# **Introduction to statistics**

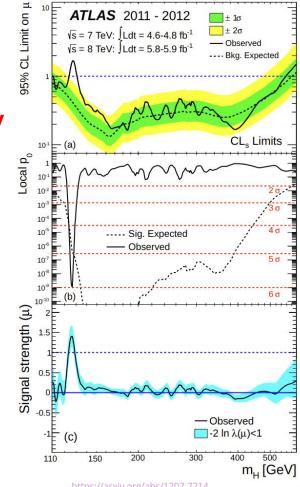
Tomas Dado (CERN)

HASCO, Goettingen, 2024

### Introduction

- Focusing on HEP statistics approaches
- Quantum mechanics/field theory = statistical theory
  - Needed for every interpretation
- Here we will go through
  - Basics of statistics
  - Hypotheses testing
  - Discovery and limit setting
  - Parameter estimation
  - <u>Unfolding</u>

• Should be able to understand these plots at the end of this presentation



#### **Useful references**

- G. Cowan, *Statistical Data Analysis*, Oxford University Press, 1998
  - Related: Cowan's Academic lectures: <u>indico link</u>
- F. James, *Statistical methods in experimental physics*, 2nd ed., World Scientific, 2006
- K. Cranmer, *Practical Statistics for the LHC*, <u>https://arxiv.org/abs/1503.07622</u>
- Cowan et al, *Asymptotic formulae for likelihood-based tests of new physics*, <u>https://arxiv.org/abs/1007.1727</u>

• Commonly used model for the binned likelihood fit in HEP: *HistFactory: A tool for creating statistical models for use with RooFit and RooStats*, <u>https://cds.cern.ch/record/1456844</u>

#### **Basics**

### **Frequentist statistics**

• Probability = outcomes of repeatable observations

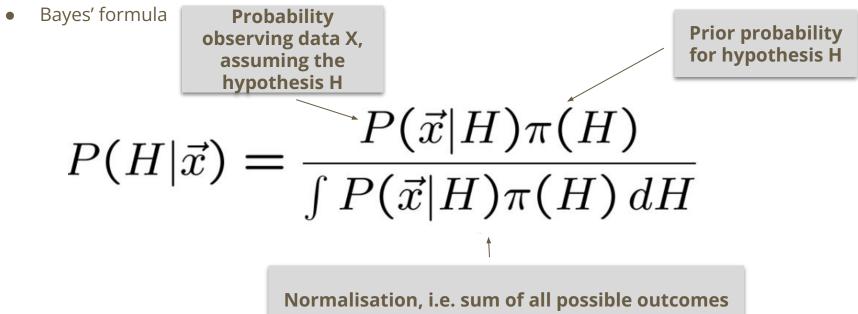
$$P(x) = \lim_{n \to \infty} \frac{\text{number of outcomes of } x}{n}$$

- I.e. we need **repeatable events**
- <u>Does Higgs boson exist?</u> Is the mass of the top quark between 172 and 173 GeV? ...?
  - It is **either true or false** but we do not know which
  - The frequentists tools tell us about outcomes of (hypothetical) **repeated experiments**

• The **preferred theories** (models, hypotheses, ...) are those for which our observations would be considered "**usual**"

# **Bayesian statistics**

- Interpretation of probability extended to a degree of belief
  - The degree of belief is updated based on the observations



# **Bayesian statistics example**

- Assume 2% of the population have COVID19 in a given time
- The tests for COVID19 detect the virus in 90% of the cases and give false-positive (show positive result even when there is no COVID19 virus) in 5% of the cases
- The test result is positive, what is the probability that the person has the COVID19 virus?

We can use the Bayes' formula for this

- P(H) = 0.02 this is the prior probability, i.e. before we do the test
- P(x,H) = 0.9 i.e. if the person is positive, what is the likelihood of getting a positive result
- Normalisation = 0.9 x 0.02 + 0.05 x 0.98 i.e. has the virus and positive test + does not have virus and has a positive test
- Using the Bayes' formula:

$$rac{0.9 imes 0.02}{0.9 imes 0.02 + 0.05 imes 0.98} pprox 24\%$$

• How would the probability change if the person would do another test and it came back positive?

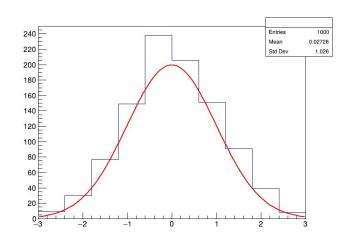
### **Frequentist vs Bayesian**

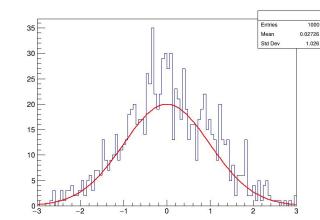
- <u>Frequentist</u>
  - Limit of a long term frequency
  - Do not need an infinite sample for the definition to be useful
  - Sometimes no ensemble exists
- <u>Bayesian</u>
  - Probability is a degree of belief
  - Intrinsically **subjective** (choice of the prior)
    - No golden rule for the choice of priors

 "Bayesians address the question everyone is interested in, by using assumptions no-one believes. Frequentists use impeccable logic to deal with an issue of no interest to anyone" - L. Lyons

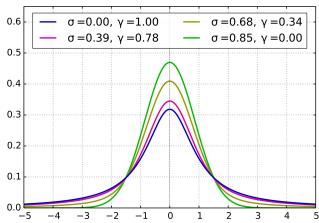
### **Binned vs unbinned - distributions**

- <u>Unbinned distributions</u>
  - Requires smooth distributions i.e. PDF
    - Often not known
    - Can use approximations
- **Binned distributions** 
  - Approximate distributions
  - Binning choice **resolution vs available statistics**





#### Voigt function Breit-Wigner x Gauss



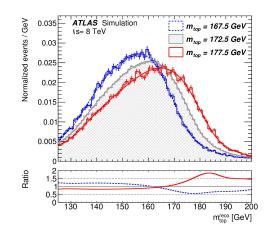
#### Likelihoods

- What we want is probability of our model describing data (frequentist)
- I.e. "likelihood":

 $P(\vec{x}|H)$ 

- Binned-likelihood
  - **Probability per bin** and combine from all bins
    - No correlations ⇔ product of the per-bin likelihoods
  - Often much simpler than unbinned
  - Depends on binning choice (corrections might be needed)
- Unbinned likelihood
  - **Probability per event** and combine for all events
    - No correlations ⇔ product over all events
  - No bin-width effects
  - Requires analytical (or approximate functions)

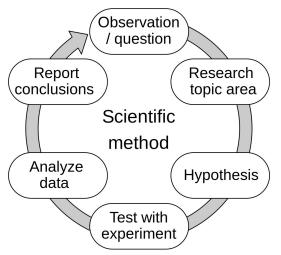
#### Eur. Phys. J. C 79 (2019) 290



# **Hypothesis testing**

# **Definitions**

• Hypothesis testing is a core of the scientific method



- **Hypothesis** *H* specifies the **probability for the data**, i.e., the outcome of the observation, *x*
- Possible values of data (*x*) form the <u>sample space</u> ("data space")
- The **probability for** *x* **given** *H* **is also called the <b>likelihood of the hypothesis, written** *L*(*x*|*H*).
  - E.g. The probability to observe N number of events with a given selection assuming the validity of the Standard Model

# **Hypothesis testing**

How to confirm a hypothesis?

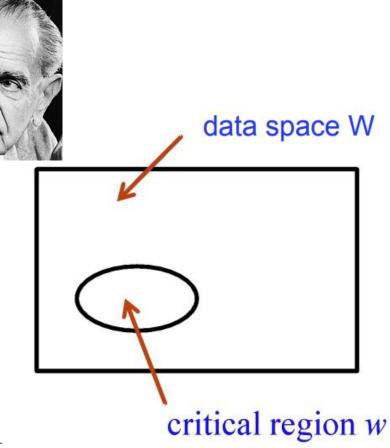
- Karl Popper: You cannot!
- But you can reject a hypothesis!



Find a region, *W*, of the data space where the is only small probability *α* to observe data *x* provided *H*<sub>0</sub> is true - this is the "critical region"

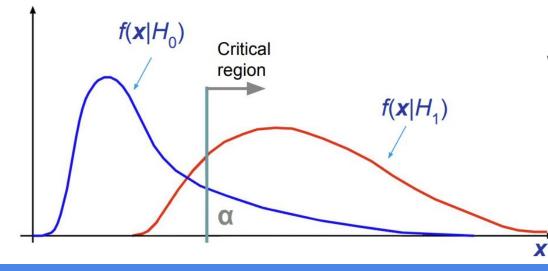
#### $P(x \in w | H_0) \leq \alpha$

- Reject hypothesis if data is observed in *W*
- $\alpha$  is called "size" or "**significance level**" of the test



# How to select the critical region?

- Infinitely many critical regions for a given hypothesis
- No unique way to select it
- Can define an **alternative hypothesis** *H*<sub>1</sub>
- Roughly speaking:
  - Choose the critical region so that the **probability of observing data under**  $H_0$  is low and **probability of observing data under**  $H_1$  is high



Rejecting  $H_0$  does not mean " $H_0$  is wrong and  $H_1$  is right"

- Frequentist only outcome of repeated experiments
- Bayesian depends on the priors

# **Type-I and type-II errors**

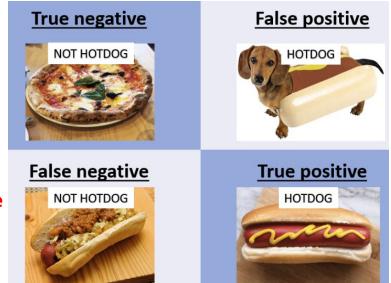
- **<u>Type-I error</u>** (false negative)
  - **Reject hypothesis** *H*<sub>0</sub> **if it is true**
  - Maximum probability for this is  $\alpha$

 $P(x \in W \mid H_0) \leq \alpha$ 

- <u>**Type-II error**</u> (false positive)
  - Accept hypothesis  $H_0$  if it is false and  $H_1$  is true
  - $\circ$  Occurs with probability  $\beta$

 $P(x \in \mathbf{S} - W | H_1) = \beta$ 

• 1 -  $\beta$  is called the "power" of the test



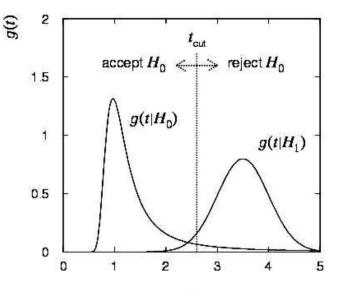
#### **Test statistics**

- Assume that for each event we have a collection of numbers
  - Number of jets, leptons, MET value, ..., have multiple bins, ...
  - Data (*x*) will follow some joint PDF for the different observables
  - The critical region is **multidimensional** cumbersome to work with
- Can define the **boundary** of the critical region using an equation of form

$$t(x_1,\ldots,x_n)=t_{\rm cut}$$

• Where  $t(x_1, ..., x_n)$  is the <u>scalar</u> test statistics

#### We have turned an N-dimensional problem to a 1-dimensional one!



#### **Optimal choice for the test statistics**

- How to choose the test statistics?
- Neyman-Pearson lemma: For a test of size  $\alpha$  of the simple hypothesis  $H_0$ , to obtain the highest power with respect to the simple alternative  $H_1$ , choose the critical region W such that the likelihood ratio satisfies

$$\frac{P(\mathbf{x}|H_1)}{P(\mathbf{x}|H_0)} \ge k$$

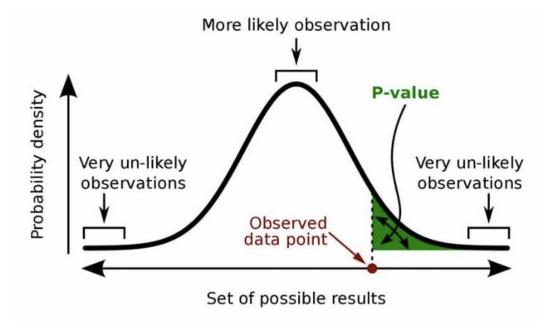
everywhere in W and is less than k else - k is a constant chosen such that the test has size  $\alpha$ 

• The optimal scalar test statistics is then

$$t(\mathbf{x}) = \frac{P(\mathbf{x}|H_1)}{P(\mathbf{x}|H_0)}$$

#### p-value

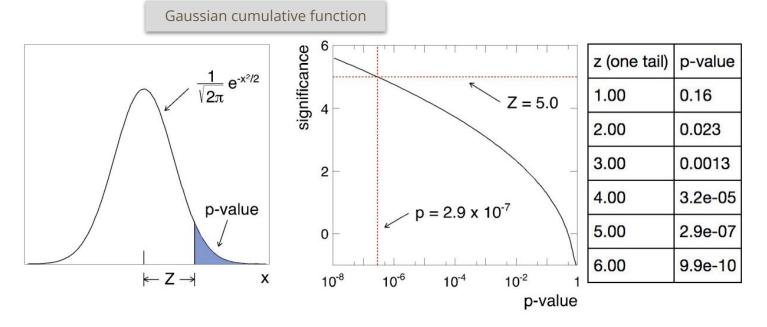
- Level of agreement (compatibility) of data and a given hypothesis (model) H
- p-value -> probability, under assumption of *H*, to observe data with equal or lesser
   compatibility with *H* relative to the data we got
  - This is NOT a probability that *H* is true!



### p-value and significance

• We can define the significance *Z* as the **number of standard deviations** ("sigmas") that a Gaussian variable would fluctuate in one direction to give the same p-value

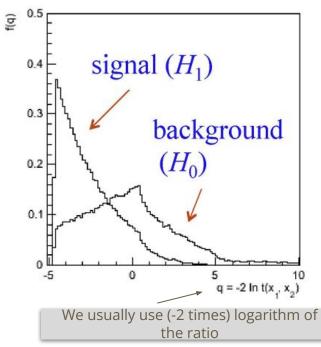
$$p = \int_{Z}^{\infty} \frac{1}{\sqrt{2\pi}} e^{-x^{2}/2} dx = 1 - \Phi(Z) \longrightarrow Z = \Phi^{-1}(1-p)$$



# **Discovery significance**

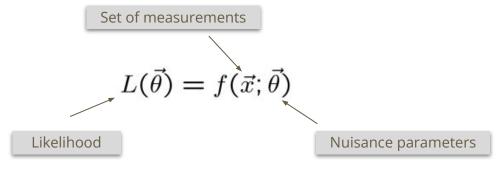
# **Discovery in HEP**

- We want to discover new physics (BSM)
- <u>Typically</u>
  - Hypothesis H<sub>0</sub>, i.e. the "null hypothesis" is the SM prediction
    - "Background-only" hypothesis
  - Alternative hypothesis H<sub>1</sub> is your favourite model
- We know what to do
  - Find the  $P(x,H_0)$  and  $P(x,H_1)$ , i.e. the *likelihood*
  - **Build the test statistics** using the ratios
  - Calculate the p-value
    - Reject/accept
- How to get the PDF?
  - Use **MC simulation**
  - Need to get a distribution of the values
    - <u>Pseudo-experiments/toys</u>!



# Let's add systematics

- So far, only considered <u>statistical uncertainty</u>
- In reality, many systematic uncertainties affect the predictions
- Can add the systematics into the likelihood
  - Define "signal strength", μ, as n = μ.s + b
    - $\mu$  = 1 means cross-section as predicted by the model
  - Add "nuisance parameters" to the likelihood
    - Parameters that impact the likelihood, but we are not interested in them, e.g. systematic uncertainties
    - Usually, "subsidiary" or "auxiliary" measurements are used to constrain NPs

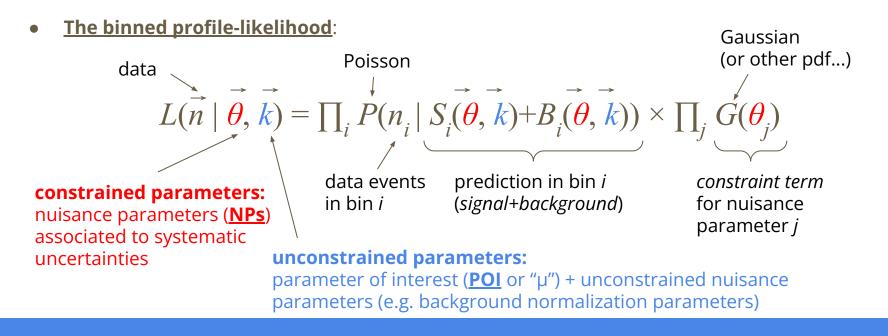


$$= rac{\sigma_{obs.}}{\sigma_{pred.}}$$

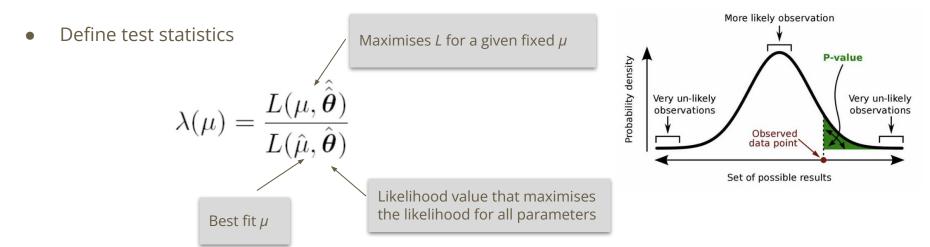
 $\mu$ 

# **Commonly used model**

- More and more common approach for including systematics in HEP statistical analysis:
  - include **systematic uncertainties as unknown parameters in the model**
  - **nuisance parameters** modifying expectations in a **parametric** way
  - nuisance parameters constrained by <u>subsidiary</u> measurements



# **Profile-likelihood significance**



- Observing new physics  $\Leftrightarrow$  excluding background-only hypothesis  $\Leftrightarrow$  excluding  $\mu = 0$
- Only consider upward fluctuations

$$q_0 = \begin{cases} -2\ln\lambda(0) & \hat{\mu} \ge 0\\ 0 & \hat{\mu} < 0 \end{cases} \qquad p_0 = \int_{q_{0,\text{obs}}}^{\infty} f(q_0|0) \, dq_0$$

# Wald's approximation

- Running the **fit can take a long time**
- We need a PDF for the test statistics ⇔ many fits to toy data
  - $\circ$  For 5 sigma discovery we need ~10<sup>7</sup> toys!
- Luckily, there is a **powerful approximation** Wald's approximation
- For large *n*, the likelihood ratio is approximately chi-square distributed!
  - Does not require the likelihood to be chi-square or gaussian distributed!

• Under this assumption, the significance is simply

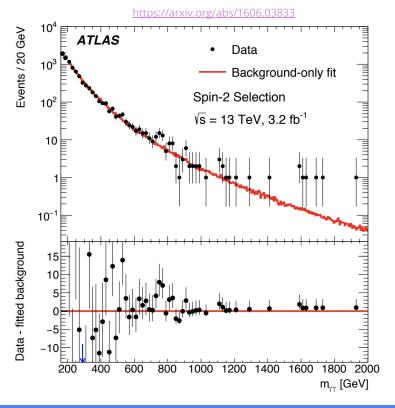
$$Z = \Phi^{-1}(1 - p_0) = \sqrt{q_0}$$

Usually a good approximation as long as number events in each bin is greater than ~10

- I.e. need to **run the fit only twice unconditional** and **with**  $\mu$  **fixed to 0** 
  - Get the -2 ln *L* values for the fits and take the square root of the difference

### Look-elsewhere effect

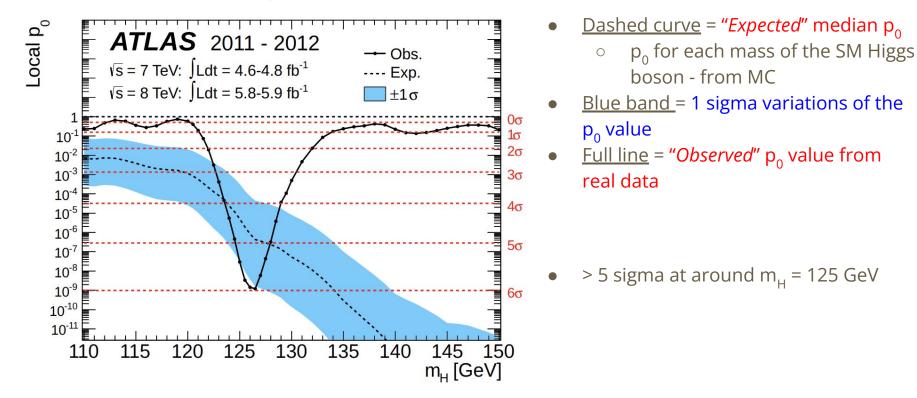
- What if we are looking for a resonance with an unknown mass and see an excess in some mass?
  - Should we just quote the **significance for that mass point**?



- Need to take into account the "*trials*"
  - We are **"testing" multiple bins**
  - $\circ$  We have more options to find an excess
  - Need to correct for this!
- Significance for a fixed mass point ⇔ local significance
- Significance for the floating mass ⇔ global significance
  - Global significance <= local significance</li>
- How to relate local significance to the global one?
  - No simple recipe
  - Need to **run toys** 
    - Usually only 100s, not millions

# **Reading significance plots**

#### https://arxiv.org/abs/1207.7214



# **Setting limits**

# **Setting limits**

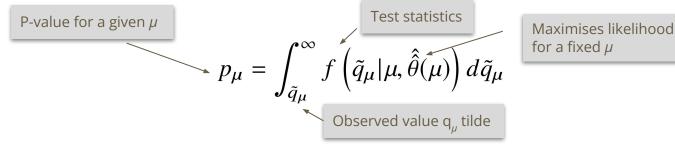
- What if we do not see any significant excess?
  - We can **set limits**!
- What values of  $\mu$  can be excluded with the observed data?
  - I.e. the **implied rate for a given** *µ* **would be very high for the observed data**
  - One-sided test provide an "upper limit"
- Slightly modify the test statistics used for discovery
  - If  $\mu$  comes out negative (unphysical) we can compare to the closest model with  $\mu$  = 0

$$\tilde{\lambda}(\mu) = \begin{cases} \frac{L(\mu, \hat{\hat{\boldsymbol{\theta}}})}{L(\hat{\mu}, \hat{\boldsymbol{\theta}})} & \hat{\mu} \ge 0, \\ \frac{L(\mu, \hat{\hat{\boldsymbol{\theta}}})}{L(0, \hat{\boldsymbol{\theta}})} & \hat{\mu} < 0. \end{cases} \qquad \tilde{q}_{\mu} = \begin{cases} -2\ln\tilde{\lambda}(\mu) & \hat{\mu} \le \mu \\ 0 & \hat{\mu} > \mu \end{cases}$$

This is the test statistics commonly used (e.g. Higgs combinations)

# **Setting limits - continued**

- Settings limits = finding the highest value of  $\mu$  that results in p-value not smaller than  $\gamma$ 
  - y is usually chosen as 0.05, i.e. 95% confidence level (CL)
  - $\circ$  "What is the largest value of  $\mu$  that is still compatible with the data?"



- <u>Need to solve for  $\mu$ </u>
  - Nasty integral equation
  - Can run pseudo-experiments to get the distribution of the test statistics
    - Find  $\mu$  that leads to  $p_{\mu} = 0.05$

# Asymptotic limit settings

- Can use the Wald's approximation
  - The test statistics approaches chi-square

$$q_{\mu} = \begin{cases} \frac{(\mu - \hat{\mu})^2}{\sigma^2} & \hat{\mu} < \mu \\ 0 & \hat{\mu} > \mu \end{cases} \quad \tilde{q}_{\mu} = \begin{cases} \frac{\mu^2}{\sigma^2} - \frac{2\mu\hat{\mu}}{\sigma^2} & \hat{\mu} < 0 \\ \frac{(\mu - \hat{\mu})^2}{\sigma^2} & 0 \le \hat{\mu} \le \mu \\ 0 & \hat{\mu} > \mu \end{cases}$$

- Limit estimation in practice (simplified)
  - Get the best fit value of  $\mu$  and its uncertainty (more on this later)
  - Set  $\mu$  to +2 sigma (approximately 95%) this is a starting point of the iterative estimation

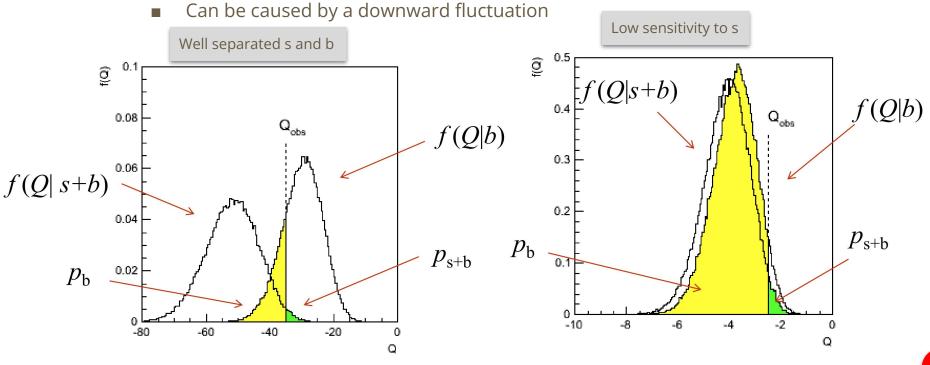
 $q_{\mu}$ 

 $\mu$ 

- $\circ$  Calculate the p-value for this this  $\mu$ 
  - If p-value too small, decrease  $\mu$ , if p-value too large increase  $\mu$
  - Repeat!
  - Stop when the p-value is sufficiently close to 0.05
- Usually requires O(10) fits
- If the asymptotic approximation is not valid, have to use toy experiments

### The CLs issue

- Suppose we have a low sensitivity to a particular signal
  - Test statistics for **s+b** is **very similar to background-only**
  - There is non-negligible **probability to exclude s+b even when we have low sensitivity**



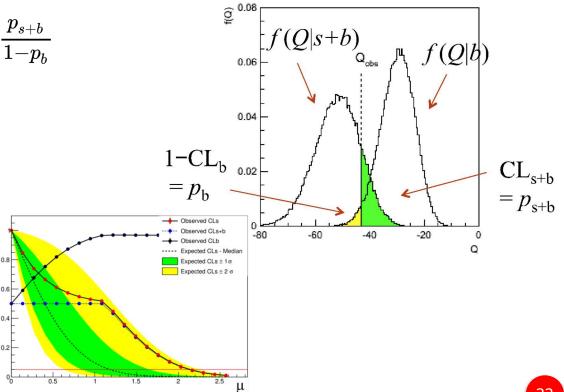
### The CLs procedure A. Read et al.

- **Solution** to the issue: do not use only p-value for the s+b but divide by p-value for b-only
- Define CLs

$$CL_s=rac{CL_{s+b}}{CL_b}=rac{p_{s+b}}{1-p_b}$$

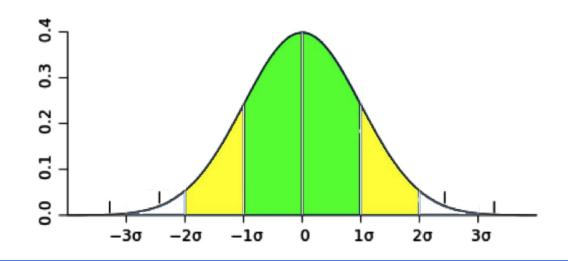
• Reject s+b hypothesis if CLs < α

- <u>Reduces "effective p-value"</u>
  - If low sensitivity
- Ratio of p-values
  - Not liked by statisticians
- Used in almost all HEP searches

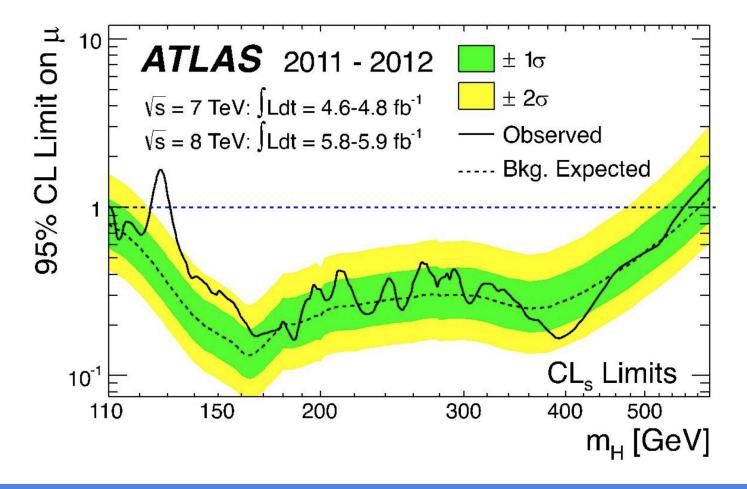


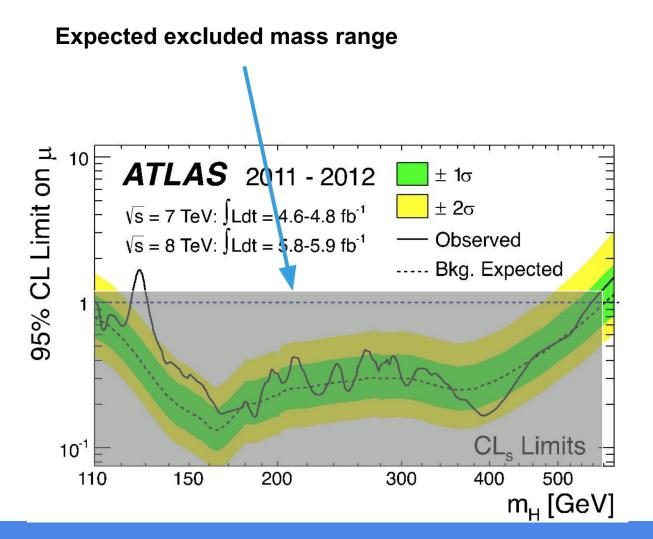
#### **Expected limits**

- **Expected limits** can be calculated using the MC prediction
  - Assume background only, what would be the limit on  $\mu$  in case data = MC?
  - Can do it for several models, e.g. different masses of the Higgs boson
- Frequentist approach
  - Distribution of the p-value ⇔ distribution of the 95% CL limits
  - Can quote **median expected limit** and **± 1(2) sigma variations**

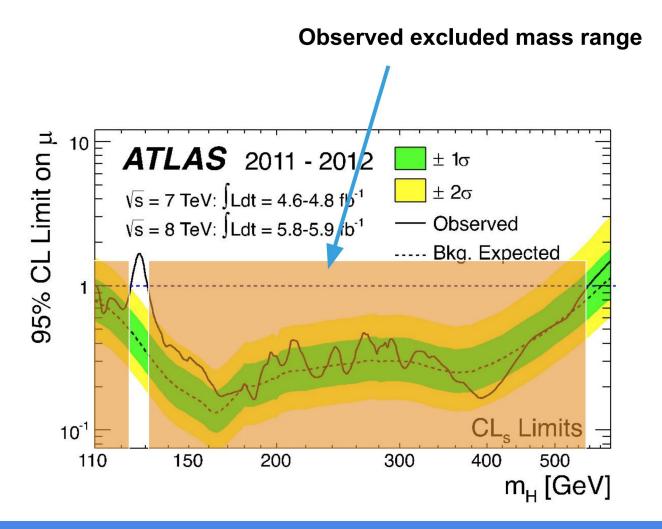








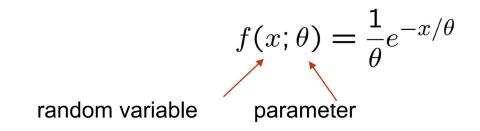
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#### **Parameter estimation**

#### **Estimators**

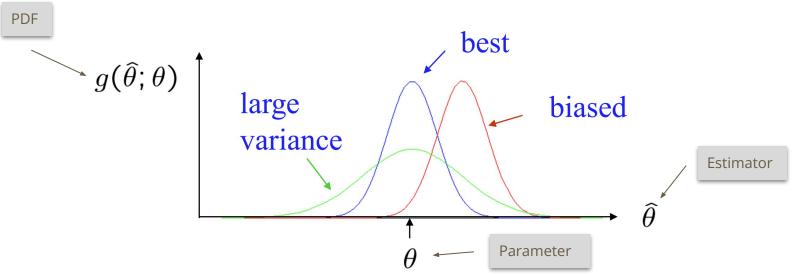
- Often not searching for a new process
  - E.g. Measuring top-quark mass, CKM matrix elements, ...
- How to get the parameters from the model with their uncertainties?
- We need the PDF of the estimation
- **Parameters** are **constants of the estimator** that characterise the shape



- We want to find some function of data to estimate the parameter(s):  $\hat{\theta}(\vec{x})$ 
  - Estimator written with a hat

#### **Estimators continued**

• <u>Repeating the measurement -> get PDF</u>



- We want **unbiased** estimator (bias = 0) with **small variance** (small statistical uncertainty)
  - Generally: conflicting requirements

#### Maximum-likelihood estimate

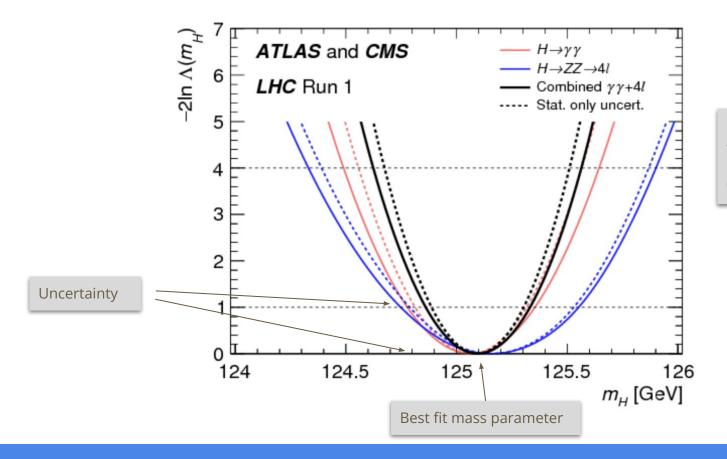
- **Maximum-likelihood estimate** ⇔ values of parameters that maximize the likelihood
  - Usually: use negative log likelihood
  - <u>Frequentists statistics</u>: **Minimise the NLL (i.e "fit")** 
    - Use minimiser tools, e.g. <u>Minuit</u>



- <u>Bayesian statistics</u>: **Sample posterior likelihood**, using Markov-chain Monte Carlo (MCMC)
- If the hypothesized  $\theta$  is close to the true value, then we expect a high probability to get data like that which we actually found
- **ML estimators are not guaranteed** to have any 'optimal' properties
  - In practice they're very good

- <u>Uncertainty of the parameter?</u>
  - Value of θ where the negative log likelihood shifts by one half (1 sigma = 0.5, 2 sigma = 2, 3 sigma = 4.5, ...)
    - Motivated by the Normal distribution where shift of 0.5 happens at exactly 1 sigma

### Example: Higgs mass measurement - https://arxiv.org/abs/1503.07589



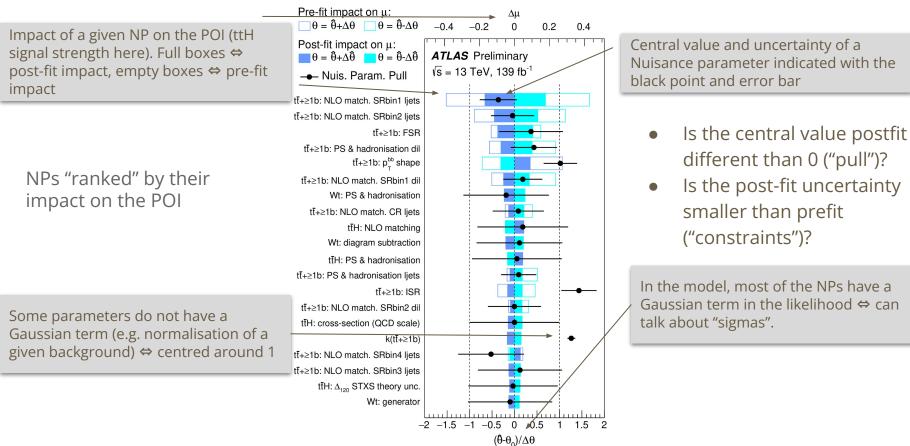
Likelihood scan wider when systematic uncertainties are added (next slide)

### **Adding systematic uncertainties**

- Nuisance parameters (systematic uncertainties) can be added to the likelihood
  - Recall the common model  $L(\vec{n} \mid \theta, k) = \prod_{i} P(n_i \mid S_i(\theta, k) + B_i(\theta, k)) \times \prod_{i} G(\theta_i)$
- <u>Maximum-likelihood</u> ⇔ also the NPs get their best fit value and an uncertainty
  - **Covariance matrix** of all parameters (including NPs)
    - Can also get correlations of the parameters ("post-fit")
  - Lot of physics in these values!

- The uncertainty (likelihood shifts by one half) includes stat+syst
  - How to get an impact of individual sources of the uncertainties?
  - Fix a given NP value to +- 1 sigma, repeat the minimisation and check impact on the parameter of interest
    - Repeat for all NPs
  - Stat-only uncertainty can be obtained by fixing all NPs to their fitted values and repeating the fit and getting the uncertainty on the POI

## Reading pull/ranking plots ATLAS-CONF-2020-058

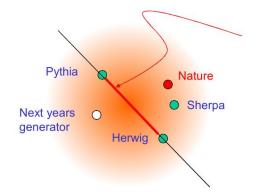


# **Dangers of constraining systematic uncertainties**

- Post-fit uncertainty smaller than prefit ⇔ **constraint** 
  - Reduces total uncertainty good!
  - Is it reliable?

#### 2-point variations especially problematic!

- Should the measurements have power to constrain a given uncertainty?
- Is the measurements "better" than dedicated calibrations?
- Are the variation granular enough?
- Usually: pass nominal and +- 1 sigma variations
  - Interpolation/extrapolation to get **continuous** impact
  - Might not have enough freedom to fit the real shape
    - Systematic might not be granular enough
    - Propagating impacts from high statistic regions?

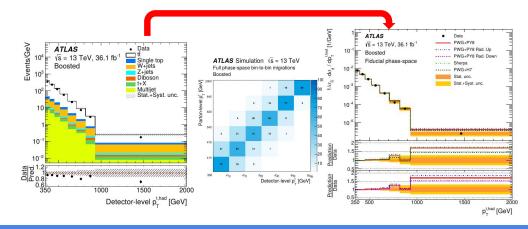




Slides from: Michele Pinamonti

### What is *unfolding* about?

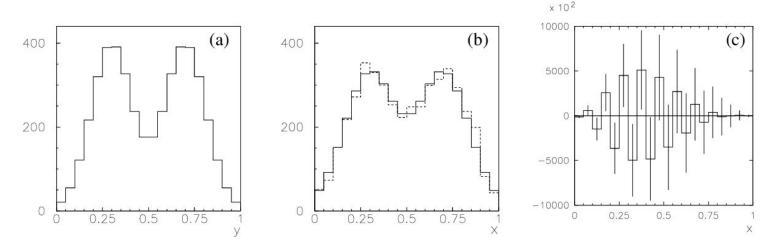
- Unfolding is:
  - removal of detector resolution effects from observed distribution, to extract (our best-guess of) underlying true distribution
  - i.e. extraction of a **differential cross-section**
- Can be done to extract:
  - total-phase-space or fiducial-phase-space cross-sections
  - cross-sections vs. variable defined at particle-level or at parton-level
- The unfolding problem can be essentially reduced to a **response-matrix**-inversion problem



### The regularization concept

"To regularize of not to regularize? This is the question..."

- Most delicate point is the so-called *regularization*:
  - introduced to avoid *amplification of statistical fluctuations* in unfolded data (*oscillations*), happening when just inverting response matrix



- Regularization techniques always imply some level of *assumptions* ⇒ inevitable **bias** 
  - Variance-bias optimisation

#### **Tikhonov regularisation**

- Recall the unfolding problem  $Aec{x}=ec{b}$
- This can be reformulated as a **minimisation** problem (chi-square):  $\chi^2 = (A\vec{x} \vec{b})^T (A\vec{x} \vec{b}) = \min$ 
  - $\circ$  Can minimise to find the best fit for  $ec{x}$
  - Can **impose some additional constraint** (will bias the result!)

$$L(ec{x})\equiv\chi^2(ec{x})+\Phi(ec{x}) o {
m min}$$

• **Common choice** for the constraint: **second discrete derivative (Tikhonov)** 

$$\Phi(ec{x}) = au \sum_i (x_{i-1} - 2x_i + x_i)^2$$

- Choice of  $\tau \Leftrightarrow$  strength of the regularisation
- Different choices of  $\Phi(ec{x})$  possible e.g. SVD  $\longrightarrow A = U\,S\,V^T$ 
  - See e.g. <u>https://arxiv.org/abs/hep-ph/9509307</u>

#### **Impact of regularisation** Taken from: https://arxiv.org/abs/1611.01927 Truth Truth N<sup>event</sup> / GeV 200 400F - MC - MC e G data data bin bin inversion → 300 ~ 300 **-** Tikhonov τ=0.0068 test wrt data: test wrt data: Overflow **Dverflow** $\chi^2$ /16=0.8 prob=0.701 $\chi^2$ /16=1.7 prob=0.032 20 20 100 $\mathbf{0}$ 30 40 50 40 20 N 20 4() $P_{\tau}$ / GeV P<sub>T</sub> / GeV

#### 50

# **Iterative Bayesian Unfolding (IBU)**

• Frequently used in high-signal measurements

true

distribution

• Uses Bayes theorem iteratively:

#### Systematics:

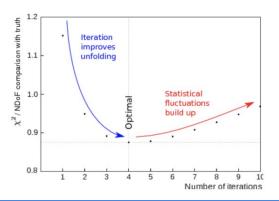
- not included in the formalism
- accessed via ensamble test

 $p_1(T|D) \propto \mathcal{L} \cdot \pi(T)$ 

 $p_2(T|D) \propto \mathcal{L} \cdot p_1(T|D)$ 

 $p_3(T|D) \propto \mathcal{L} \cdot p_2(T|D)$ 

- prior based on theoretical prediction in first iteration
- following iterations use result of previous ones as prior



#### **Regularization:**

posterior

data ("reco")

distribution

achieved by stopping after a few iterations

response

matrix

 $(N_{iter} \rightarrow \infty \Rightarrow$  unregularized unfolding, i.e. matrix inversion)

prior

 finding optimal stopping point is an important feature of using IBU

 $p(T|D, \mathcal{M}) \propto \mathcal{L}(D|T, \mathcal{M}) \cdot \pi(T)$ 

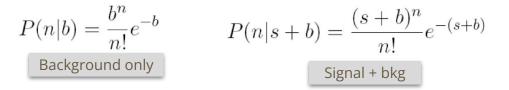
likelihood

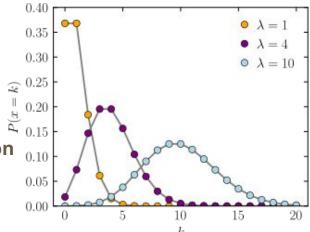
# Thank you for your attention Questions?

"If your experiment needs a statistician, you need a better experiment." — Ernest Rutherford

### Simple example

- Suppose we are doing a *counting experiment* 
  - Predicted number of background events is **b**
  - Predicted number of signal events is **s**
  - Observed number of events will follow **Poisson distribution**





- We observe **n** instances of **x**
- <u>Likelihoods for the hypotheses</u> • Background only • Signal + bkg  $L_b = \frac{b^n}{n!} e^{-b} \prod_{i=1}^n f(\mathbf{x}_i | \mathbf{b})$   $L_{s+b} = \frac{(s+b)^n}{n!} e^{-(s+b)} \prod_{i=1}^n (\pi_s f(\mathbf{x}_i | \mathbf{s}) + \pi_b f(\mathbf{x}_i | \mathbf{b}))$ (Prior) probabilities for an event to be signal or bkg

### Simple example continued

• Define test statistics (-2 logarithm of the likelihood ratio)

$$Q = -2\ln\frac{L_{s+b}}{L_b} = -s + \sum_{i=1}^n \ln\left(1 + \frac{s}{b}\frac{f(\mathbf{x}_i|\mathbf{s})}{f(\mathbf{x}_i|\mathbf{b})}\right)$$

#### • HEP standard

- Claim discovery at 5 sigma
- Reject B-only hypothesis when p- value is  $< 2.9 \times 10^{-7}$

