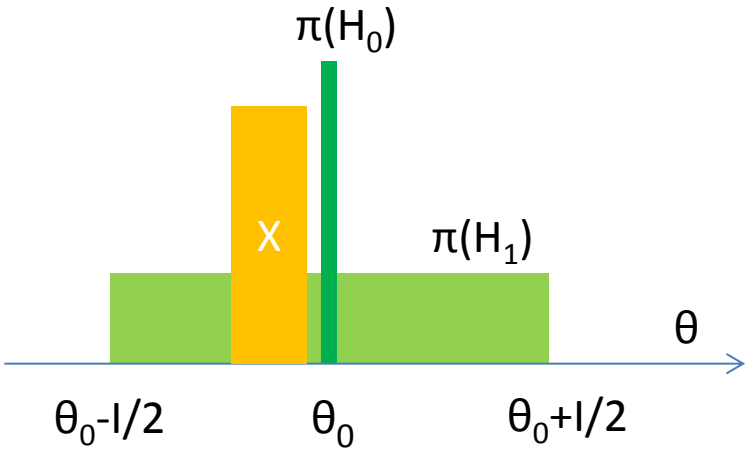
Take $X_1...X_n$ i.i.d. as $X_i|\theta \sim N(\theta,\sigma^2)$, and a prior belief on θ constituted by a mixture of a point mass p at θ_0 and (1-p) uniformly distributed in $[\theta_0-I/2,\theta_0+I/2]$.

In classical hypothesis testing the "critical values" of the sample mean delimiting the rejection region of $H_0:\theta=\theta_0$ in favor of $H_1:\theta<>\theta_0$ at significance level α are

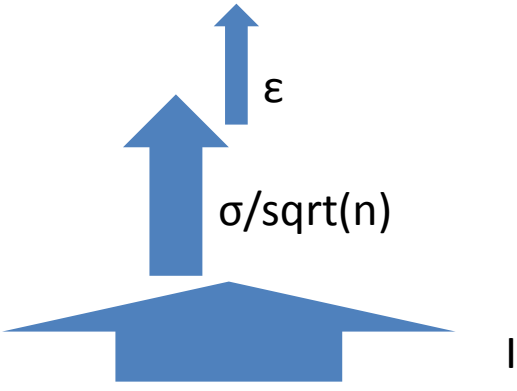
$$\bar{X} = \theta_0 \pm (\sigma/\sqrt{n})z_{\alpha/2}$$

where $z_{\alpha/2}$ is the significance corresponding to test size α for a two-tailed normal distribution

Given the above, it can be proven that the **posterior probability that H_0 is true** conditional on the data in the critical region (i.e. excluded by a classical α-sized test) **approaches 1 as the sample size becomes arbitrarily large**.



As evidenced by Bob Cousins[23], the paradox arises if there are <u>three different scales in the problem</u>, **ε << σ/sqrt(n) << I**, i.e. the width of the point mass, the measurement uncertainty, and the scale **I** of the prior for the alternative hypothesis



The three scales are usually independent in HEP!!

Proof (in case you need it...)

$$P\quad (H_0|\bar{X}=\bar{x}=\theta_0+(\sigma/\sqrt{n})z_{\alpha/2})\quad =\quad \frac{P(H_0)P(data|H_0)}{P(H_0)P(data|H_0))+P(H_A)P(data|H_A)}$$

$$=\quad \frac{p\ \frac{\sqrt{n}}{\sqrt{2\pi}\sigma}\ e^{\{(-1/2)[(\sqrt{n}/\sigma)(\bar{x}-\theta_0)]^2\}}}{p\ \frac{\sqrt{n}}{\sqrt{2\pi}\sigma}\ e^{\{(-1/2)[(\sqrt{n}/\sigma)(\bar{x}-\theta_0)]^2\}}+(1-p)\int_{\theta_0-I/2}^{\theta_0+I/2}\frac{\sqrt{n}}{\sqrt{2\pi}\sigma}\ e^{\{(-1/2)[(\sqrt{n}/\sigma)(\bar{x}-\theta)]^2\}}\ \frac{1}{I}\ d\theta}$$

$$=\quad \frac{p\ e^{\{-(1/2)z_{\alpha/2}^2\}}}{p\ e^{\{-(1/2)z_{\alpha/2}^2\}}+\frac{(1-p)}{I}\int_{\theta_0-I/2}^{\theta_0+I/2}e^{\{(-1/2)[(\sqrt{n}/\sigma)(\theta-\bar{x})]^2\}}d\theta}$$

$$\geq\quad \frac{p\ e^{\{-(1/2)z_{\alpha/2}^2\}}}{p\ e^{\{-(1/2)z_{\alpha/2}^2\}}+\frac{(1-p)}{I}\frac{\sqrt{2\pi}\sigma}{\sqrt{n}}}\quad \rightarrow\quad 1\quad as\quad n\quad \rightarrow\quad \infty$$

In the first line the posterior probability is written in terms of Bayes' theorem;
in the second line we insert the actual priors p and (1-p) and the likelihood values in terms of the stated Normal density of the iid data X;
in the third line we rewrite two of the exponentials using the conditional value of the sample mean in terms of the corresponding significance z, and remove the normalization factors sqrt(n)/sqrt(2π)σ;
in the fourth line we maximize the expression by using the integral of the Normal.

Notes on the JL paradox

- The paradox is often used by Bayesians to criticize the way inference is drawn by frequentists:
  - Jeffreys: "***What the use of [the p-value] implies, therefore, is that a hypothesis that may be true may be rejected because it has not predicted observable results that have not occurred***" [24]
  - Alternatively, the criticism concerns the fact that no mathematical link between p and P(H|x) exists in classical HT.
- On the other hand, the problem with the Bayesian approach is that there is no clear substitute to the Frequentist p-value for reporting experimental results
  - Bayesians prefer to cast the HT problem as a Decision Theory one, where by specifying the loss function allow a quantitative and well-specified (although subjective) recipe to choose between alternatives
  - Bayes factors, which describe by how much prior odds are modified by the data, are not factorizing out the subjectivity of the prior belief when the JLP holds: even asymptotically, **they retain a dependence on the scale of the prior of H_1.**
- In their debates on the JL paradox, Bayesian statisticians have blamed the concept of a "point mass", as well as suggested n-dependent priors. There is a large body of literature on the subject
  - As assigning to it a non-zero prior is the source of the problem, statisticians tend to argue that "the precise null" is never true. However, we do believe our point nulls in HEP and astro-HEP!!
- **The JL paradox draws attention to the fact that a fixed level of significance does not cope with a situation where the amount of data increases, which is common in HEP.**

In summary, the issue is an active research topic and is not resolved. I have brought it up here to show how the trouble of defining a test size α in classical hypothesis testing is not automatically solved by moving to Bayesian territory.

So what to do with 5σ ?

To summarize the points made above:

- the LEE can be estimated analytically as well as computationally; experiments in fact now often produce "global" and "local" p-values and Z-values
  - What is then the point of protecting from large LEE ?
- In any case sometimes the trials factor is 1 and sometimes it is enormous; a one-size-fits-all is then hardly justified – it is illogical to penalize an experiment for the LEE of others
- the impact of systematic uncertainties varies widely from case to case; e.g. sometimes one has control samples (e.g. particle searches), sometimes one does not (e.g. OPERA)
- The cost of a wrong claim, as image damage or backfiring of media hype, can vary dramatically
- Some claims are intrinsically less likely to be true –eg. we have a subconscious Bayes factor at work. It depends if you are discovering an unimportant new meson or a violation of physical laws

So why a fixed discovery threshold ?

- One may take the attitude that any claim is anyway subject to criticism and independent verification anyway, and the latter is always more rigorous when the claim is steeper and/or more important; and it is good to just have a "reference value" for the level of significance of the data
- It is often held that it is a "tradition" and a useful standard.

Lyons' Table

My longtime CDF and CMS colleague Louis Lyons considered several known searches in HEP and astro-HEP, and produced a table where for each effect he listed several "inputs":

1. the degree of surprise of the potential discovery
2. the impact for the progress of science
3. the size of the trials factor at work in the search
4. the potential impact of unknown or ill-quantifiable systematics

He could then derive a "reasonable" significance level that would account for the different factors at work, for each considered physics effect [21]

- The approach is of course only meant to provoke a discussion, and the numbers in the table entirely debatable. The message is however clear: we should beware of a "one-size-fits-all" standard.

I have slightly modified his original table to reflect my personal bias

Table of searches for new phenomena and "reasonable" significance levels

Search	Surprise level	Impact	LEE	Systematics	Z-level
Neutrino osc.	Medium	High	Medium	Low	4
Bs oscillations	Low	Medium	Medium	Low	4
Single top	Absent	Low	Absent	Low	3
$B_s \rightarrow \mu\mu$	Absent	Medium	Absent	Medium	3
Higgs search	Medium	Very high	Medium	Medium	5
SUSY searches	High	Very high	Very high	Medium	7
Pentaquark	High	High	High	Medium	7
G-2 anomaly	High	High	Absent	High	5
H spin >0	High	High	Absent	Low	4
4th gen fermions	High	High	High	Low	6
V>c neutrinos	Huge	Huge	Absent	Very high	THTQ
Direct DM search	Medium	High	Medium	High	5
Dark energy	High	Very high	Medium	High	6
Tensor modes	Medium	High	Medium	High	5
Grav. waves	Low	High	Huge	High	7

THTQ: one last note about very high Nσ

Recently heard claim from respected astrophysicist "**The quantity has been measured to be non-zero at 40σ level**", referring to a measurement quoted as 0.110+-0.0027.

That is a silly statement! As N goes above 7 or so, we are rapidly losing contact with the reality of experimental situations

To claim e.g. a 5σ effect, one has to be reasonably sure to know the p-value **PDF to the 10^{-7} level**

Remember, Nσ is just as femtobarns or or attometers: a useful placeholder for small numbers

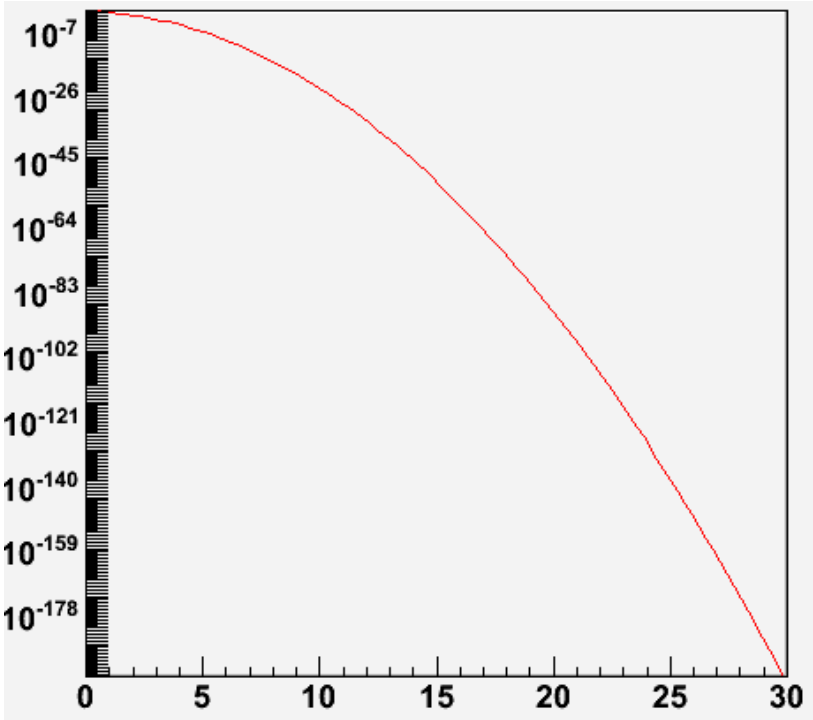
- Hence before quoting high Nσ blindly, think at what they really mean

In the case of the astrophysicist, it is not even easy to directly make the conversion, as ErfInverse() breaks down above 7.5 or so. We resort to a good approximation by Karagiannidis and Lioumpas [25],

$$Q(x) \approx \frac{\left(1 - e^{-1.4x}\right) e^{-\frac{x^2}{2}}}{1.135\sqrt{2\pi}x}, x > 0$$

For N=40 my computer still refuses to give anything above 0, but for N=38 it gives p=2.5*10^{-316}

- so he was basically saying that the data had a probability of less than a part in 10^316 of being observed if the null hypothesis held.
- That is beyond ridiculous ! We will never be able to know the tails of our systematic uncertainties to something similar.



Conclusions

- 45 years after the first suggestion of a 5-sigma threshold for discovery claims, and 20 years after the start of its consistent application, the criterion appears inadequate
  - It did not protect from steep claims that later petered out
  - It significantly delayed acceptance of some relatively uncontroversial finds
    - single top is a prime example: DZERO and CDF kept battling to be first to 5σ for 8 years of Run 2, when in fact they could have used their thinning forces better in other directions
  - It is arbitrary and illogical in many aspects

- Bayesian hypothesis testing does not appear ready to offer a robust replacement
  - JL paradox still active area of debate, no consensual view
- A single number never summarizes the situation of a measurement
  - experiments have started to publish their likelihoods, so combinations and interpretation get easier
- My suggestion is that for each considered search the community should seek a consensus on what could be an acceptable significance level for a media-hitting claim
- For searches of unknown effects and fishing expeditions, the **global** p-value is the only real weapon – but in most cases the trials factor is hard to quantify
- Probably 5-sigma are insufficient for unpredicted effects, as large experiments look at thousands of distributions, multiple times, and the experiment-wide trials factor is extremely high
  - One example: CDF lasted 25 years and got one 6-sigma effect (superjet events), plus one unexplainable event. These are roughly on par with the rate at which one would expect similar things to occur

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Backup slides

Nuts and Bolts of Higgs Combination

The recipe must be explained in steps. The first one is of course the one of writing down extensively the likelihood function!

1) One writes a global likelihood function, whose parameter of interest is the strength modifier μ. If s and b denote signal and background, and θ is a vector of systematic uncertainties, one can generically write for a single channel:

$$\mathcal{L}(\text{data}\,|\,\mu,\theta) = \text{Poisson}\,(\,\text{data}\,|\,\mu\cdot s(\theta)+b(\theta)\,)\cdot p(\tilde{\theta}|\theta)$$

Note that θ has a "prior" coming from a hypothetical auxiliary measurement.
In the LHC combination of Higgs searches, nuisances are treated in a frequentist way by taking for them the likelihood which would have produced as posterior, given a flat prior, the PDF one believes the nuisance is distributed from. This differs from the Tevatron and LEP Higgs searches.

In L one may combine many different search channels where a counting experiment is performed as the product of their Poisson factors:

$$\prod_i \frac{(\mu s_i + b_i)^{n_i}}{n_i!}\; e^{-\mu s_i - b_i}$$

or from a unbinned likelihood over k events, factors such as:

$$k^{-1}\prod_i (\mu S f_s(x_i) + B f_b(x_i))\;\cdot\; e^{-(\mu S+B)}$$

2) One then constructs a profile likelihood test statistic q_μ as $\tilde{q}_\mu = -2 \ln \frac{\mathcal{L}(\text{data}|\mu, \hat{\theta}_\mu)}{\mathcal{L}(\text{data}|\hat{\mu}, \hat{\theta})}$

Note that the denominator has L computed with the values of $\mu\hat{}$ and $\theta\hat{}$ that globally maximize it, while the numerator has $\theta=\theta\hat{}_\mu$ computed as the conditional maximum likelihood estimate, given μ.

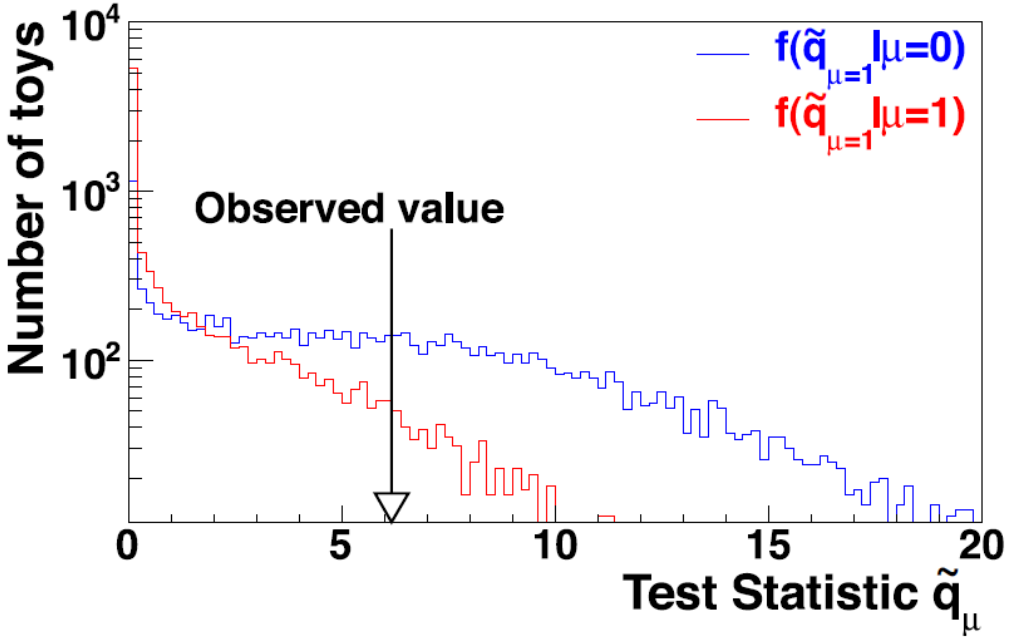
A constraint is posed on the MLE $\mu\hat{}$ to be confined in $0<=\mu\hat{}<=\mu$: this avoids negative solutions for the cross section, and ensures that best-fit values *above* the signal hypothesis μ are not counted as evidence against it.

The above definition of a test statistic for CL_s in Higgs analyses differs from earlier instantiations

- LEP: no profiling of nuisances
- Tevatron: $\mu=0$ in L at denominator

3) ML values $\theta_\mu\hat{}$ for H_1 and $\theta_0\hat{}$ for H_0 are then computed, given the data and $\mu=0$ (bgr-only) and $\mu>0$

4) Pseudo-data is then generated for the two hypotheses, using the above ML estimates of the nuisance parameters. With the data, one constructs the pdf of the test statistic given a signal of strength μ (H_1) and $\mu=0$ (H_0). This way has good coverage properties.



5) With the pseudo-data one can then compute the integrals defining p-values for the two hypotheses. For the signal plus background hypothesis H_1 one has

$$p_\mu = P(\tilde{q}_\mu \geq \tilde{q}_\mu^{obs} \,|\, \text{signal+background}) = \int_{\tilde{q}_\mu^{\text{obs}}}^{\infty} f(\tilde{q}_\mu|\mu, \hat{\theta}_\mu^{\text{obs}})\, d\tilde{q}_\mu$$

and for the null, background-only H_0 one has

$$1 - p_b = P(\tilde{q}_\mu \geq \tilde{q}_\mu^{obs} \,|\, \text{background-only}) = \int_{q_0^{\text{obs}}}^{\infty} f(\tilde{q}_\mu|0, \hat{\theta}_0^{\text{obs}})\, d\tilde{q}_\mu$$

6) Finally one can compute the value called CL_s as

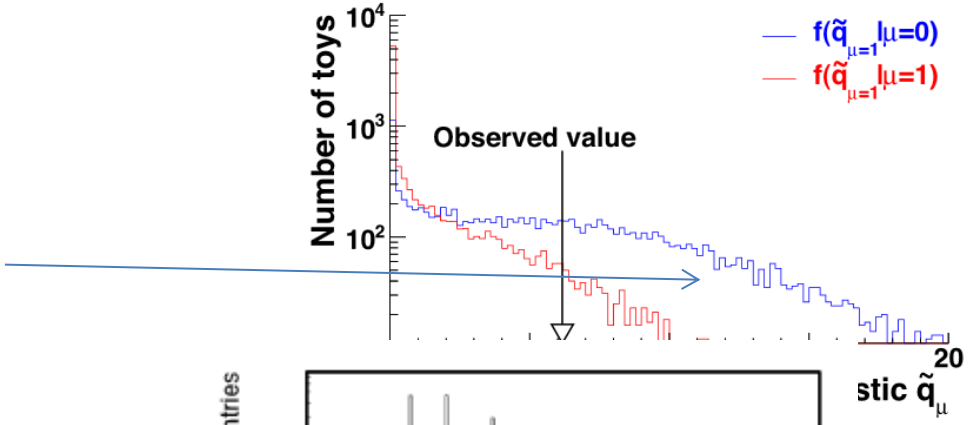
$$CL_s = p_\mu/(1-p_b)$$

CL_s is thus a "modified" p-value, in the sense that it describes how likely it is that the value of test statistic is observed under the alternative hypothesis by also accounting for how likely the null is: the drawing incorrect inferences based on extreme values of p_μ is "damped", and cases when one has no real discriminating power, approaching the limit $f(q|\mu)=f(q|0)$, are prevented from allowing to exclude the alternate hypothesis.

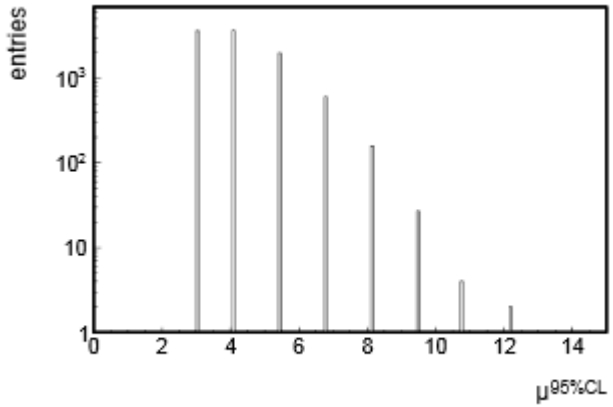
7) We can then **exclude H_1 when $CL_s < \alpha$**, the (defined in advance !) *size* of the test. In the case of Higgs searches, all mass hypotheses $H_1(M)$ for which $CL_s<0.05$ are said to be excluded (one would rather call them "disfavoured"…)

Derivation of expected limits

One starts with the **background-only hypothesis μ=0**, and determines a distribution of possible outcomes of the experiment with toys, obtaining the CLs test statistic distribution for each investigated Higgs mass point

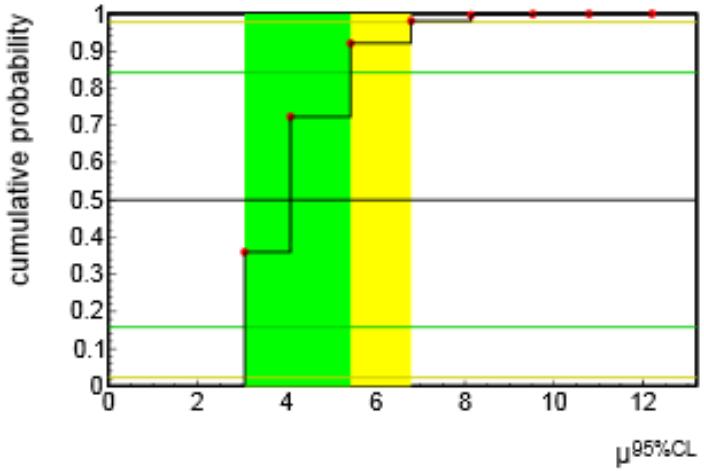


From CLs one obtains the PDF of upper limits μ^{UL} on μor each M_h. [*E.g. on the right we assumed b=1 and s=0 for μ=0, whereas μ=1 would produce <s>=1*]



Then one computes the cumulative PDF of μ^{UL}

Finally, one can derive the median and the intervals for μ which correspond to 2.3%, 15.9%, 50%, 84.1%, 97.7% quantiles. These define the “expected-limit bands” and their center.



Significance in the Higgs search

- To test for the significance of an excess of events, given a M_h hypothesis, one uses the bgr-only hypothesis and constructs a modified version of the q test statistic:

$$q_0 = -2\ln\frac{\mathcal{L}(\text{data}|0,\hat{\theta}_0)}{\mathcal{L}(\text{data}|\hat{\mu},\hat{\theta})} \quad \text{and } \hat{\mu} \geq 0.$$

- This time we are testing any $\mu>0$ versus the H_0 hypothesis. One builds the distribution $f(q_0|0,\hat{\theta}_0^{obs})$ by generating pseudo-data, and derives a p-value corresponding to a given observation as

$$p_0 = P(q_0 \geq q_0^{obs}) = \int_{q_0^{obs}}^{\infty} f(q_0|0,\hat{\theta}_0^{\text{obs}})\, dq_0.$$

One then converts p into Z using the relation

$$p = \int_Z^{\infty} \frac{1}{\sqrt{2\pi}} \exp(-x^2/2)\, dx = \frac{1}{2} P_{\chi_1^2}(Z^2)$$

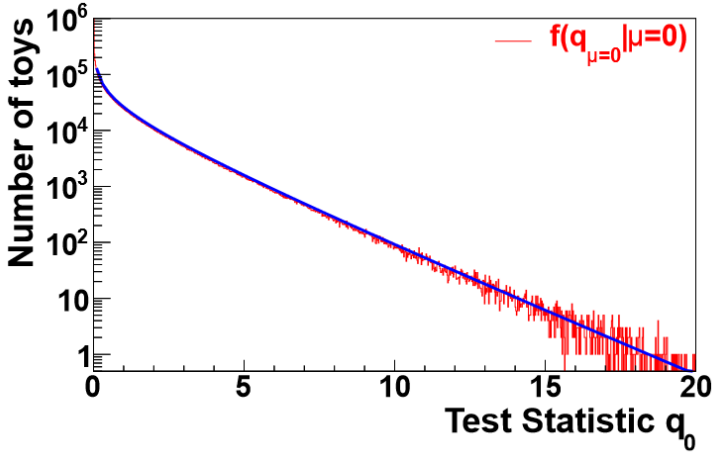
where p_χ^2 is the survival function for the 1-dof chi2.

Often it is impractical to generate large datasets given the complexity of the search (dozens of search channels and sub-channels, correlated among each other). One then relies on a very good asymptotic approximation:

$$p^{estimate} = \frac{1}{2}\left[1 - \text{erf}\left(\sqrt{q_0^{\text{obs}}/2}\right)\right]$$

The derived p-value and the corresponding Z value are "local": they correspond to the specific hypothesis that has been tested (a specific M_h) as q_0 also depends on M_h (the search changes as M_h varies)

When dealing with many searches, one needs to get a global p-value and significance, i.e. **evaluate a trials factor.**



JLP example: Charge bias of a tracker

- Imagine you want to investigate whether your tracker has a bias in reconstructing positive versus negative curvature. Say we work with a zero-charge initial state at a lepton collider (e^+e^-). You take a unbiased set of collisions, and count how many positive and negative curvature tracks you have reconstructed in a set of n=1,000,000 events.
- You get n^+=498,800, n^-=501,200. You want to test the hypothesis that R=0.5 with a size **α=0.05**.
- Bayesians will **need a prior** to make a statistical inference: their typical choice would be to **assign equal probability** to the chance that R=0.5 and to it being different (R<>0.5): a "*point mass*" of p=1/2 at R=0.5, and a uniform distribution of the remaining p=1/2 in [0,1]
- We are in high-statistics regime and away from 0 or 1, so Gaussian approximation holds for the Binomial. The probability to observe a number of positive tracks n^+ can then be written, with $x=n^+/n$, as $N(x,\sigma)$ with $\sigma^2=x(1-x)/n$.

  The posterior probability that R=0.5 is then

$$P(R=\frac{1}{2}\,|\,x,n) \approx \frac{\frac{1}{2}\frac{e^{-\frac{(x-\frac{1}{2})^2}{2\sigma^2}}}{\sqrt{2\pi}\sigma}}{\left[\frac{1}{2}\frac{e^{-\frac{(x-\frac{1}{2})^2}{2\sigma^2}}}{\sqrt{2\pi}\sigma}+\frac{1}{2}\int_0^1 \frac{e^{-\frac{(x-R)^2}{2\sigma^2}}}{\sqrt{2\pi}\sigma}dR\right]} = 0.9781\epsilon$$

from which a Bayesian concludes that there is **no evidence against R=0.5,** and actually the data strongly supports the null hypothesis (P>1-α)

JLP charge bias: frequentist solution

- Frequentists will not need a prior, and just ask themselves how often a result "at least as extreme" as the one observed arises by chance, if the underlying distribution is N(R,σ) with R=1/2 and σ^2=x(1-x)/n as before.
- One then has

$$P(x \leq 0.4988 | R = \frac{1}{2}) = \int_0^{0.4988} \frac{e^{-\frac{(t-\frac{1}{2})^2}{2\sigma^2}}}{\sqrt{2\pi}\sigma} dt = 0.00819$$

$$\Rightarrow P'(x | R = \frac{1}{2}) = 2 * P = 0.01639$$

(we multiply by two since we would be just as surprised to observe an excess of positives as a deficit).

From this, frequentists conclude that the tracker is biased, since there is a less-than 5% probability, P'<α, that a result as the one observed could arise by chance!

A frequentist thus draws the **opposite conclusion** that a Bayesian draws from the same data .