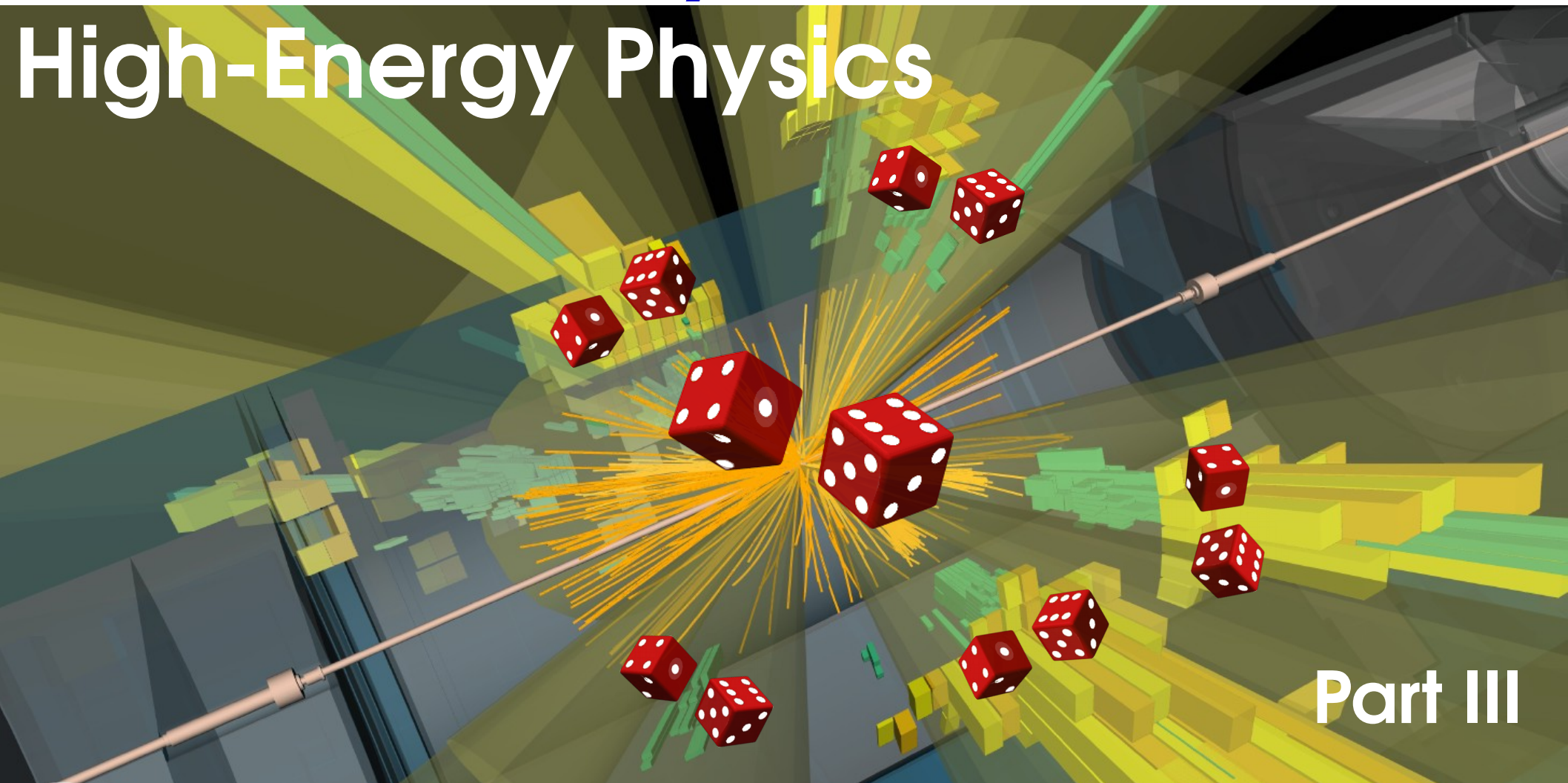


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# Statistical analysis methods in High-Energy Physics



Part III

Nicolas Berger (LAPP Annecy)

# Outline

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## Profiling

Look-Elsewhere Effect

Bayesian methods

## Statistical modeling in practice

Building binned likelihoods

Choosing PDFs in unbinned likelihoods

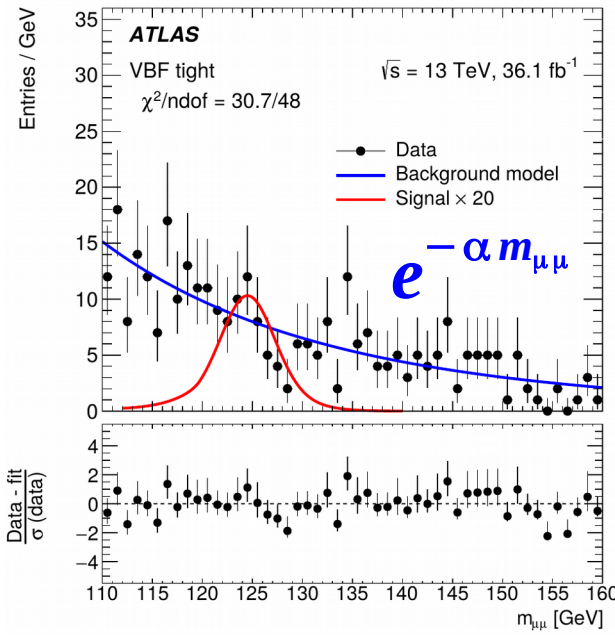
Implementing systematics

***BLUE***

# Nuisances and Systematics

Likelihood typically includes

- **Parameters of interest** (POIs) :  $\mathbf{S}, \sigma \times \mathbf{B}, m_W, \dots$
- **Nuisance parameters** (NPs) : other parameters needed to define the model
  - Ideally, **constrained by data** like the POI
  - e.g. shape of  $H \rightarrow \mu\mu$  continuum bkg



## What about systematics ?

= what we don't know about the random process

⇒ **Parameterize using additional NPs**

→ By definition, **not constrained by the data**

⇒ Cannot be free, or would spoil the measurement (lumi free ⇒ no  $\sigma \times B$  measurement!)

⇒ **Introduce a constraint in the likelihood:**

"Systematic uncertainty is, in any statistical inference procedure, the uncertainty due to the incomplete knowledge of the probability distribution of the observables.  
G. Punzi, *What is systematics ?*

$$L(\underbrace{\mu}_{\text{POI}}, \underbrace{\theta}_{\text{Systematics NP}}; \text{data}) = \underbrace{L_{\text{measurement}}(\mu, \theta; \text{data})}_{\text{Measurement Likelihood}} \underbrace{C(\theta)}_{\text{NP Constraint term}}$$

⇒ penalty for  $\theta \neq \theta^{\text{nominal}}$

# Frequentist Constraints

**Prototype:** NP measured in a separate *auxiliary experiment*

e.g. luminosity measurement

→ Build the combined likelihood of the main+auxiliary measurements

$$L(\boldsymbol{\mu}, \boldsymbol{\theta}; \text{data}) = L_{\text{main}}(\boldsymbol{\mu}, \boldsymbol{\theta}; \text{main data}) L_{\text{aux}}(\boldsymbol{\theta}; \text{aux. data})$$

Independent  
measurements:  
⇒ just a product

**Gaussian** form often used by default:  $L_{\text{aux}}(\boldsymbol{\theta}; \text{aux. data}) = G(\theta^{\text{obs}}; \boldsymbol{\theta}, \sigma_{\text{syst}})$

In the combined likelihood, **systematic NPs are constrained**

→ now same as other NPs: **all uncertainties statistical in nature**

→ Often no clear setup for auxiliary measurements

e.g. theory uncertainties on missing HO terms from scale variations

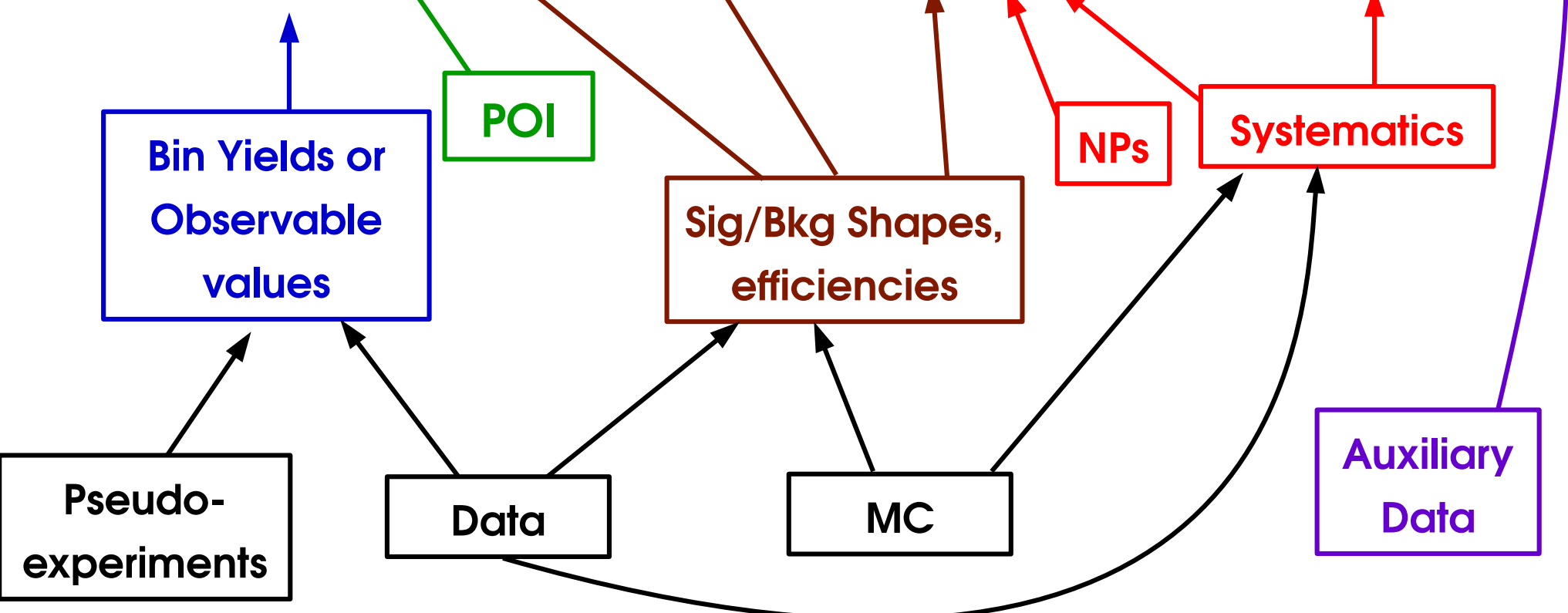
→ **Implemented in the same way nevertheless** (“pseudo-measurement”)

# Likelihood, the full version (binned case)

$$L(\boldsymbol{\mu}, \{\boldsymbol{\theta}_j\}_{j=1 \dots n_{NP}}; \{n_i^{(k)}\}_{i=1 \dots n_{data}^{(k)}}^{k=1 \dots n_{cat}}, \{\boldsymbol{\theta}_j^{obs}\}_{j=1 \dots n_{NP}}) =$$

Expected bin yield

$$\prod_{k=1}^{n_{cat}} P[n_i; \boldsymbol{\mu} \epsilon_{i,k}(\vec{\boldsymbol{\theta}}) N_{S,i,k}(\vec{\boldsymbol{\theta}}) + B_{i,k}(\vec{\boldsymbol{\theta}})] \prod_{j=1}^{n_{syst}} G(\boldsymbol{\theta}_j^{obs}; \boldsymbol{\theta}_j; \mathbf{1})$$



\* number of categories!

# Wilks' Theorem

The likelihood usually has NPs:

- **Systematics**
- Parameters fitted in data

→ **What values to use when defining the hypotheses ?** →  $H(S=0, \theta=?)$

**Answer: let the data choose** ⇒ use the best-fit values (*Profiling*)

⇒ **Profile Likelihood Ratio** (PLR)

$$t_{\mu_0} = -2 \log \frac{L(\mu = \mu_0, \hat{\theta}_{\mu_0})}{L(\hat{\mu}, \hat{\theta})}$$

$\hat{\theta}_{\mu_0}$  best-fit value for  $\mu = \mu_0$  (conditional MLE)  
 $\hat{\theta}$  overall best-fit value (unconditional MLE)

**Wilks' Theorem: PLR also follows a  $\chi^2$  !**  $f(t_{\mu_0} | \mu = \mu_0) = f_{\chi^2(n_{dof}=1)}(t_{\mu_0})$   
**also with NPs present**

→ Profiling “builds in” the effect of the NPs

⇒ Can treat the PLR as a **function of the POI only**

# Gaussian Profiling

**Recall:** Gaussian counting, no syst:  $t_{S_0} = \left( \frac{S_0 - \hat{S}}{\sigma_S} \right)^2$

Counting exp. with background uncertainty:  $\mathbf{n} = \mathbf{S} + \boldsymbol{\theta}$  :

$$\left. \begin{array}{l} \rightarrow \text{Main measurement: } \mathbf{n} \sim \mathbf{G}(\mathbf{S} + \boldsymbol{\theta}, \sigma_{\text{stat}}) \\ \rightarrow \text{Aux. measurement: } \boldsymbol{\theta}^{\text{obs}} \sim \mathbf{G}(\boldsymbol{\theta}, \sigma_{\text{syst}}) \end{array} \right\} L(S, \theta) = G(n; S + \theta, \sigma_{\text{stat}}) G(\theta^{\text{obs}}; \theta, \sigma_{\text{syst}})$$

Then:  $\lambda(S, \theta) = \left( \frac{n - (S + \theta)}{\sigma_{\text{stat}}} \right)^2 + \left( \frac{\theta^{\text{obs}} - \theta}{\sigma_{\text{syst}}} \right)^2$

For  $S = \hat{S}$ , matches MLE as it should

**MLEs:**  $\hat{S} = n - \theta^{\text{obs}}$       **Conditional MLE:**  $\hat{\theta}(S) = \theta^{\text{obs}} + \frac{\sigma_{\text{syst}}^2}{\sigma_{\text{stat}}^2 + \sigma_{\text{syst}}^2} (\hat{S} - S)$   
 $\hat{\theta} = \theta^{\text{obs}}$

**PLR:**  $t_{S_0} = -2 \log \frac{L(S=S_0, \hat{\theta}_{S_0})}{L(\hat{S}, \hat{\theta})}$

$$= \lambda(S_0, \hat{\theta}(S_0)) - \lambda(\hat{S}, \hat{\theta}) = \frac{(S_0 - \hat{S})^2}{\sigma_{\text{stat}}^2 + \sigma_{\text{syst}}^2} \quad \sigma_S = \sqrt{\sigma_{\text{stat}}^2 + \sigma_{\text{syst}}^2}$$

Stat uncertainty (on n) and syst (on  $\theta$ ) add in quadrature as expected

# Effect of Profiling

Systematics still affect the result even after profiling their NPs!

e.g. **again counting experiment**:  $N(S, \theta) = S + \theta$ , measure  $n$ , constraint on  $\theta \sim 0$ .

**1. No NP**:  $N(S) = S$   $t_{S_0} = -2 \log \frac{L(S_0)}{L(\hat{S})}$

→  $\hat{S}$  fit: adjust  $S$  to  $N(\hat{S}) = \hat{S} = n$

→  $S=S_0$  fit:  $S=S_0$  fixed  $\Rightarrow N(S_0) = S_0$ , **cannot adjust**

⇒ **tension** between  $N(S_0)=S_0$  and  $n \Rightarrow$  large  $t_{S_0} \Rightarrow$  **strong exclusion of  $H(S_0)$**

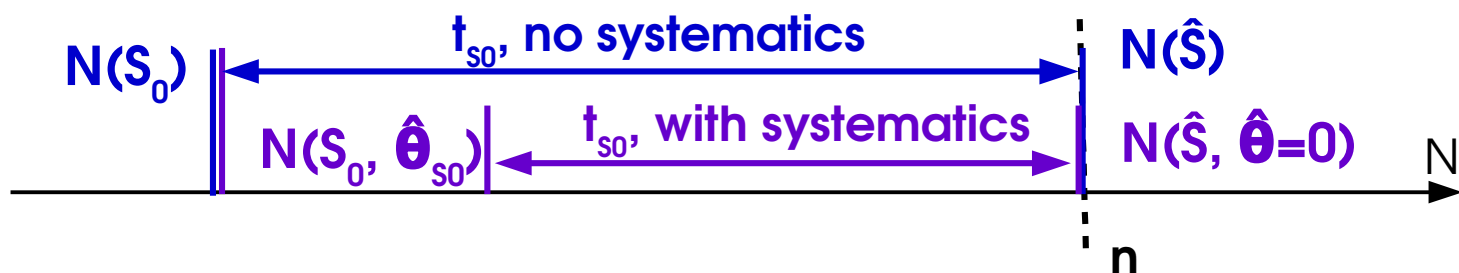
$$t_{S_0} = -2 \log \frac{L(S=S_0, \hat{\theta}_{S_0})}{L(\hat{S}, \hat{\theta})}$$

**2. With NP**:  $N(\mu, \theta) = S + \theta$

→  $\hat{S}$  fit adjust  $N(\hat{S}, \hat{\theta}) = N(\hat{S}, \hat{\theta}=0) = n$  using  $S$  only (avoid penalty on  $\theta$ )

→  $S=S_0$  fit:  $S=S_0$  fixed, but  $\hat{\theta}(S_0)$  **can still pull  $N(S_0, \hat{\theta}(S_0))$  towards  $n$**

⇒ smaller  $t_{S_0} \Rightarrow$  **reduced exclusion of  $H(S_0)$**



More freedom  
⇒ Weaker exclusion



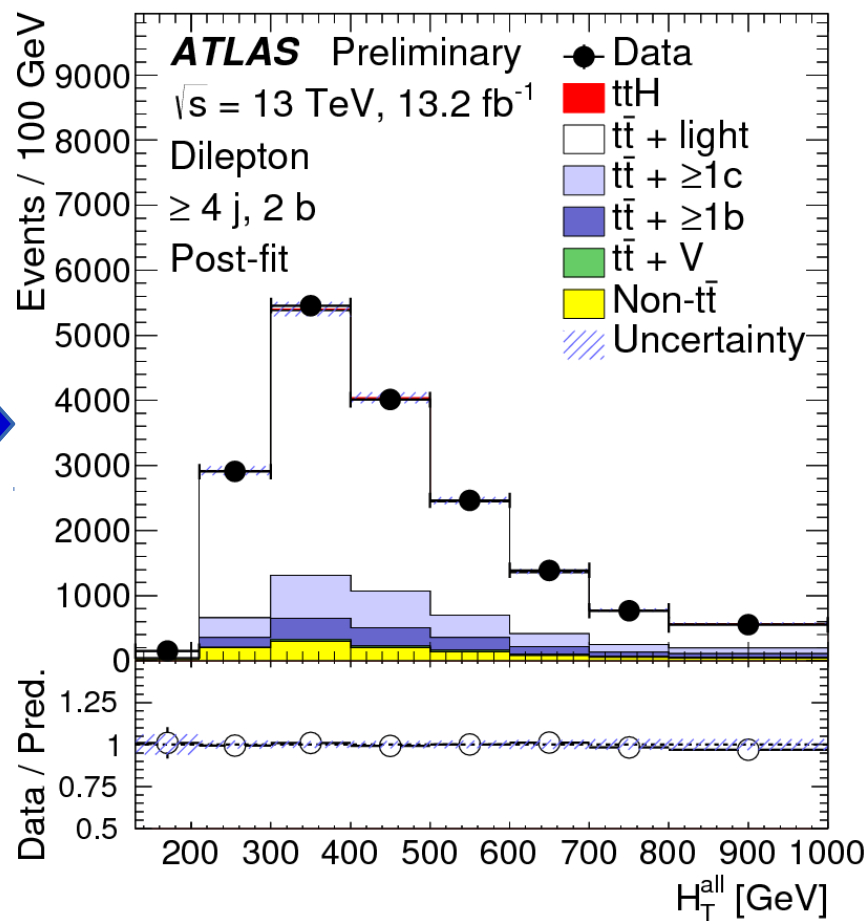
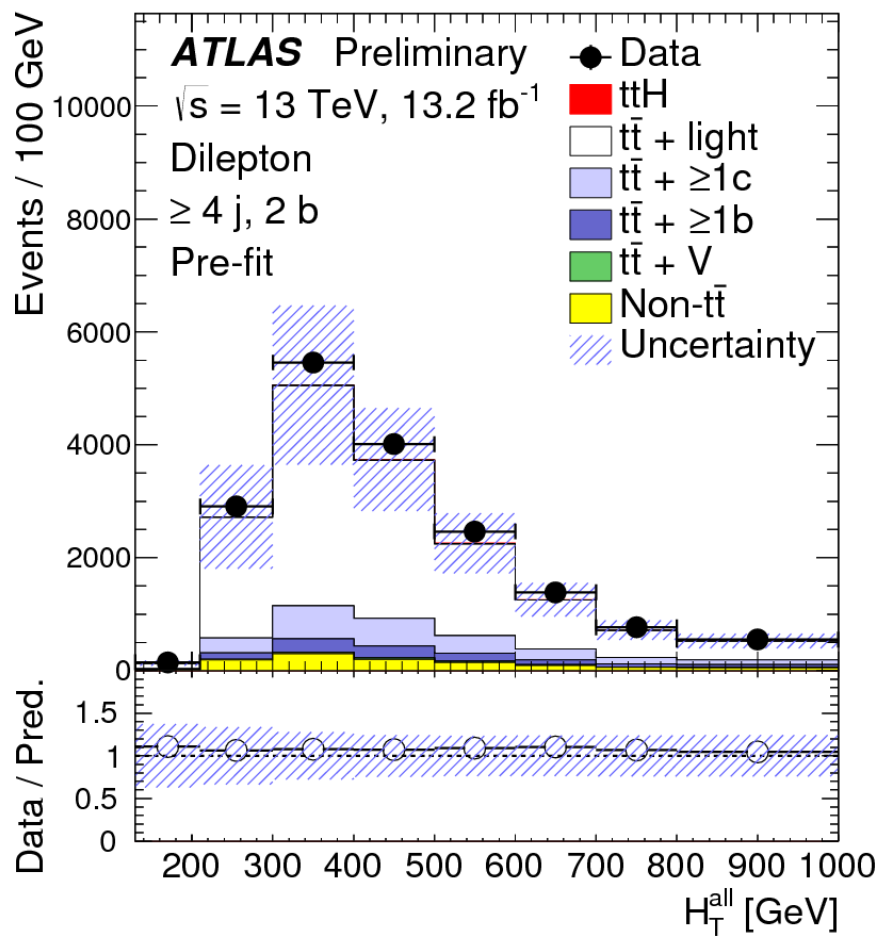
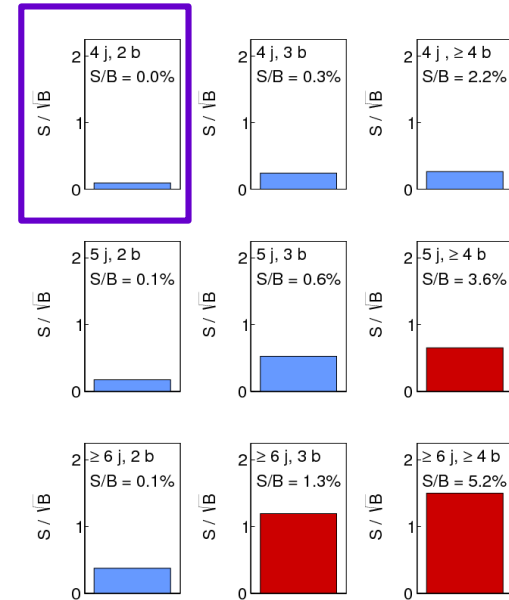
# Profiling Example: $t\bar{t}H \rightarrow bb$

Analysis uses low-S/B categories to constrain backgrounds.

→ **Reduction in large uncertainties on  $t\bar{t}$  bkg**

→ **Propagates to the high-S/B categories** through the statistical modeling

⇒ **Care needed in the propagation** (e.g. different kinematic regimes)



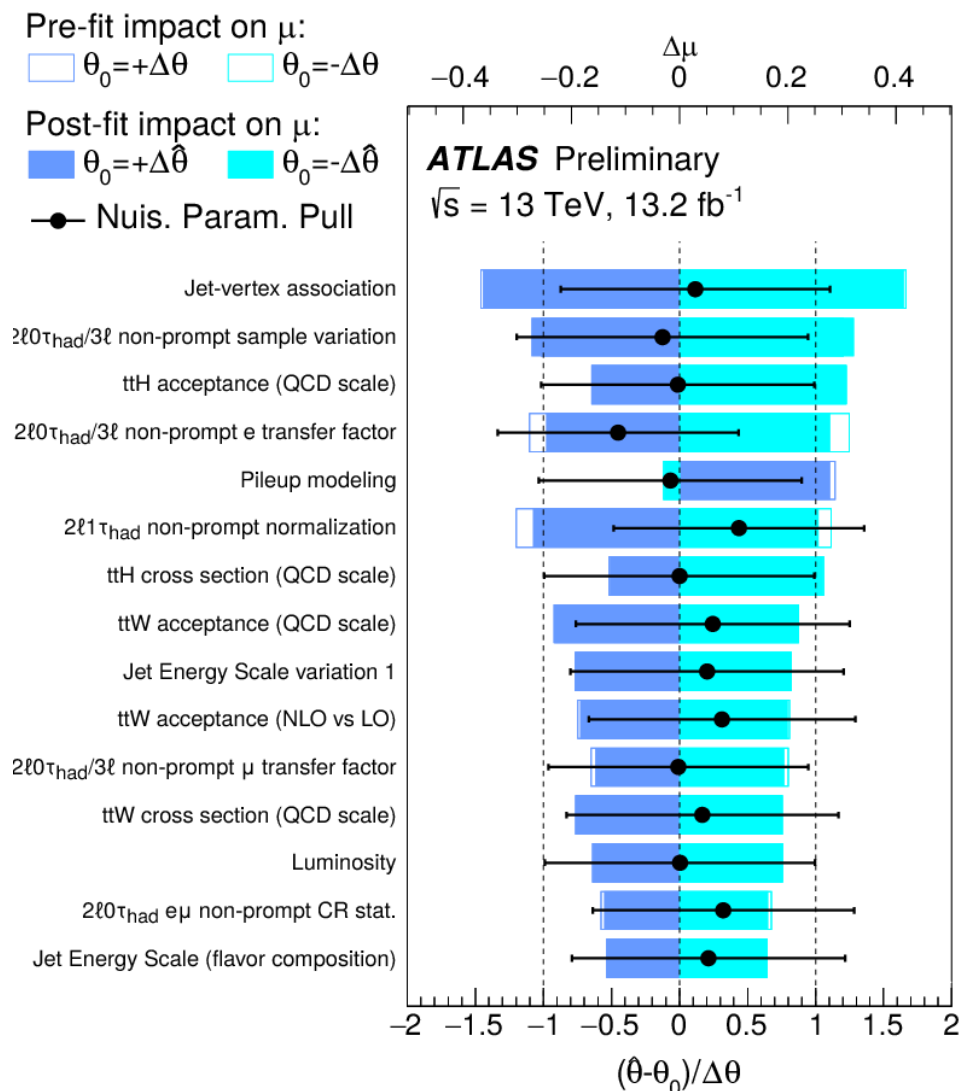
Systematics are described by NPs included in the fit. Nominally:

- **NP central value = 0** : corresponds to the pre-fit expectation (usually MC)
- **NP uncertainty = 1** : since NPs normalized to the value of the syst. :

$$N = N_0 (1 + \sigma_{\text{syst}} \theta), \theta \sim G(0, 1)$$

Fit results provide information on impact of the systematic on the result:

- **If central value  $\neq 0$** : some data feature absorbed by nonzero value  $\Rightarrow$  Need investigation if large pull
- **If uncertainty  $< 1$**  : systematic is constrained by the data  $\Rightarrow$  Needs checking if this legitimate or a modeling issue
- **Impact on result** of  $\pm 1\sigma$  shift of NP



# Pull/Impact plots

Systematics are described by NPs included in the fit. Nominally:

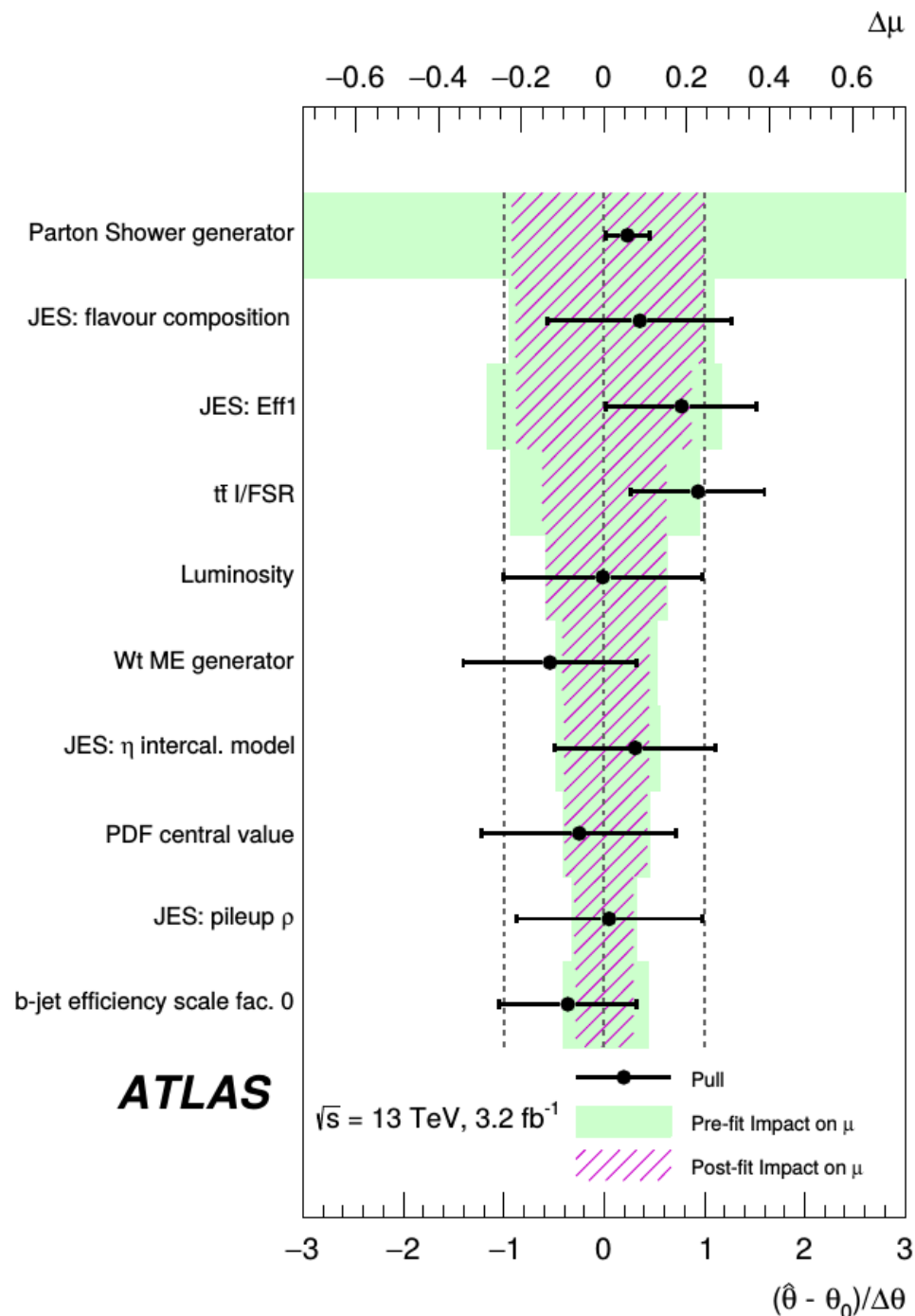
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- **Impact on result** of  $\pm 1\sigma$  shift of NP

13 TeV single- $t$  XS (arXiv:1612.07231)



# Profiling Takeaways

**Systematic** = NP with an external constraint (auxiliary measurement).

→ No special treatment, treated like any other NP: statistical and systematic uncertainties represented in the same way.

When testing a hypothesis, use the best-fit values of the nuisance parameters: *Profile Likelihood Ratio*.

$$\frac{L(\mu = \mu_0, \hat{\theta}_{\mu_0})}{L(\hat{\mu}, \hat{\theta})}$$

**Wilks' Theorem**: the PLR has the same asymptotic properties as the LR without systematics: can profile out NPs and just deal with POIs.

Profiling systematics includes their effect into the total uncertainty. Gaussian:

$$\sigma_{\text{total}} = \sqrt{\sigma_{\text{stat}}^2 + \sigma_{\text{syst}}^2}$$

Guaranteed to work only as long as everything is Gaussian, but typically robust against non-Gaussian behavior.

**Profiling can have unintended effects – need to carefully check behavior**

# Beyond Asymptotics: Toys

Asymptotics usually work well, but break down in some cases – e.g. **small event counts**.

**Solution:** generate **pseudo data (toys)** using the PDF, under the tested hypothesis

→ Also randomize the observable

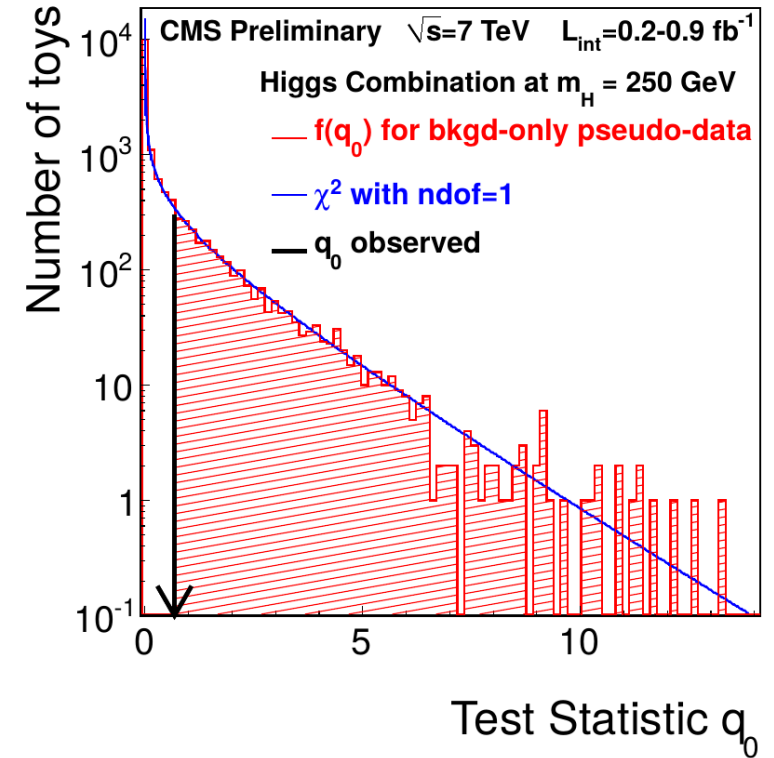
( $\theta^{obs}$ ) of each auxiliary experiment:  $G(\theta^{obs}; \theta, \sigma_{syst})$

→ Samples the true distribution of the PLR

⇒ Integrate above observed PLR to get the p-value

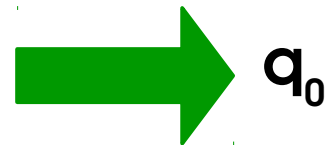
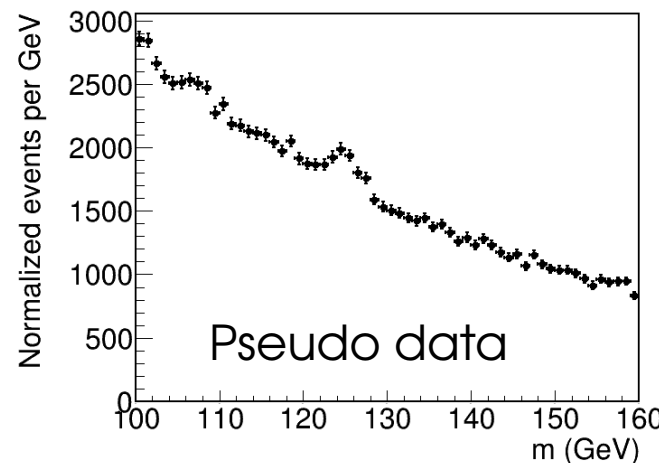
→ Precision limited by number of generated toys,

**Small p-values** ( $5\sigma : p \sim 10^{-7}$ !) ⇒ **large toy samples**

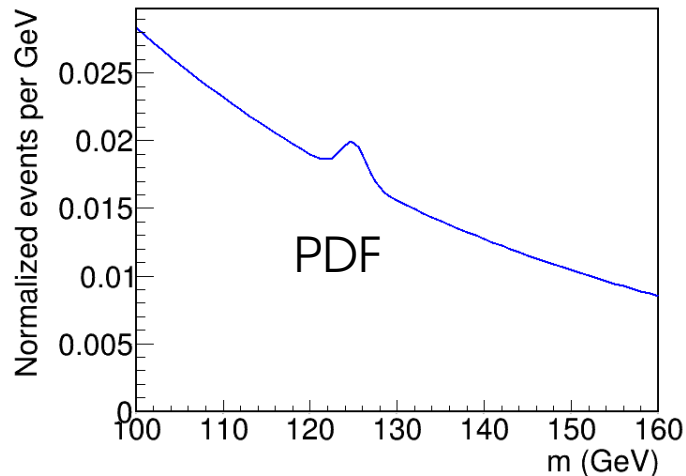


Repeat  $N_{toys}$  times

$p(\text{data} | x)$



$q_0$

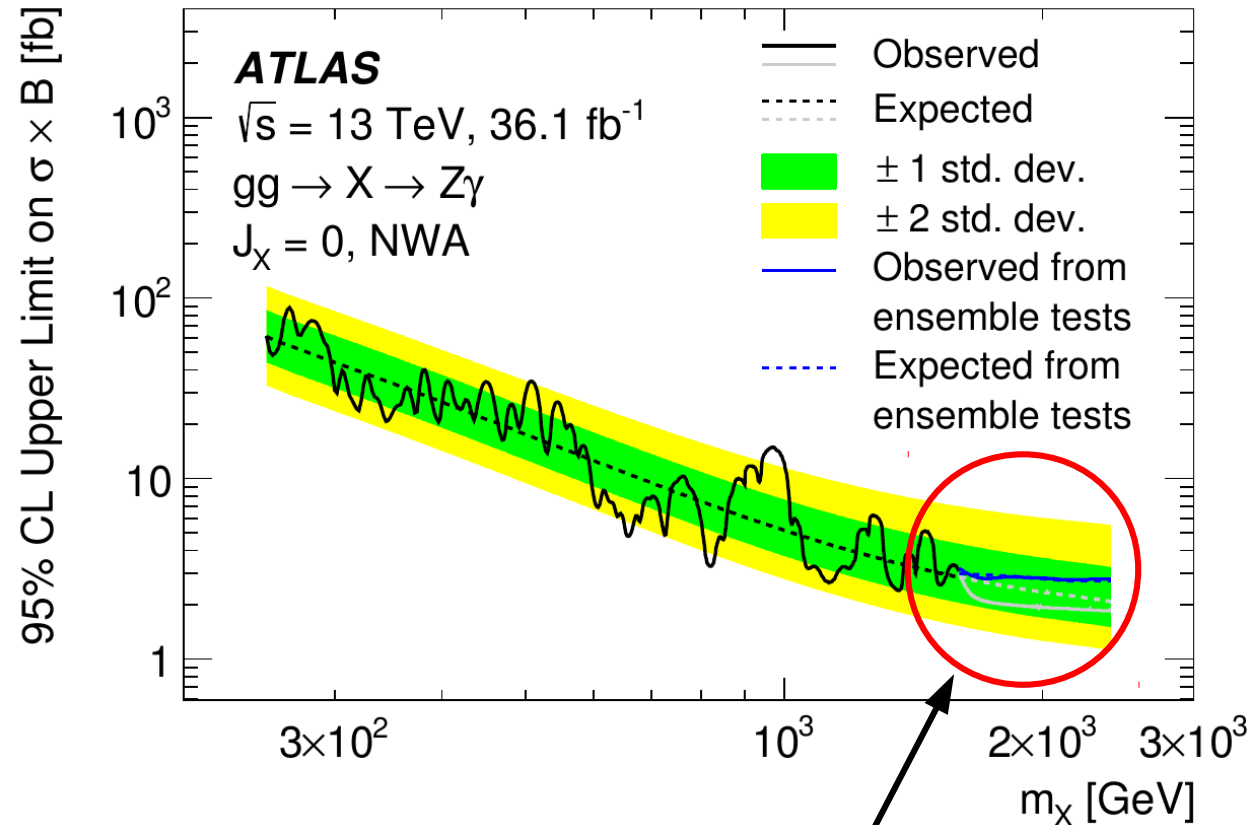
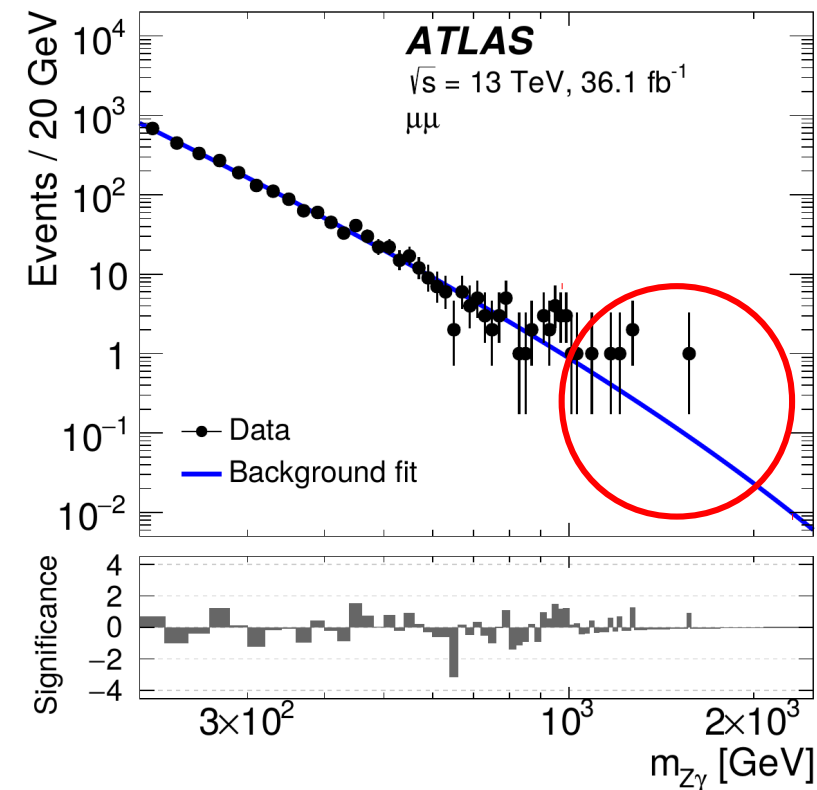


# Toys: Example

arXiv:1708.00212

ATLAS  $X \rightarrow Z\gamma$  Search: covers  $200 \text{ GeV} < m_X < 2.5 \text{ TeV}$

$\rightarrow$  for  $m_X > 1.6 \text{ TeV}$ , low event counts  $\Rightarrow$  derive results from toys



Asymptotic results (in gray) give optimistic result compared to toys (in blue)

# Summary of Statistical Results Computation

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Methods provide:

→ **Optimal use of information from the data under general hypotheses**

→ **Arbitrarily complex/realistic models (up to computing constraints...)**

→ **No Gaussian assumptions in the measurements**

Still often assume Gaussian behavior of PLR – but weaker assumption and can be lifted with toys

Systematics treated as auxiliary measurements – modeling can be tailored as needed

→ **Single PLR-based framework for all usual classes of measurements**

Discovery testing

Upper limits on signal yields

Parameter estimation

# Outline

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Profiling

**Look-Elsewhere Effect**

Bayesian methods

**Statistical modeling in practice**

Building binned likelihoods

Choosing PDFs in unbinned likelihoods

Implementing systematics

***BLUE***



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# Look-Elsewhere Effect

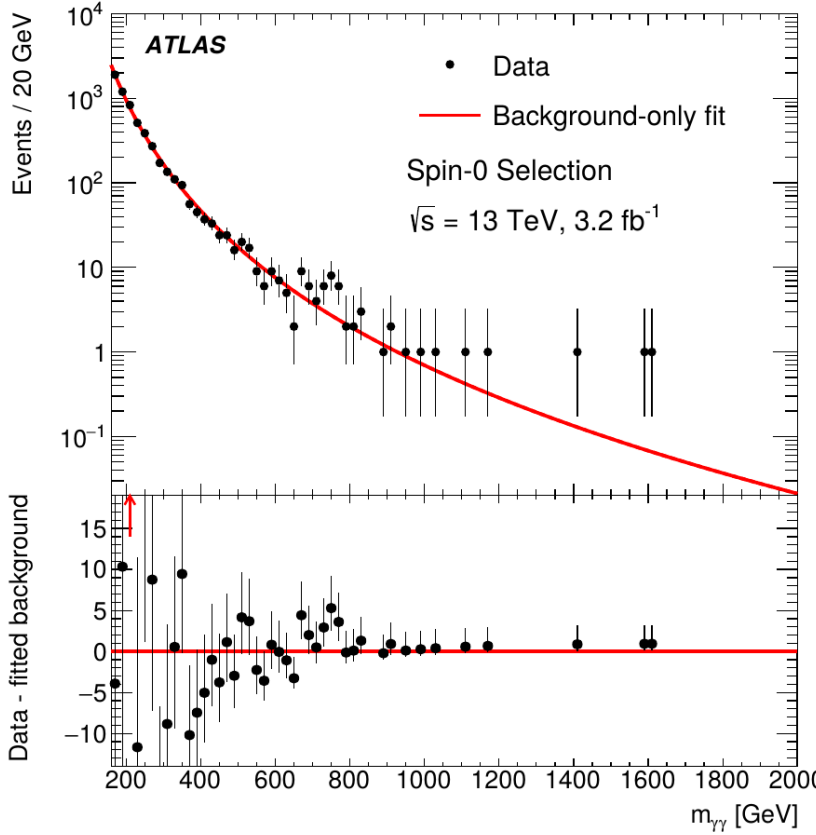
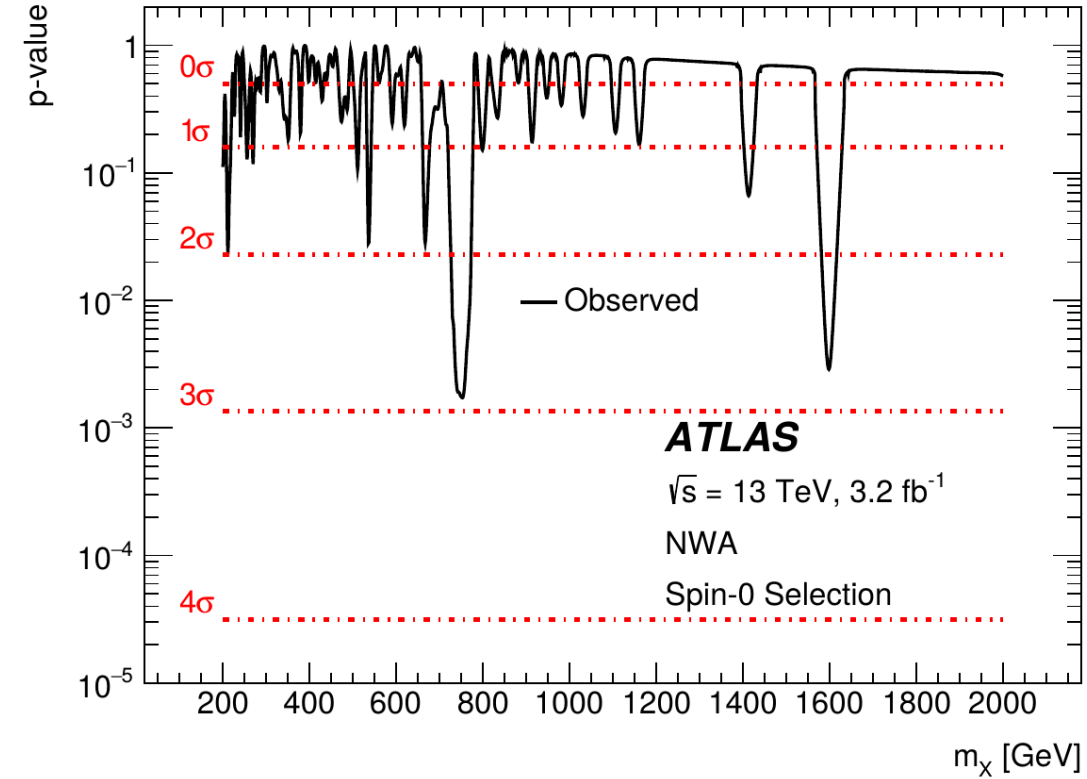
# Look-Elsewhere effect

Sometimes, unknown parameters in signal model

e.g. p-values as a function of  $m_x$

⇒ Effectively performing **multiple, simultaneous searches**

→ If e.g. small resolution and large scan range, **many independent experiments**

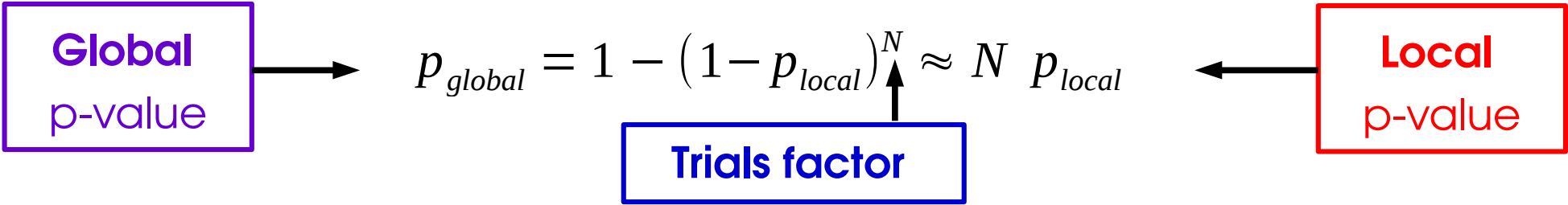


→ More likely to find an excess **anywhere in the range**, rather than in a **predefined** location  
 ⇒ **Look-elsewhere effect** (LEE)

Testing the same  $H_0$ , but against different alternatives  
 ⇒ different p-values

# Global Significance

Probability for a fluctuation **anywhere** in the range → **Global** p-value.  
 at a given location → **Local** p-value

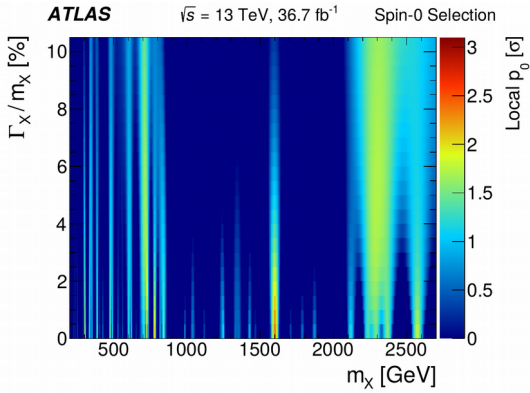


→  $p_{global} > p_{local} \Rightarrow Z_{global} < Z_{local}$  – global fluctuation more likely ⇒ less significant

**Trials factor**: **naively** = # of independent intervals:  $N_{trials} = N_{indep} = \frac{\text{scan range}}{\text{peak width}}$   
 However this is usually **wrong** – more on this later

For searches over a parameter range,  $p_{global}$  is the relevant p-value

→ Depends on the scanned parameter ranges  
**e.g.**  $X \rightarrow \gamma\gamma$ :  $200 < m_X < 2000 \text{ GeV}$ ,  $0 < \Gamma_X < 10\% m_X$ .  
 → However what comes out of the usual asymptotic formulas is  $p_{local}$ .



**How to compute  $p_{global}$  ?** → **Toys** (brute force) or **asymptotic formulas**.

# Global Significance from Toys

**Principle:** repeat the analysis in toy data:

- generate pseudo-dataset
- perform the search, scanning over parameters as in the data
- report the largest significance found
- repeat many times

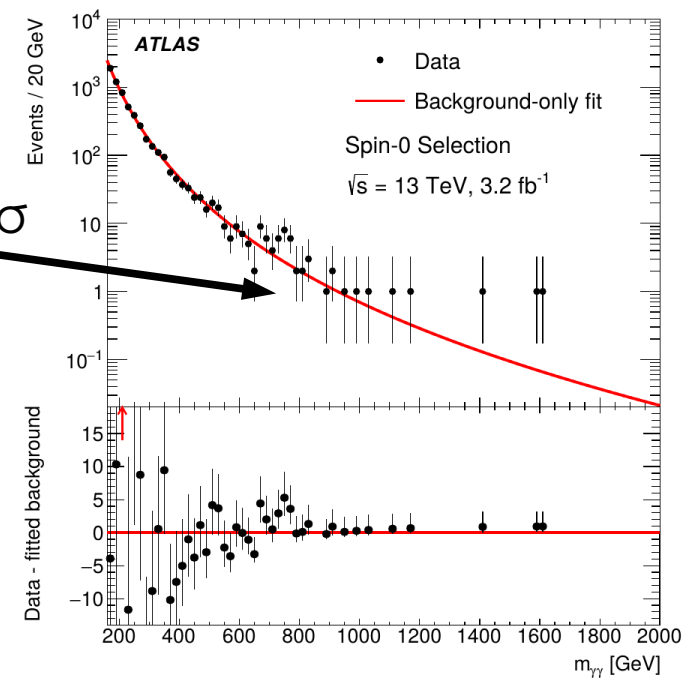
⇒ The frequency at which a given  $Z_0$  is found *is* the global p-value

e.g.  **$X \rightarrow \gamma\gamma$  Search:**  $Z_{\text{local}} = 3.9\sigma$  ( $\Rightarrow p_{\text{local}} \sim 5 \cdot 10^{-5}$ ),  
scanning  $200 < m_X < 2000$  GeV and  $0 < \Gamma_X < 10\% m_X$

→ In toys, find such an excess 2% of the time

⇒  $p_{\text{global}} \sim 2 \cdot 10^{-2}$ ,  $Z_{\text{global}} = 2.1\sigma$  Less exciting...

**Local**  $3.9\sigma$



⊕ **Exact treatment**

⊖ **CPU-intensive** especially for large Z (need  $\sim O(100)/p_{\text{global}}$  toys)

# Global Significance from Asymptotics

**Principle:** approximate the global p-value in the asymptotic limit

→ reference paper: **Gross & Vitells, EPJ.C70:525-530,2010**

$$N_{indep} = \frac{\text{scan range}}{\text{peak width}}$$

**Asymptotic trials factor** (1 POI):

$$N_{trials} = 1 + \sqrt{\frac{\pi}{2}} N_{indep} Z_{local}$$

→ Trials factor is **not just**  $N_{indep}$ ,  
also depends on  $Z_{local}$  !

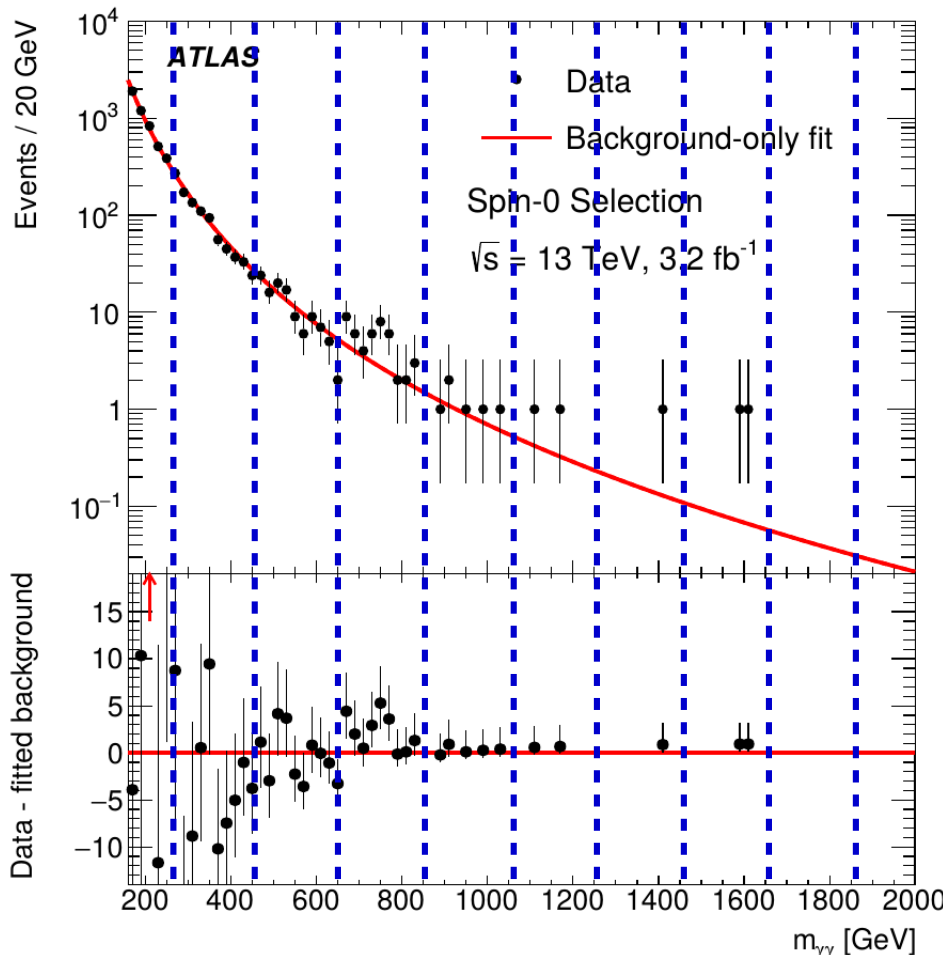
**Why ?**

- slice scan range into  $N_{indep}$  regions of size  $\sim$  peak width
- search for a peak in each region

⇒ Indeed gives  $N_{trials} = N_{indep}$

However this misses peaks sitting on **edges between regions**

⇒ true  $N_{trials}$  is **>**  $N_{indep}$  !



# Global Significance from Asymptotics

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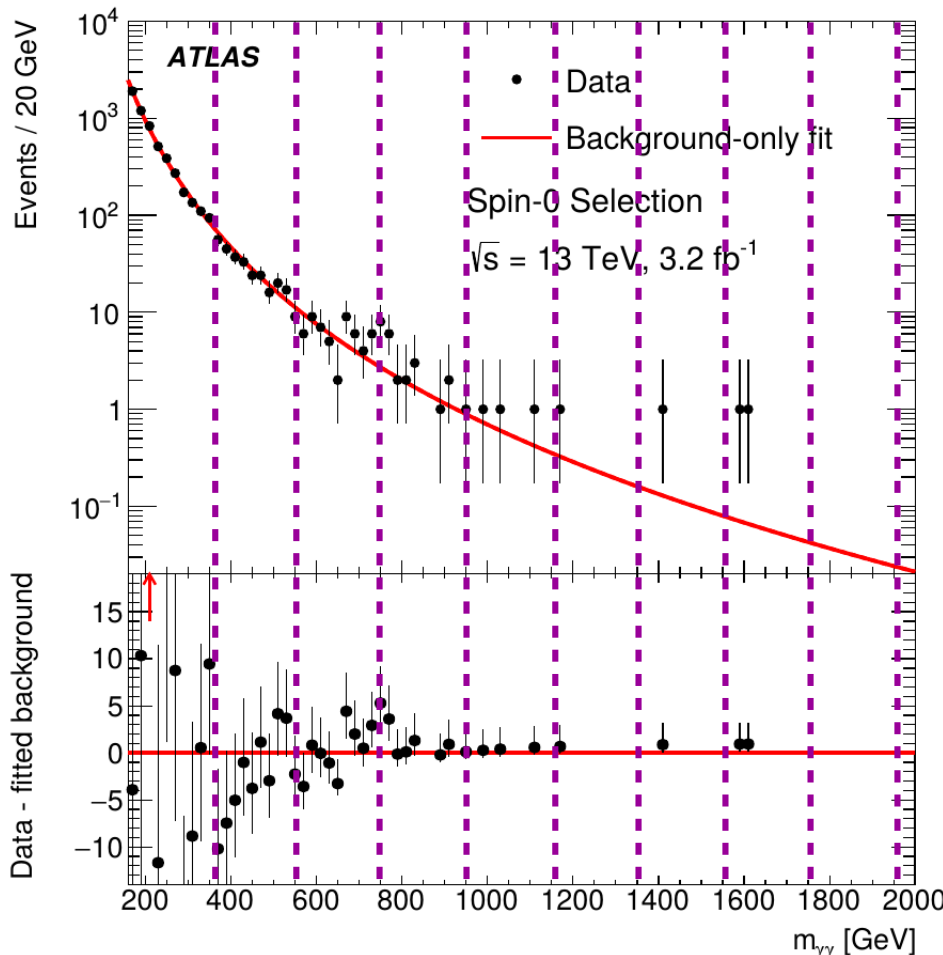
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However this misses peaks sitting on **edges between regions**

⇒ true  $N_{\text{trials}}$  is **>**  $N_{\text{indep}}$  !



# Illustrative Example

**Test on a simple example:** generate toys with

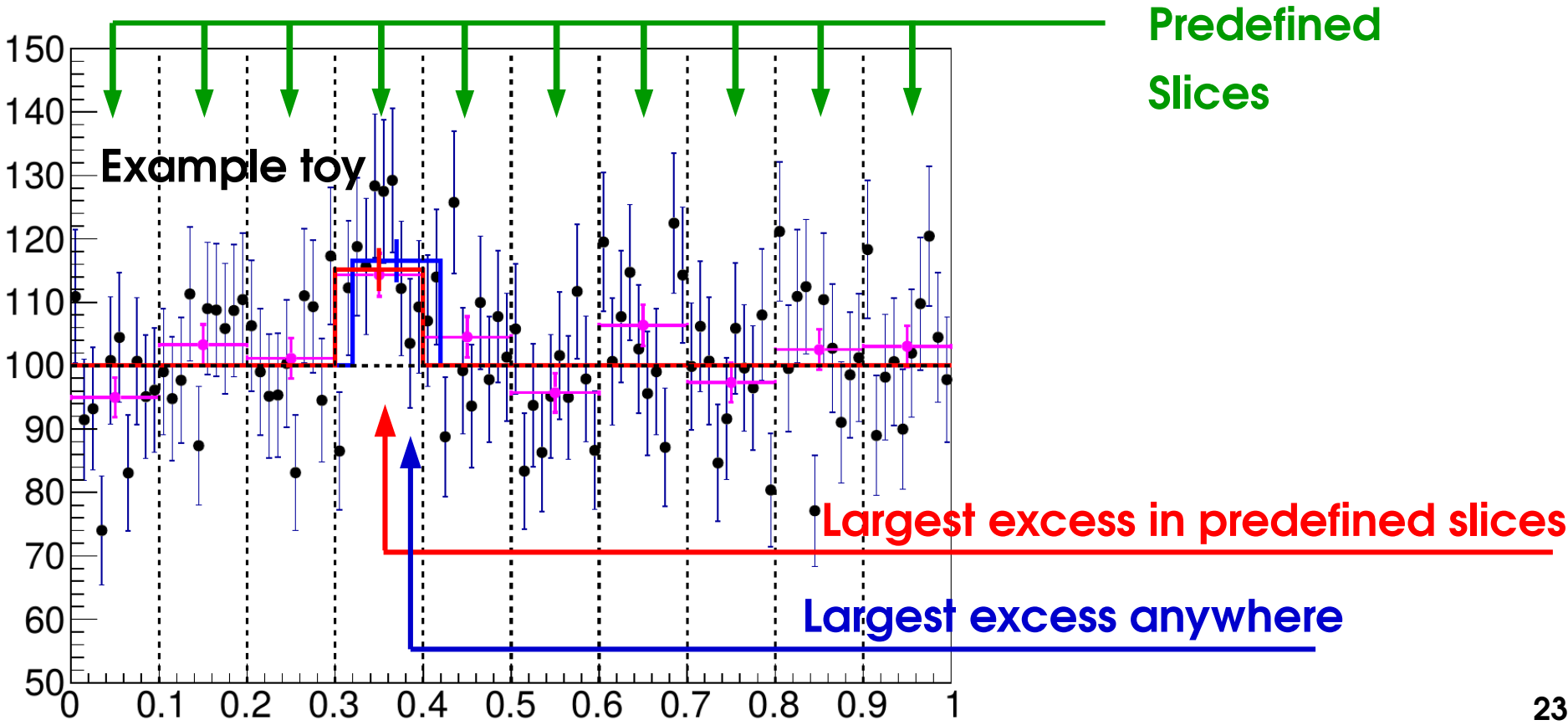
→ flat background (100 events/bin)

→ count events in a fixed-size sliding window, look for excesses

**Two configurations:**

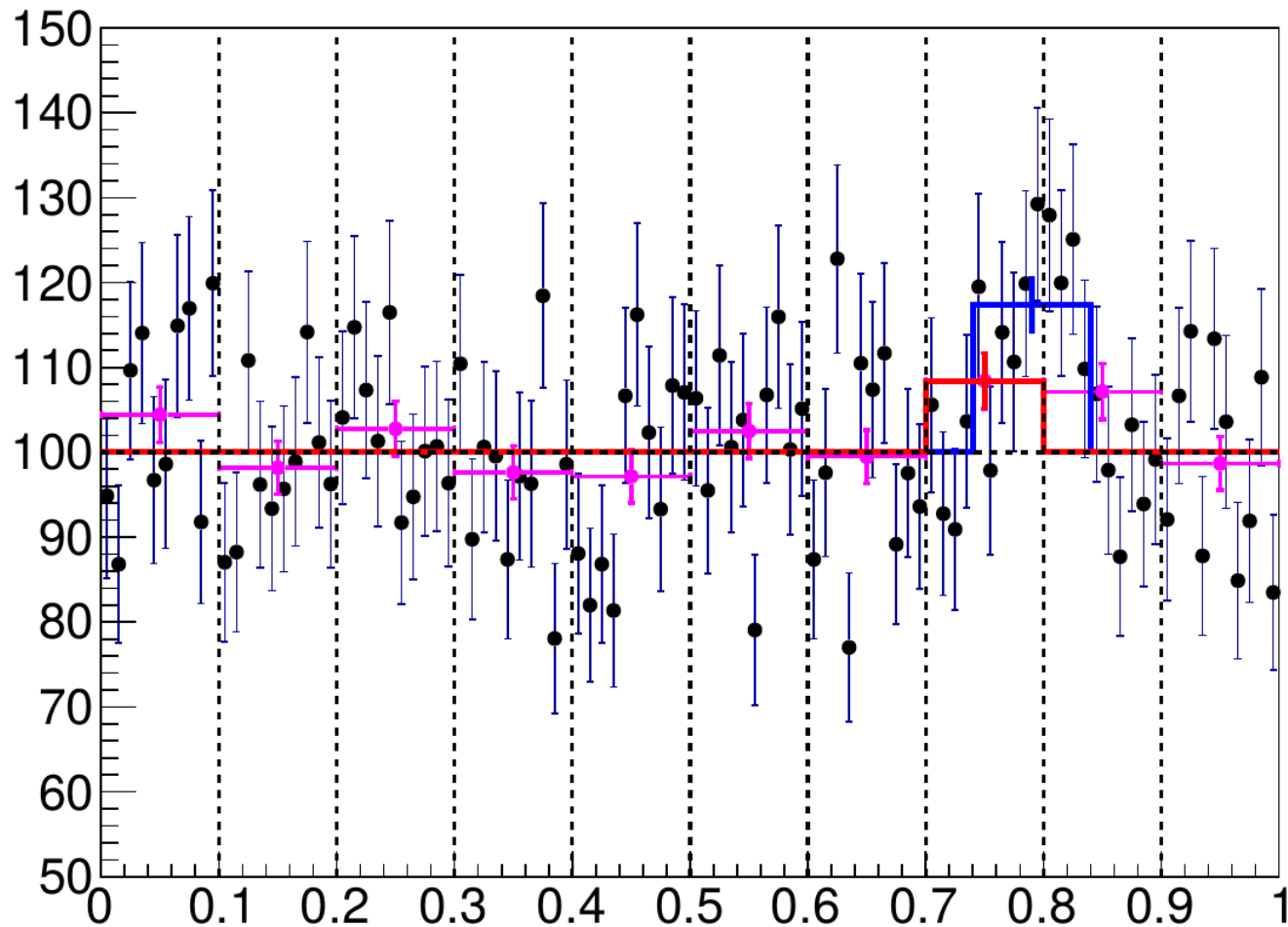
1. Look only in 10 slices of the full spectrum

2. Look in any window of same size as above, anywhere in the spectrum



# Illustrative Example (2)

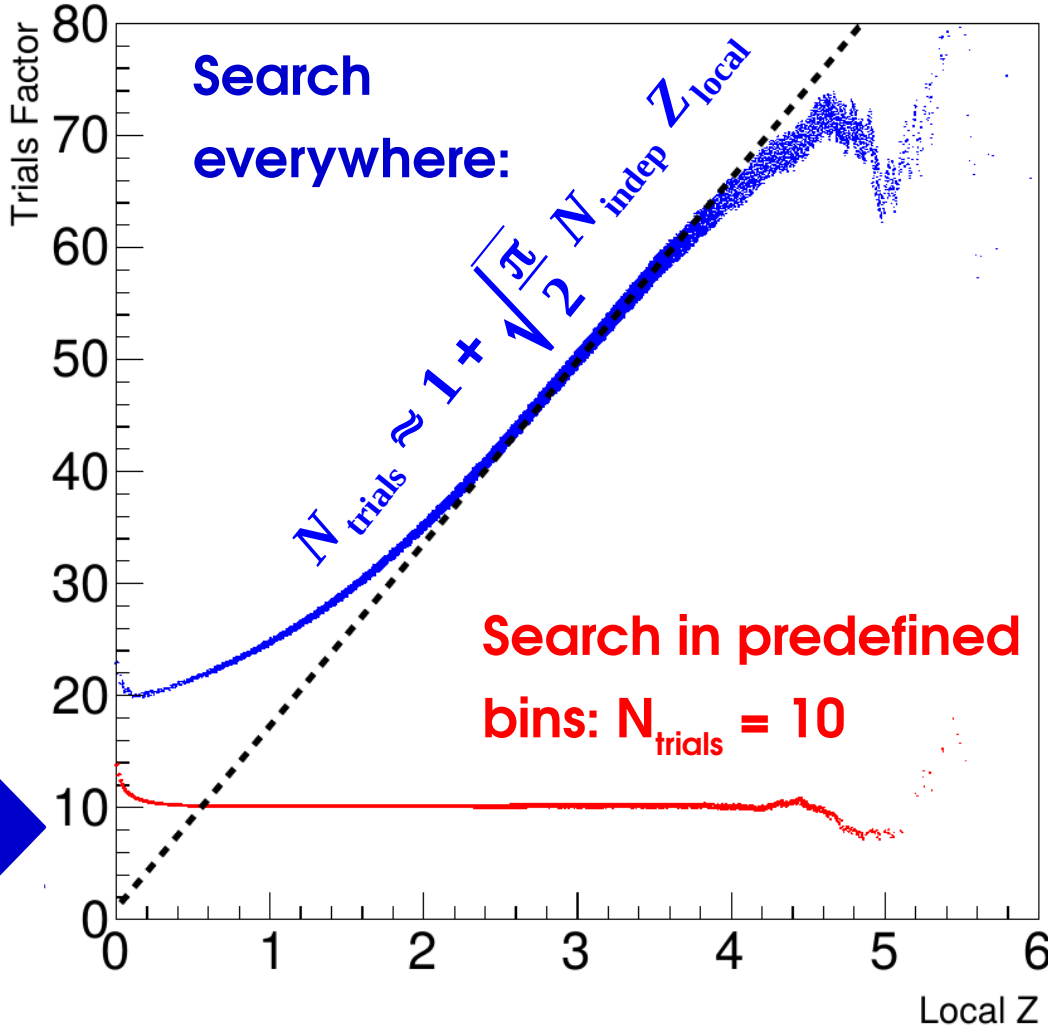
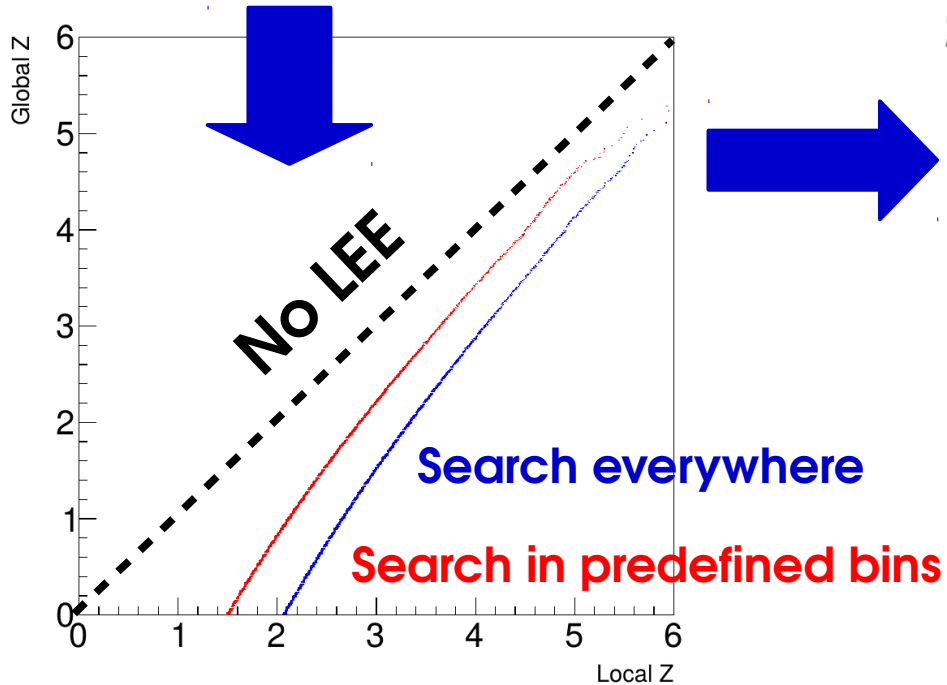
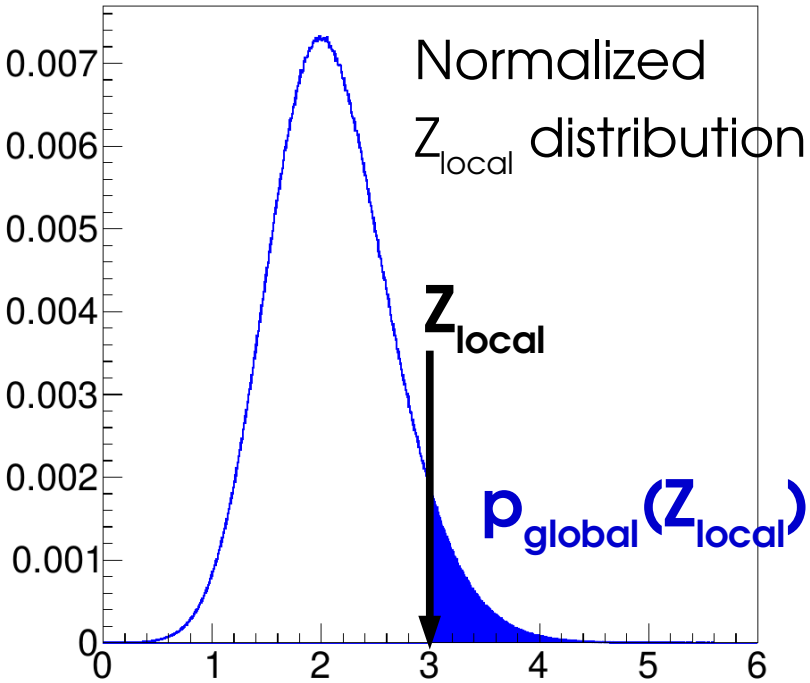
Very different results if the excess is **near a boundary** :



1. Look only in 10 slices of the full spectrum
2. Look in any window of same size as above, anywhere in the spectrum



# Illustrative Example (3)



Searching everywhere gives the extra  $Z_{\text{local}}$  dependence

# $Z_{\text{Global}}$ Asymptotics Extrapolation

Asymptotic trials factor (1 POI):  $N_{\text{trials}} = 1 + \sqrt{\frac{\pi}{2}} N_{\text{indep}} Z_{\text{local}}$

How to get  $N_{\text{indep}}$ ? Usually work with a slightly different formula:

$$N_{\text{trials}} = 1 + \frac{1}{P_{\text{local}}} \langle N_{\text{up}}(Z_{\text{test}}) \rangle e^{\frac{Z_{\text{local}}^2 - Z_{\text{test}}^2}{2}}$$

Number of excesses with  $Z > Z_{\text{test}}$

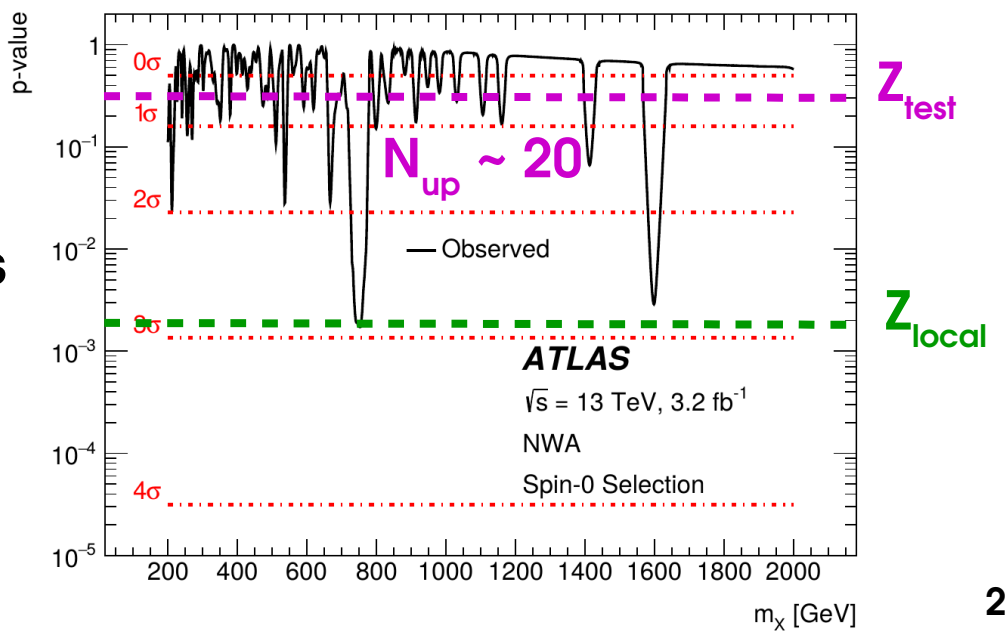
⇒ calibrate for small  $Z_{\text{test}}$ , apply result to higher  $Z_{\text{local}}$

Can choose arbitrarily small  $Z_{\text{test}}$

- ⇒ many excesses
- ⇒ can measure  $N_{\text{up}}$  in data (1 "toy")

Can also measure  $\langle N_{\text{up}} \rangle$  in multiple toys

if large stat uncertainty from too few excesses

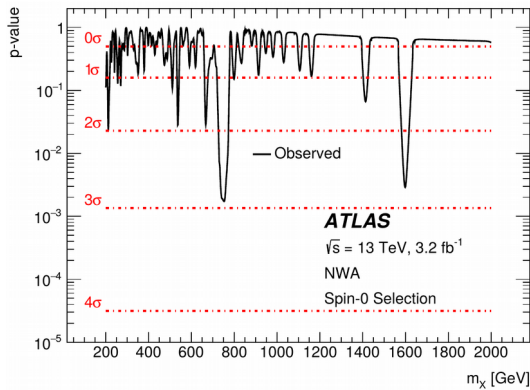


**Generalization to 2D scans:** consider sections at a fixed  $Z_{\text{test}}$ , compute its

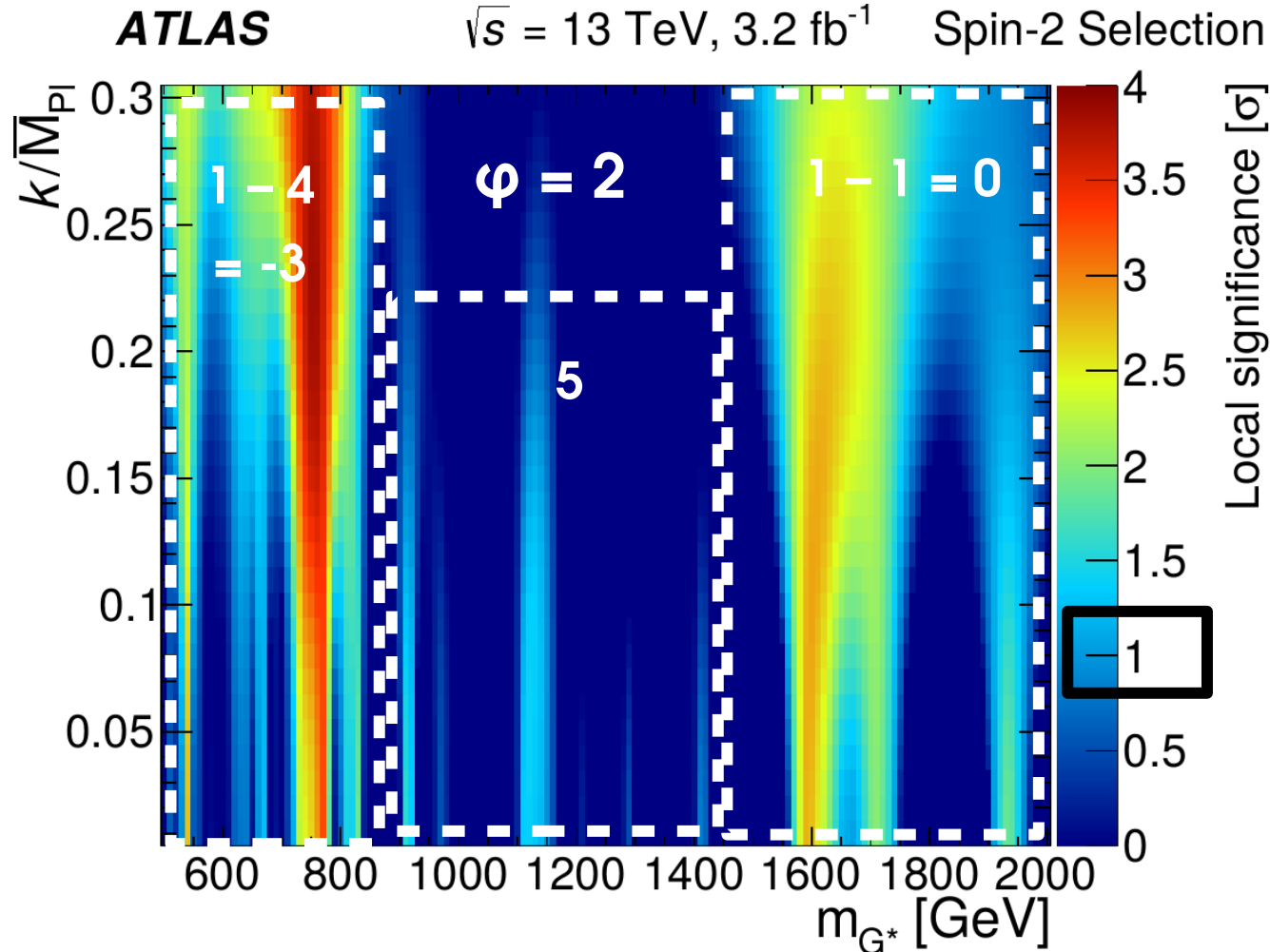
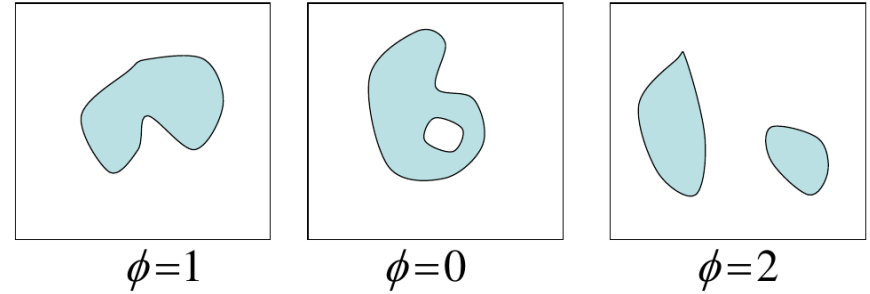
**Euler characteristic**  $\phi$ , and use

$$p_{\text{global}} \approx E[\phi(A_u)] = p_{\text{local}} + e^{-u/2}(N_1 + \sqrt{u}N_2)$$

→ Generalizes 1D bump counting



Now need to determine 2 constants  $N_1$  and  $N_2$ , from Euler  $\phi$  measurements at 2 different  $Z_{\text{test}}$  values.



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Profiling

Look-Elsewhere Effect

**Bayesian methods**

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***BLUE***

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# Bayesian Methods

# Frequentist vs. Bayesian

All methods described so far are **frequentist**

- Probabilities (p-values) refer to outcomes if the experiment were **repeated identically many times**
- Parameters value are **fixed but unknown**
- Probabilities apply to measurements:

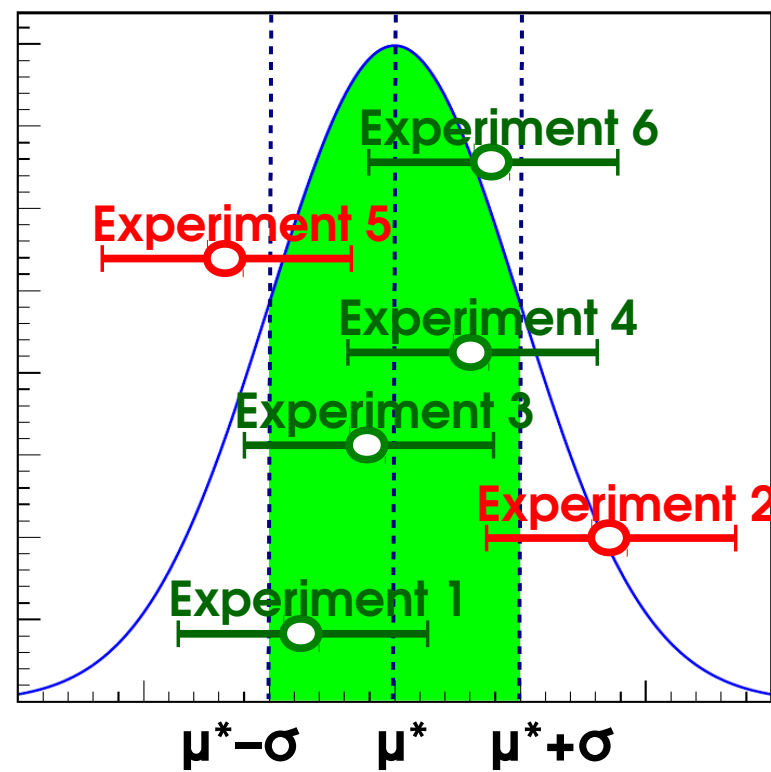
→ “ **$m_H = 125.09 \pm 0.24 \text{ GeV}$** ” :

→ i.e.  $[125.09 - 0.24 ; 125.09 + 0.24 ] \text{ GeV}$  has  $p=68\%$  to contain **the** true  $m_H$ .

→ if we repeated the experiment many times, we would get different intervals, 68% of which would contain the true  $m_H$ .

→ “ **$5\sigma$  Higgs discovery**”

- if there is really no Higgs, such fluctuations observed in  $3 \cdot 10^{-7}$  of experiments



Not exactly the crucial question – what we would really like to know is

***What is the probability that the excess we see is a fluctuation***

→ we want **P(no Higgs | data)** – but all we have is **P(data | no Higgs)**

# Frequentist vs. Bayesian

Can use **Bayes' theorem** to address this:

$$P(\mu | data) = \frac{P(data | \mu)}{P(data)} P(\mu)$$

same as in the frequentist formalism (=likelihood)

Prior Probability

irrelevant normalization factor

Can compute  $P(\mu | data)$ , **if we provide  $P(\mu)$**

→ Implicitly, we have now made  $\mu$  into a random variable

- Is  $m_H$ , or the presence of H(125), randomly chosen ?
- In fact, different definition of p: **degree of belief**, not from frequencies.
- $P(\mu)$  **Prior degree of belief** – critical ingredient in the computation

Compared to frequentist PLR:

- ⊕ answers the “right” question
- ⊖ answer depends on the prior

“Bayesians address the questions everyone is interested in by using assumptions that no one believes. Frequentist use impeccable logic to deal with an issue that is of no interest to anyone.” - **Louis Lyons**

# Bayesian methods

**Probability distribution** (= likelihood) : same form as frequentist case, but

**P( $\theta$ ) constraints** now **priors for the systematics NPs**,  $P(\theta)$

not auxiliary measurements  $P(\theta^{\text{mes}}; \theta)$

⊕ Simply integrate them out, no need for profiling:  $P(\mu) = \int P(\mu, \theta) d\theta$

→ Use probability distribution  $P(\mu)$  directly for limits, credibility intervals

e.g. define 68% CL (“Credibility Level”) interval (A, B) by:  $\int_A^B P(\mu) d\mu = 68\%$

⊖ No simple way to test for discovery

⊖ Integration over NPs can be CPU-intensive

**Priors** : most analyses still using flat priors in the analysis variable(s)

⇒ **Parameterization-dependent**: if flat in  $\sigma \times B$ , then not flat in  $\kappa \dots$

→ Can use the Jeffreys’ or reference priors, but difficult in practice

**Frequentist-Bayesian Hybrid methods** (“Cousins-Highland”)

- Integrate out NPs as in Bayesian measurements

- Once only POIs left, Use  $P(\text{data} | \mu)$  in a frequentist way

→ “Bayesian NPs, frequentist POIs”

- Some use in Run 1, now phased out in favor of frequentist PLR.



# Bayesian methods and $CL_s$ : $CL_s$ computation

Gaussian counting with systematic on background:  $n = S + B + \sigma_{\text{syst}} \theta$

$$L(n; S, \theta) = G(n; S + B + \sigma_{\text{syst}} \theta, \sigma_{\text{stat}}) G(\theta_{\text{obs}} = 0; \theta, 1)$$

$$\text{MLE: } \hat{S} = n - B$$

$$\text{Conditional MLE: } \hat{\theta}(\mu) = \frac{\sigma_{\text{syst}}}{\sigma_{\text{stat}}^2 + \sigma_{\text{syst}}^2} (n - S - B) \quad \left. \vphantom{\hat{\theta}(\mu)} \right\} \text{PLR: } \lambda(\mu) = \left( \frac{S + B - n}{\sqrt{\sigma_{\text{stat}}^2 + \sigma_{\text{syst}}^2}} \right)^2$$

Gaussian  $\Rightarrow$  from previous studies,  $CL_s$  limit is

$$CL_s: \quad S_{\text{up}}^{CL_s} = n - B + \left[ \Phi^{-1} \left( 1 - 0.05 \Phi \left( \frac{n - B}{\sqrt{\sigma_{\text{stat}}^2 + \sigma_{\text{syst}}^2}} \right) \right) \right] \sqrt{\sigma_{\text{stat}}^2 + \sigma_{\text{syst}}^2}$$

# Bayesian methods and CL<sub>s</sub>: Bayesian case

Gaussian counting with systematic on background:  $n = S + B + \sigma_{\text{syst}} \theta$

$$P(n | S, \theta) = G(n; S + B + \sigma_{\text{syst}} \theta, \sigma_{\text{stat}}) G(\theta | 0, 1)$$

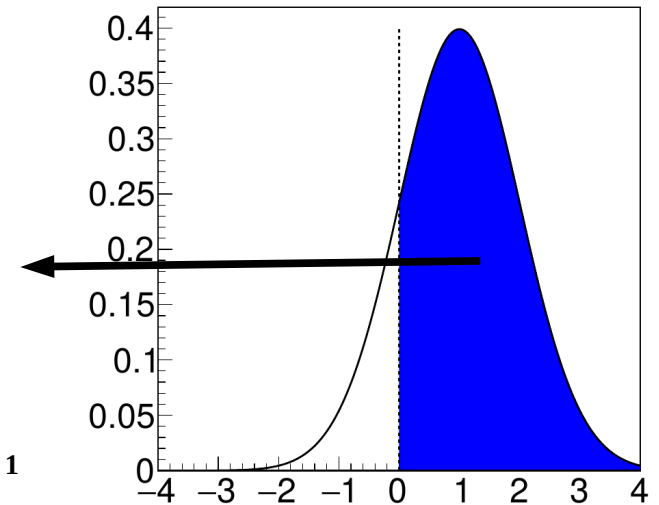
**Bayesian:**  $G(\theta)$  is actually a **prior** on  $\theta \Rightarrow$  perform integral (**marginalization**)

$$P(n | S) = G(S; n - B, \sqrt{\sigma_{\text{stat}}^2 + \sigma_{\text{syst}}^2}) \quad \text{same effect as profiling!}$$

Need  $P(S | n) \Rightarrow$  a prior for  $S$  – take flat PDF over  $S > 0$

$\Rightarrow$  Truncate Gaussian at  $S=0$ :  $P(S | n) = P(n | S) P(S)$

$$P(S | n) = G(S; n - B, \sqrt{\sigma_{\text{stat}}^2 + \sigma_{\text{syst}}^2}) \left[ \Phi \left( \frac{n - B}{\sqrt{\sigma_{\text{stat}}^2 + \sigma_{\text{syst}}^2}} \right) \right]^{-1}$$



**Bayesian Limit:**

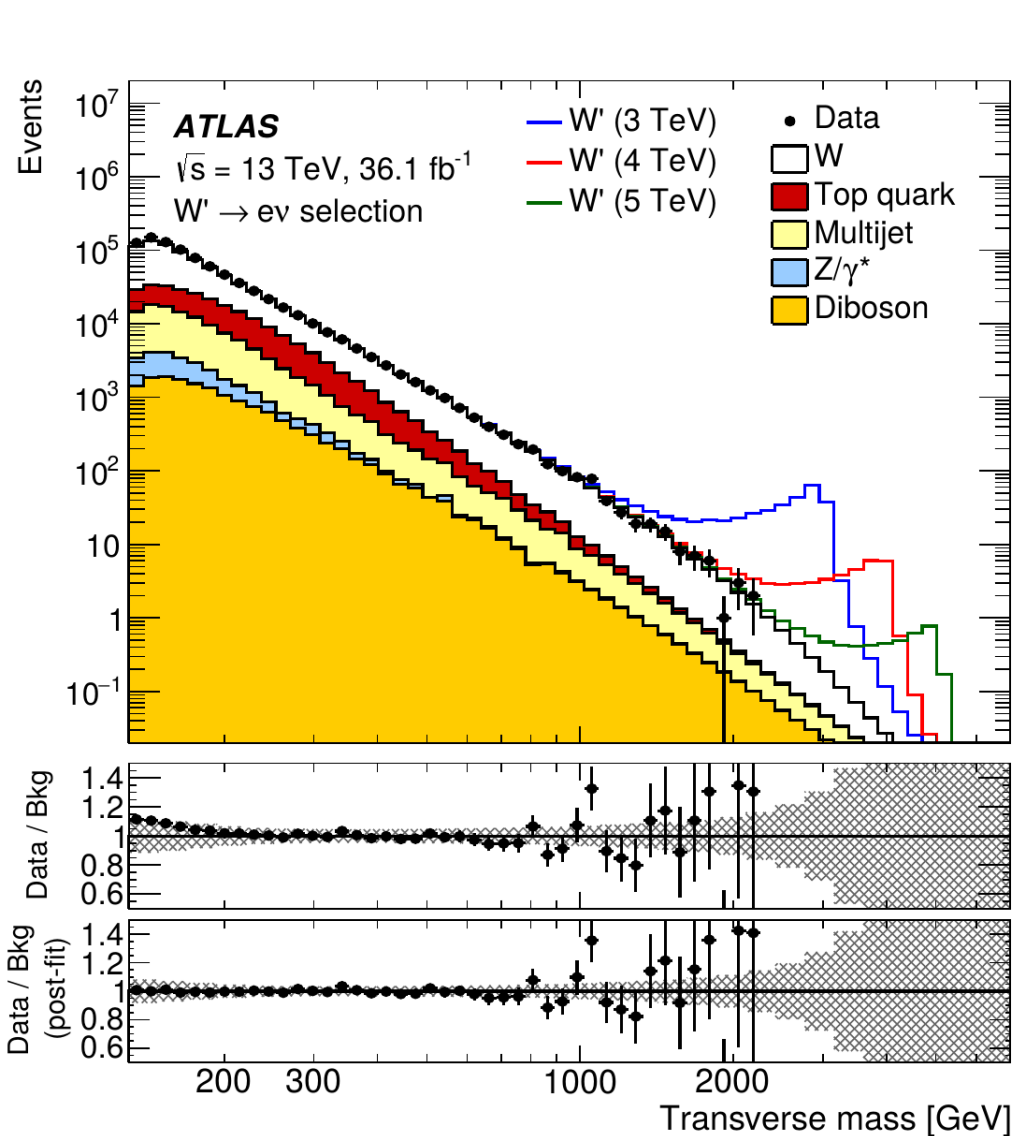
$$\int_{S_{\text{up}}}^{\infty} P(S | n) dS = 5\% = \left[ 1 - \Phi \left( \frac{S_{\text{up}} - (n - B)}{\sqrt{\sigma_{\text{stat}}^2 + \sigma_{\text{syst}}^2}} \right) \right] \left[ \Phi \left( \frac{n - B}{\sqrt{\sigma_{\text{stat}}^2 + \sigma_{\text{syst}}^2}} \right) \right]^{-1}$$

$$S_{\text{up}}^{\text{Bayes}} = n - B + \left[ \Phi^{-1} \left( 1 - 0.05 \Phi \left( \frac{n - B}{\sqrt{\sigma_{\text{stat}}^2 + \sigma_{\text{syst}}^2}} \right) \right) \right] \sqrt{\sigma_{\text{stat}}^2 + \sigma_{\text{syst}}^2}$$

same result as CL<sub>s</sub>!

# Example: $W' \rightarrow l\nu$ Search

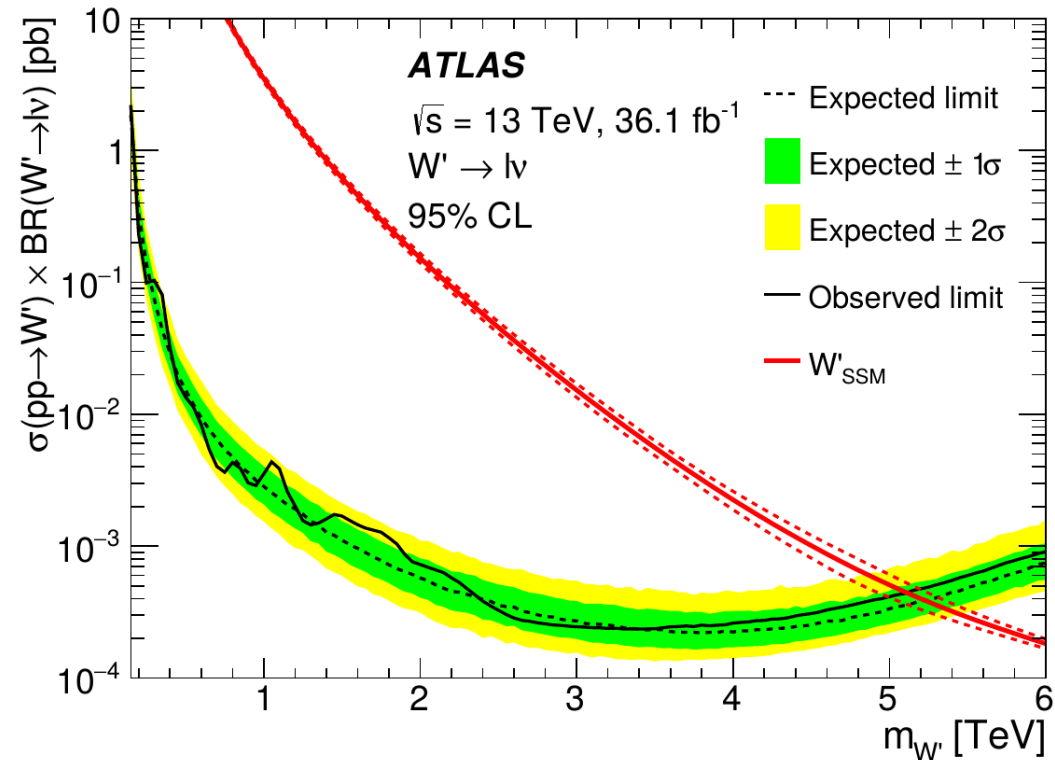
- **POI:**  $W' \sigma \times B$  → use flat prior over  $[0, +\infty[$ .
- **NPs:** syst on **signal  $\epsilon$**  (6 NPs), **bkg** (6), **lumi** (1) → integrate over Gaussian priors



Trigger  
 Lepton reconstruction and identification  
 Lepton momentum scale and resolution  
 $E_T^{\text{miss}}$  resolution and scale  
 Jet energy resolution  
 Pile-up

Multijet background  
 Top extrapolation  
 Diboson extrapolation  
 PDF choice for DY  
 PDF variation for DY  
 EW corrections for DY

Luminosity



# Why $5\sigma$ ?

One-sided discovery:  $5\sigma \Leftrightarrow p_0 = 3 \cdot 10^{-7} \Leftrightarrow 1 \text{ chance in } 3.5\text{M}$

→ Overly conservative ?

→ Do we even know the sampling distributions so far out ?

**Local**  $3.9\sigma$ ,  $p_0 = 5\text{E-}5$

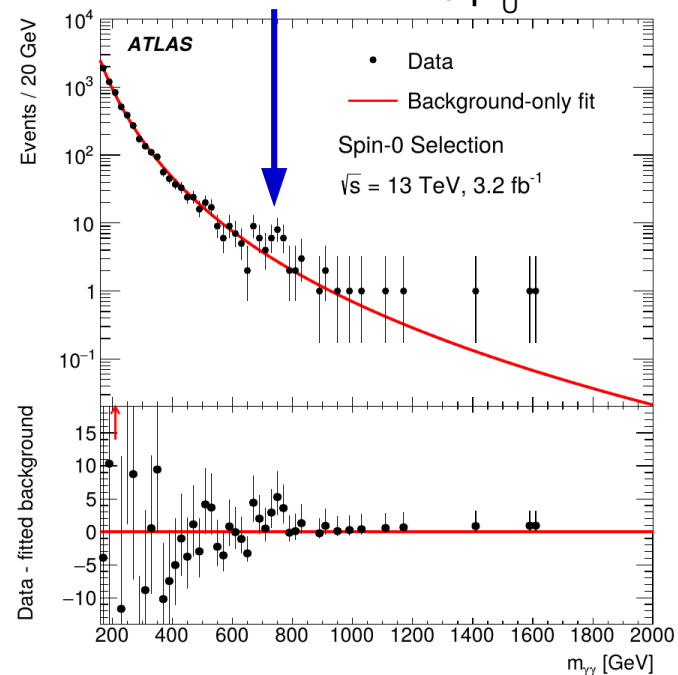
**Global**  $2.1\sigma$ ,  $p_0 = 2\text{E-}2$

**Reasons for sticking with  $5\sigma$**  (from Louis Lyons):

- **LEE** : searches typically cover multiple independent regions  
 ⇒ Global p-value is the relevant one

$N_{\text{trials}} \sim 1000$  : **local  $5\sigma \Leftrightarrow O(10^{-4})$**  more reasonable

- **Mismodeled systematics**: factor 2 error in syst-dominated analysis ⇒ factor 2 error on Z...
- **History**:  $3\sigma$  and  $4\sigma$  excesses do occur regularly, for the reasons above
- **“Subconscious Bayes Factor”** : p-value should be at least as small as the subjective  $p(S)$ :



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

**Extraordinary claims require extraordinary evidence**

⇒ **Stay with  $5\sigma$ ...**

# Outline

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Profiling

Look-Elsewhere Effect

Bayesian methods

## **Statistical modeling in practice**

Building binned likelihoods

Choosing PDFs in unbinned likelihoods

Implementing systematics

***BLUE***

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# Statistical Modeling: in Practice

# Bulding statistical models

---

So far focus has been on concepts, but building a statistical model also requires **numerical** inputs:

- **Data PDFs** for all model components
- **Constraint PDFs** for all sources systematics
- **Impact** of each systematic uncertainty on all relevant model parameters

*→ Statistical methods are only as accurate (and/or optimal) as the description provided by the model!*

Technically, MC simulation provides most of these inputs. However 2 problematic issues:

- **Potential MC/data differences**
- **Limited MC statistics**

Which need to be addressed with (yet more) systematics.

---

# Statistical Modeling:

## I. Component PDFs



# PDFs : Binned likelihood

Binned case:

→ PDF usually just a normalized histogram, from

- **MC sample** or
- **Data control region (CR)**

⇒ **Statistical uncertainties** on the prediction:

- **Data CR:** counts as **statistical** uncertainty
- **MC sample:** uncertainty can be reduced without collecting more data (just need more CPU!) ⇒ Counted as **systematic**

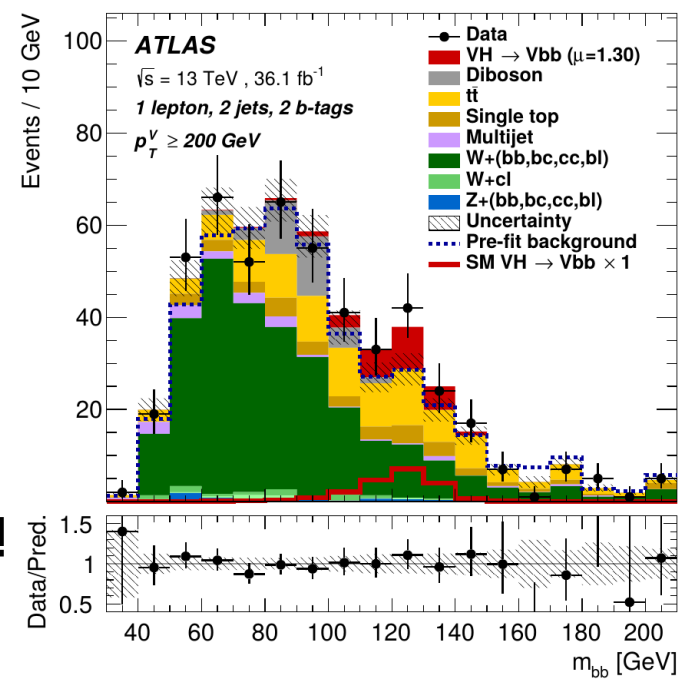
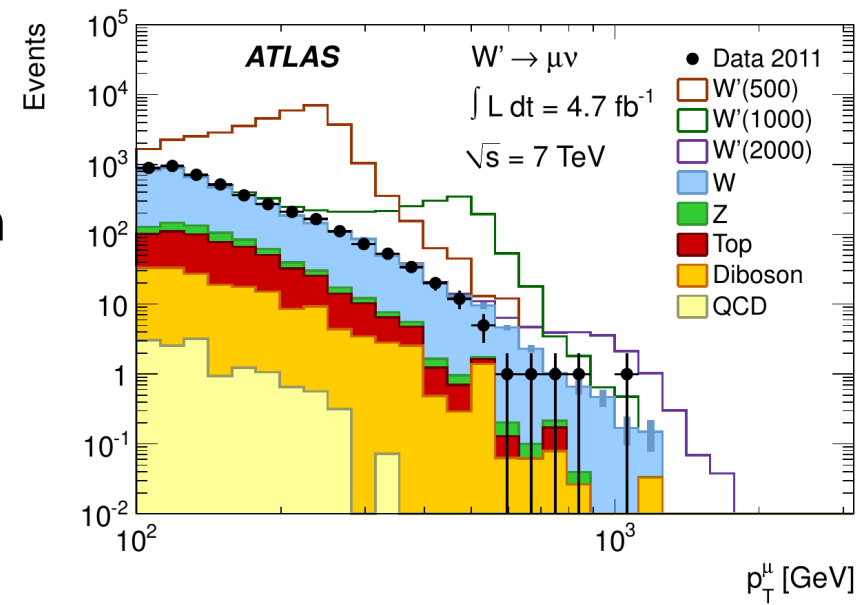
Independent counts in each bin

⇒ a separate **MC statistics NP** in each bin

→ Poisson constraints **Pois( $N_i^{MC}$ ;  $N_i^{true}$ )**

$$\text{Total uncertainty} \sim \sqrt{\sigma_{\text{data stats}}^2 + \sigma_{\text{MC stats}}^2 + \dots}$$

⇒ need enough MC to avoid spoiling the sensitivity!



# MC Statistics Requirements

e.g. **Discovery**: Total uncertainty:  $\sigma_S^2 \sim \sqrt{\sigma_{\text{data stats}}^2 + \sigma_{\text{MC stats}}^2 + \dots}$

⇒ need  $\sigma_{\text{MC stats}} \ll \sigma_{\text{data stats}}$   
 $B_{\text{MC}} \gg B_{\text{data}}$

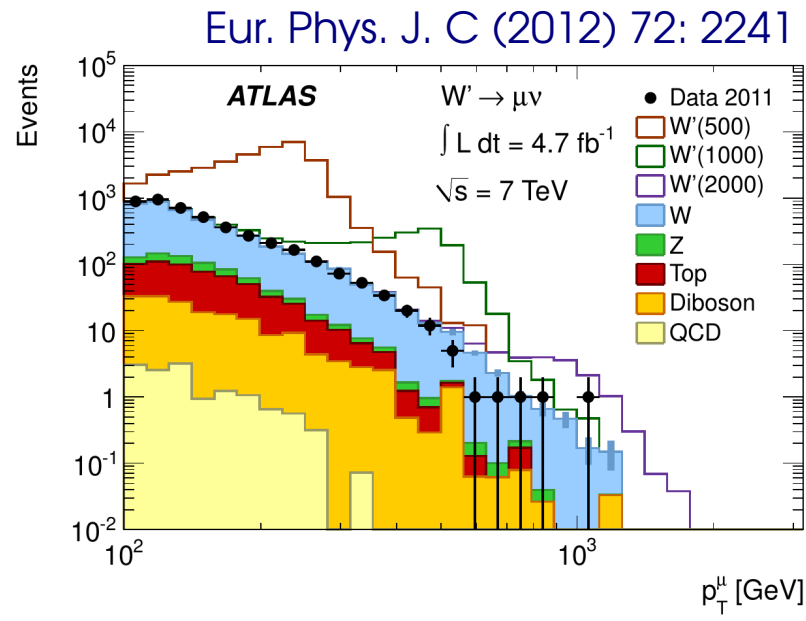
$B_{\text{MC}}/B_{\text{data}}$ ( $\alpha$ )	$\sigma_{\text{MC stats}}/\sigma_{\text{data stats}}$ ( $1/\sqrt{\alpha}$ )	$\sigma_{\text{data+MC stats}}/\sigma_{\text{data stats}}$ ( $\sqrt{1+\alpha^{-1}}$ )
1	1	<b>1.41</b>
4	0.5	<b>1.12</b>
25	0.2	<b>1.02</b>

By how much ?

In the presence of a signal (e.g. limit-setting,  $N_{\text{sig}}$  measurement), relevant uncertainty is  $\sqrt{(S+B)}$   
 ⇒ **S/B** also matters:

$$\frac{\sigma_S}{S} \sim \sqrt{1 + \frac{S}{B} + \frac{B_{\text{data}}}{B_{\text{MC}}} \frac{1}{1+S/B}}$$

- **low S/B** : same problem as for discovery
- **high S/B** : no issue, dominated by uncertainty on signal itself.



# PDF shapes: Unbinned likelihood

**Smooth backgrounds** : Describe distribution using appropriate **function**  
 ⇒ **Unbinned likelihood**. Describes sideband + signal region in one fit.

Phys. Rev. Lett. 118 (2017), 191801

Phys. Lett. B241 (1990) 278-282

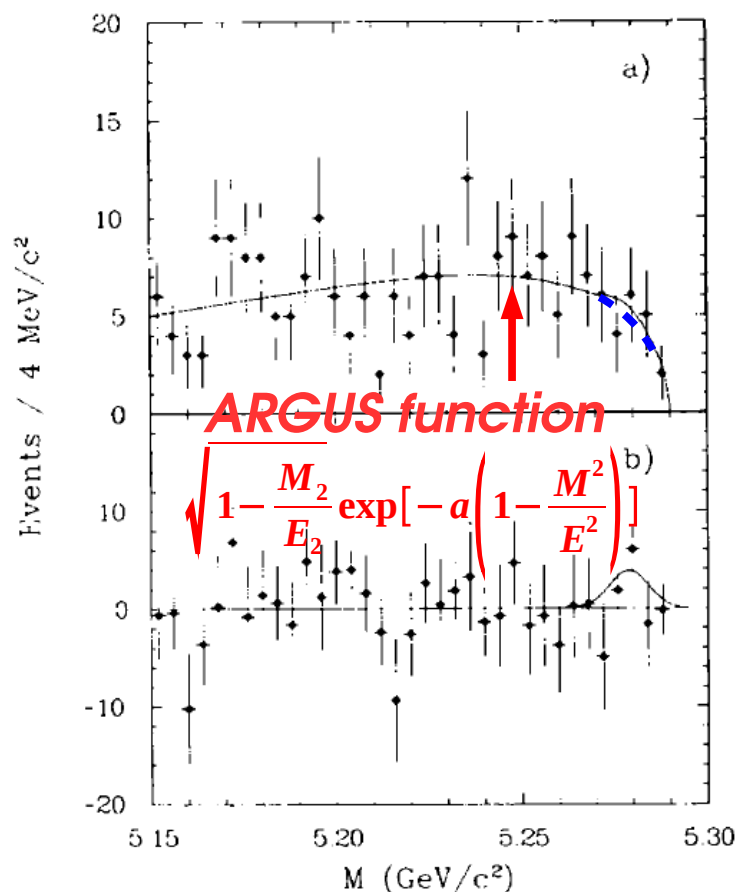
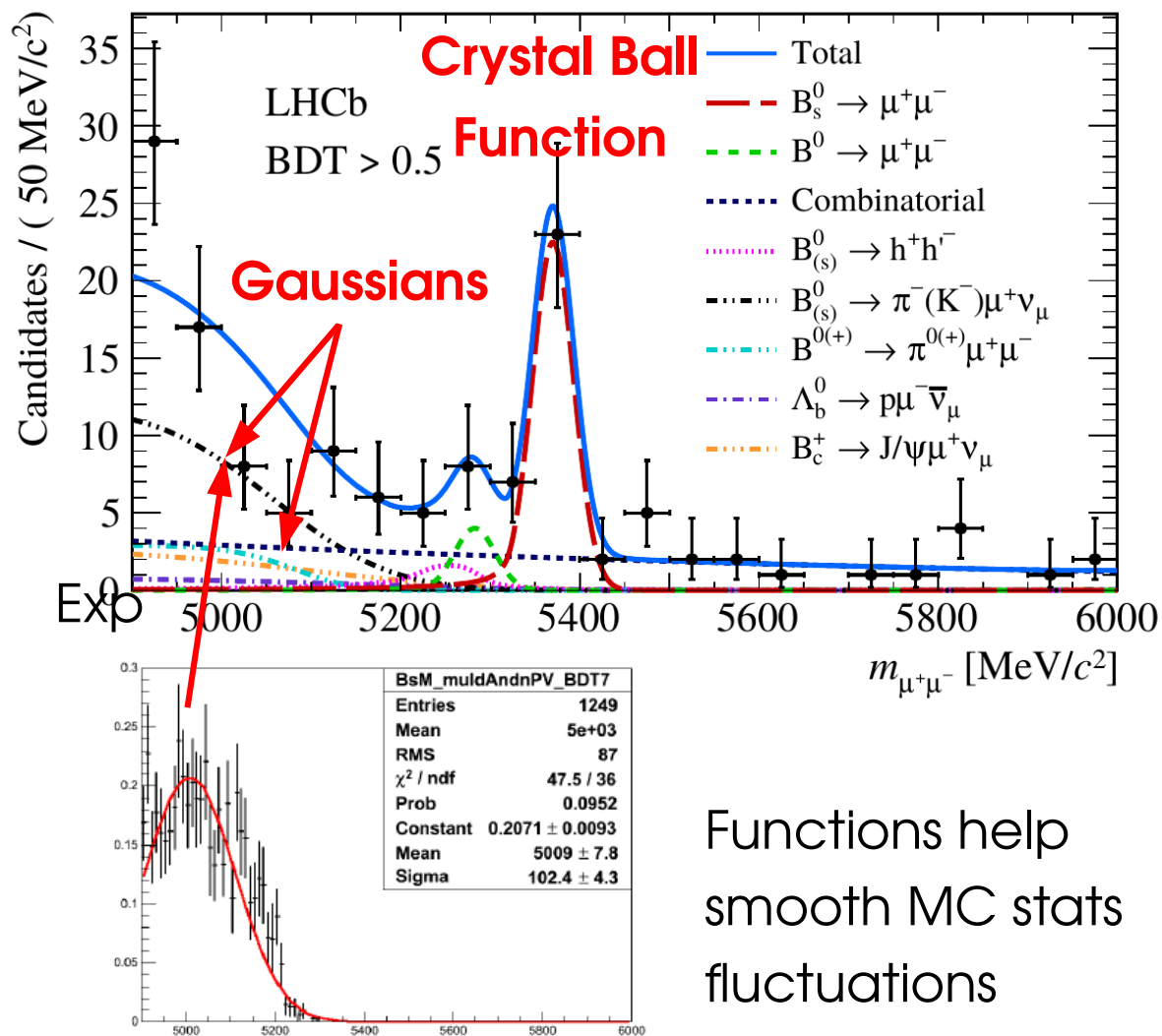


Fig. 1. Invariant mass distribution of the decay  $B^+ \rightarrow \pi^+ \pi^0$ . (a) At the  $\Upsilon(4S)$ ; the curve shows the result of the maximum likelihood fit described in the text. (b) After subtraction of the continuum contribution. The gaussian curve represents the 90% CL upper limit on the signal from the above fit (see table 1).

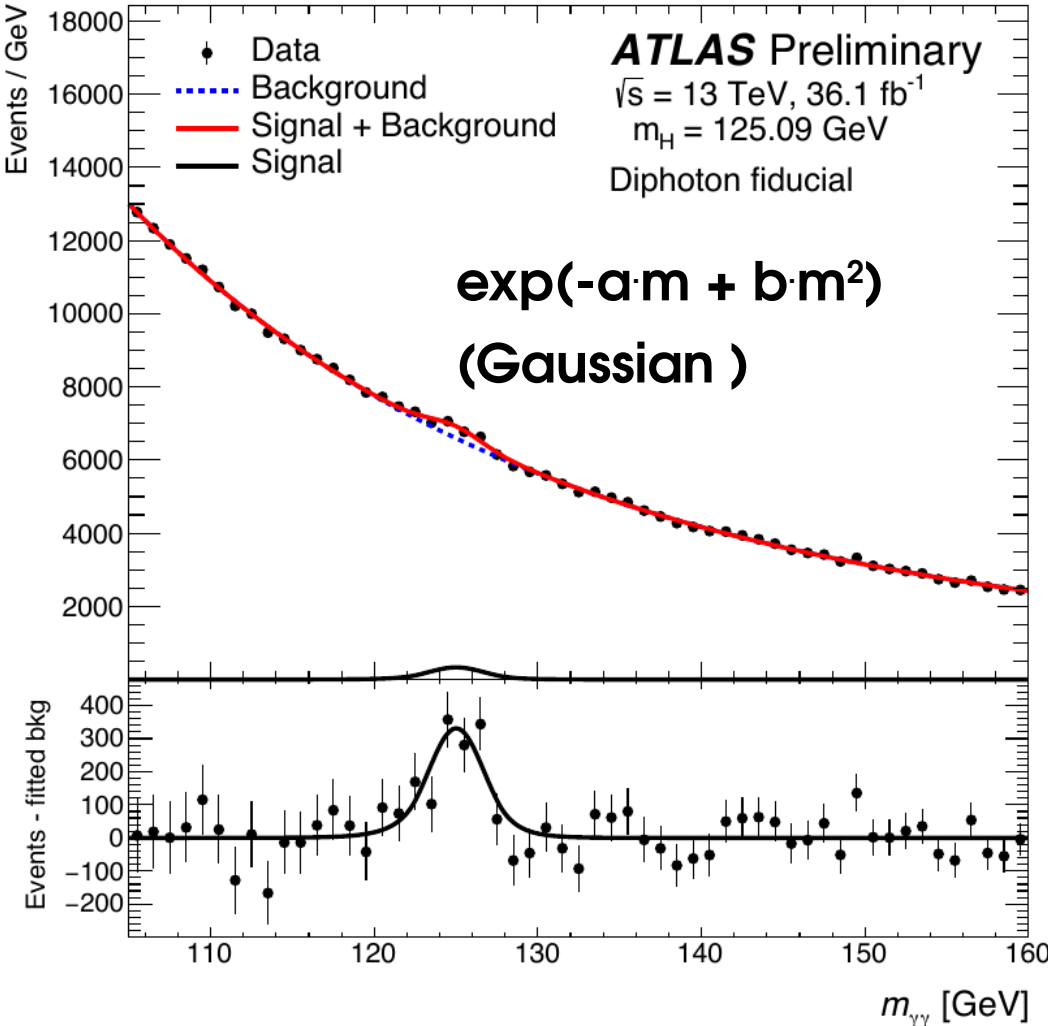


Functions help  
smooth MC stats  
fluctuations

# PDF Shapes: Unbinned likelihood

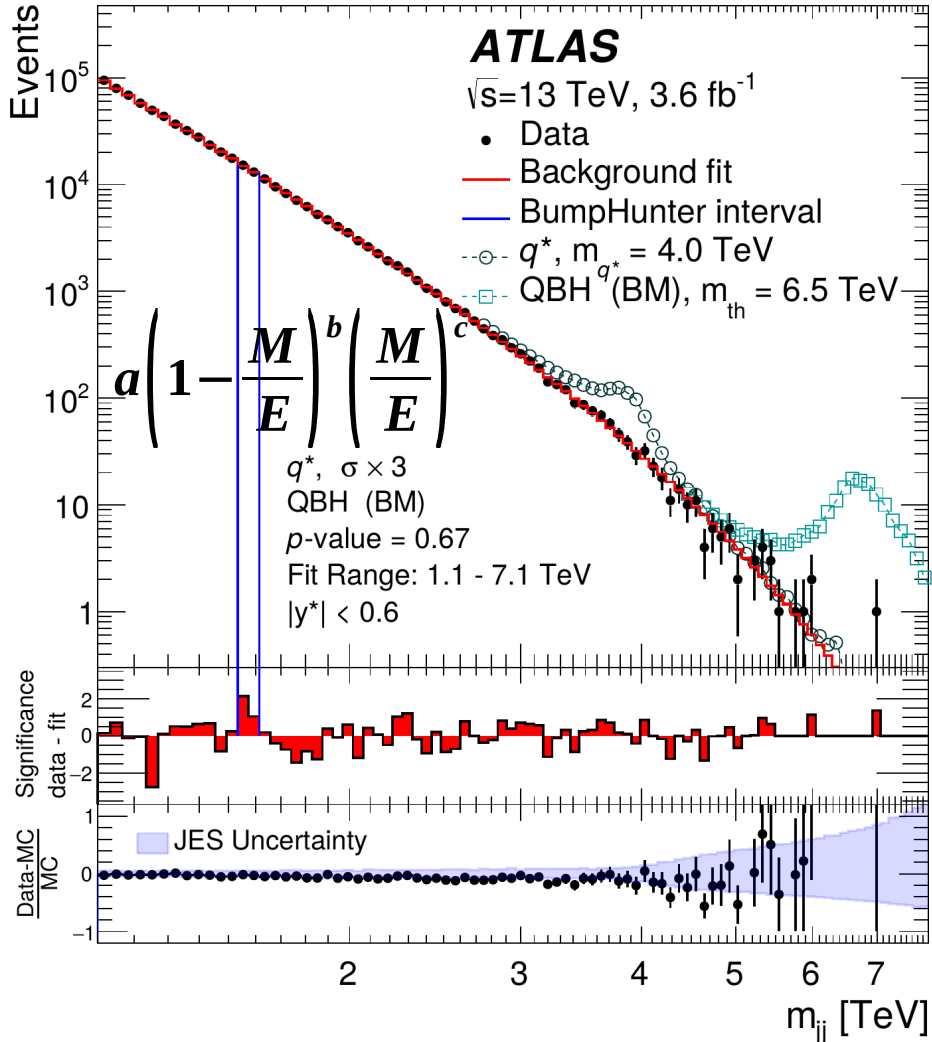
Widely used in HEP for smooth backgrounds (→ no resonances or threshold)

## H → γγ Measurements



## X → jj Search

Phys.Lett. B754 (2016) 302-322



# Signal Bias in Unbinned likelihoods

Function usually ad-hoc (no closed form expression for (theory  $\otimes$  detector effects), or usually even theory by itself...)

→ may not accurately describe the data

⇒ Introduce free parameters, fit in sidebands

→ Biases may still remain due to functional form itself

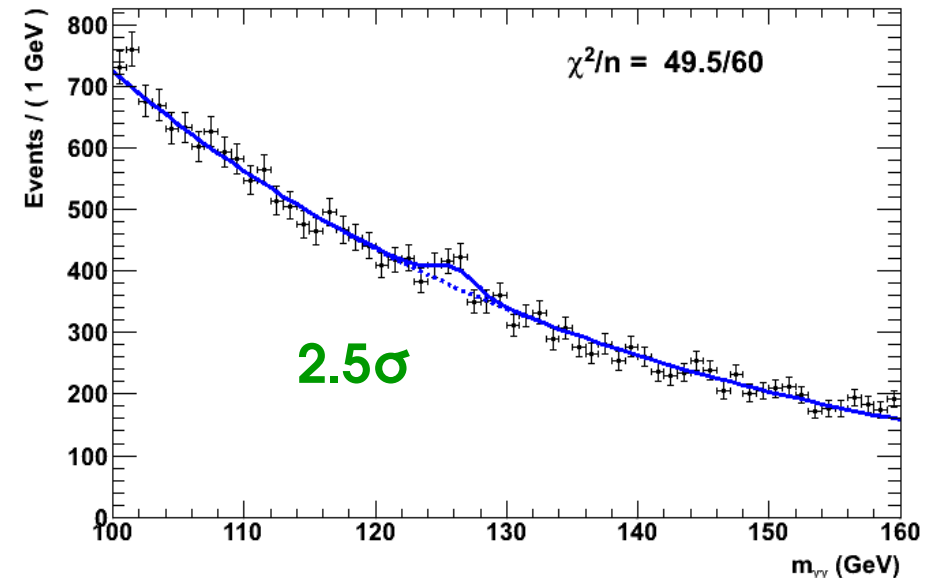
Jan 2012 Higgs search paper  
(4.9 fb<sup>-1</sup> of 2011 data)

exponential

Problematic especially for **low S/B**

→ small mismodelings of B can be large compared to S.

→  **$\chi^2$  test in sideband may not help**: even a large bias on the scale of S ( $\ll$  B) may remain within stat errors in the sideband!



Situation doesn't improve with more luminosity:

→ Reduced statistical uncertainties in sideband, but

→ Also reduced  $\sigma_s$ , in the same proportion

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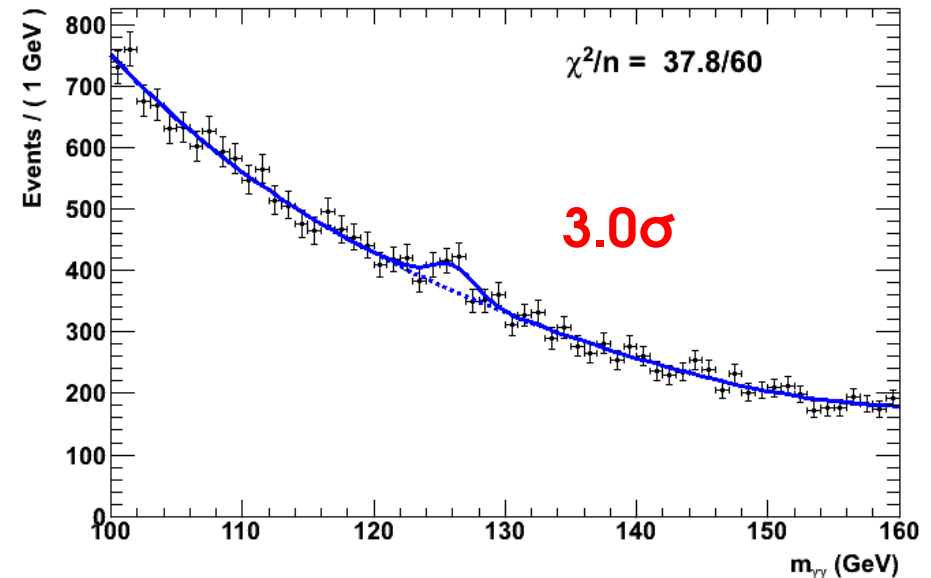
Jan 2012 Higgs search paper  
(4.9 fb<sup>-1</sup> of 2011 data)

polynomial

Problematic especially for **low S/B**

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Situation doesn't improve with more luminosity:

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# Signal Bias in Unbinned likelihoods

If data cannot fix B shape, **use MC**  
 → Measure signal bias  $N_{ss}$  on “credible” shapes taken from MC (**Spurious signal**)  
 → take the maximum bias as systematic

Works well if the true distribution is somewhere in the space of MC distributions scanned...

Also **Impose:**

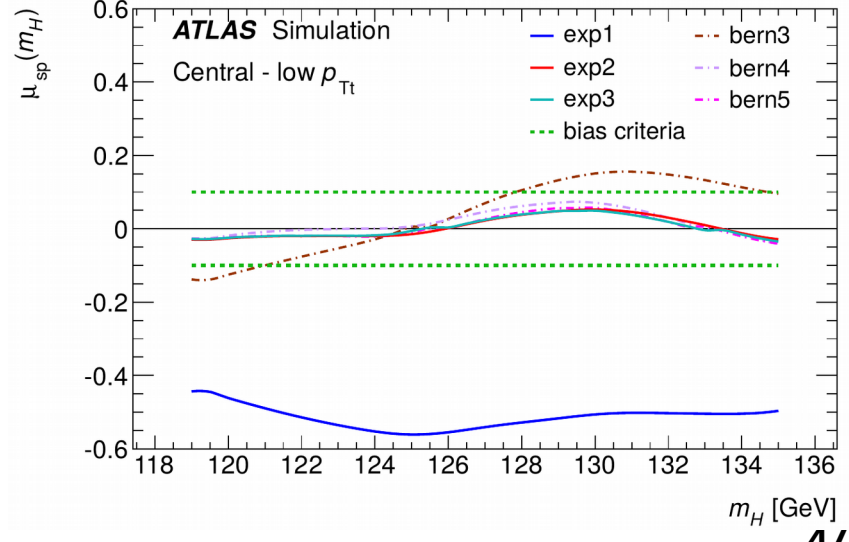
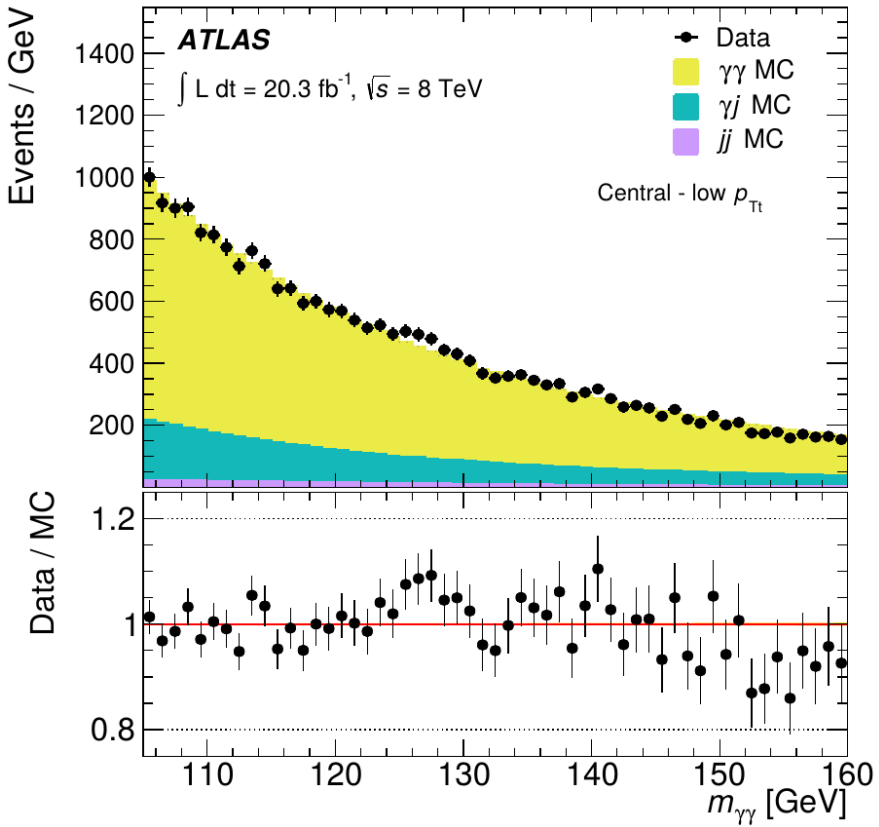
$N_{ss} < 20\% \sigma_{stat}$  (small contribution to  $\sigma_{total}$ )

**OR**

$N_{ss} < 10\% S_{exp}$  (small bias on measured S)

Second criterion more stringent at higher  $S/\sqrt{B}$ .

If criteria are not met, move to more complex functions (→ more free parameters)



# Signal Bias in Unbinned likelihoods

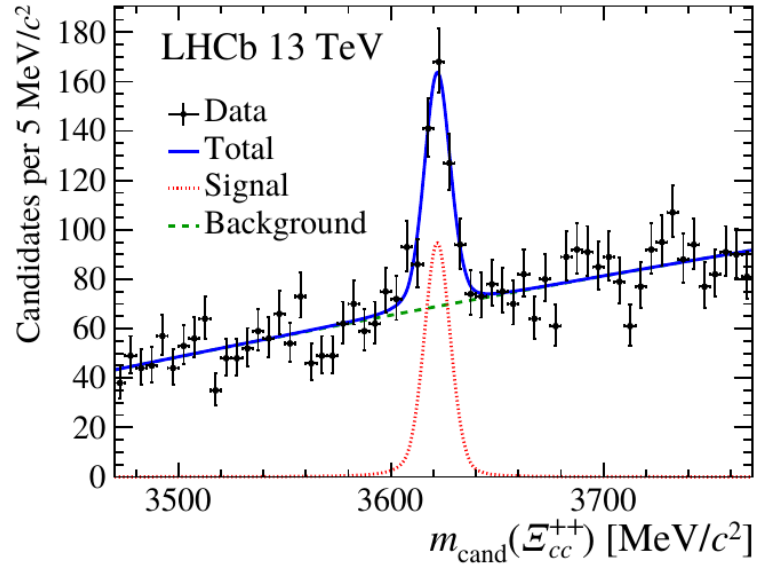
**Problem:** for small MC stats, measured bias dominated by fluctuations  
 → again, need high MC stats ( $B_{MC} > 25 B_{data}$ ) when S/B is low.

$B_{MC}/B_{data}$ ( $\alpha$ )	$\sigma_{MC\ stats}/\sigma_{data\ stats}$ ( $1/\sqrt{\alpha}$ )	$\sigma_{data+MC\ stats}/\sigma_{data\ stats}$ ( $\sqrt{1+\alpha^{-1}}$ )
1	100%	1.41
4	50%	1.12
25	20%	1.02

←  $N_{SS} < 20\% \sigma_{stat}$

→ Can compromise on criterion level  
 (50% instead of 20% ?)

→ As before, better situation at at high S/B



Phys. Rev. Lett. 118, 182001 (2017)



**Polynomials:** various basis choices (Chebyshev, Bernstein,...)

**Bernstein basis:**

$$B_{k,n}(x) = \binom{n}{k} x^k (1-x)^{n-k} \text{ for } 0 \leq x \leq 1$$

→ **Positive coefficients** ⇒ **positive polynomial everywhere**, useful to avoid numerical issues in  $-2 \log(\text{PDF})$  computation

**Exponential family** :  $\exp(\text{polynomial})$

**Power laws** :  $x^\alpha, x^\alpha(1-x)^\beta, \dots$

**Gaussians**

**Crystal Ball Functions**

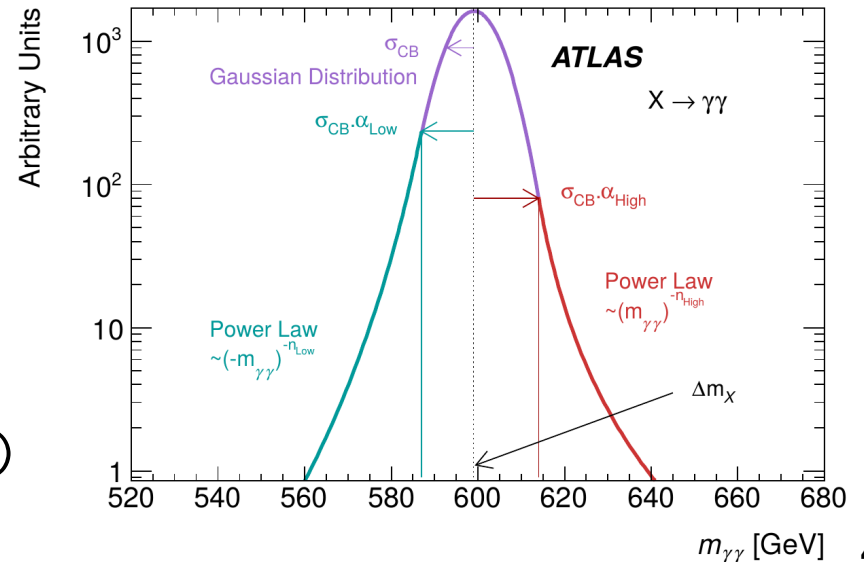
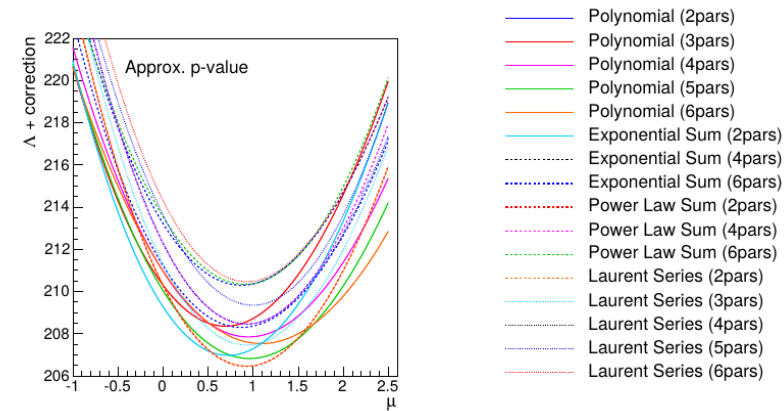
$$t = (m_{\gamma\gamma} - \mu_{\text{CB}}) / \sigma_{\text{CB}}$$

$$N \cdot \begin{cases} e^{-0.5t^2} & \text{if } -\alpha_{\text{low}} \leq t \leq \alpha_{\text{high}} \\ e^{-0.5\alpha_{\text{low}}^2} \left[ \frac{\alpha_{\text{low}}}{n_{\text{low}}} \left( \frac{n_{\text{low}}}{\alpha_{\text{low}}} - \alpha_{\text{low}} - t \right) \right]^{-n_{\text{low}}} & \text{if } t < -\alpha_{\text{low}} \\ e^{-0.5\alpha_{\text{high}}^2} \left[ \frac{\alpha_{\text{high}}}{n_{\text{high}}} \left( \frac{n_{\text{high}}}{\alpha_{\text{high}}} - \alpha_{\text{high}} + t \right) \right]^{-n_{\text{high}}} & \text{if } t > \alpha_{\text{high}}, \end{cases}$$

→ **Sums of the above**

→ **Convolutions** (resolution  $\otimes$  Breit-Wigner, ...)

JINST 10 (2015) no.04, P04015



# Discrete Profiling

**Idea:** treat the **type of function** and **number of parameters** as discrete NPs, profiled in data

→ **Let data choose the best shape**

→ Similar principle as other NPs, except for discrete nature

→ Need a **penalty on  $N_{\text{pars}}$**  to avoid always choosing functions with high  $N_{\text{pars}}$

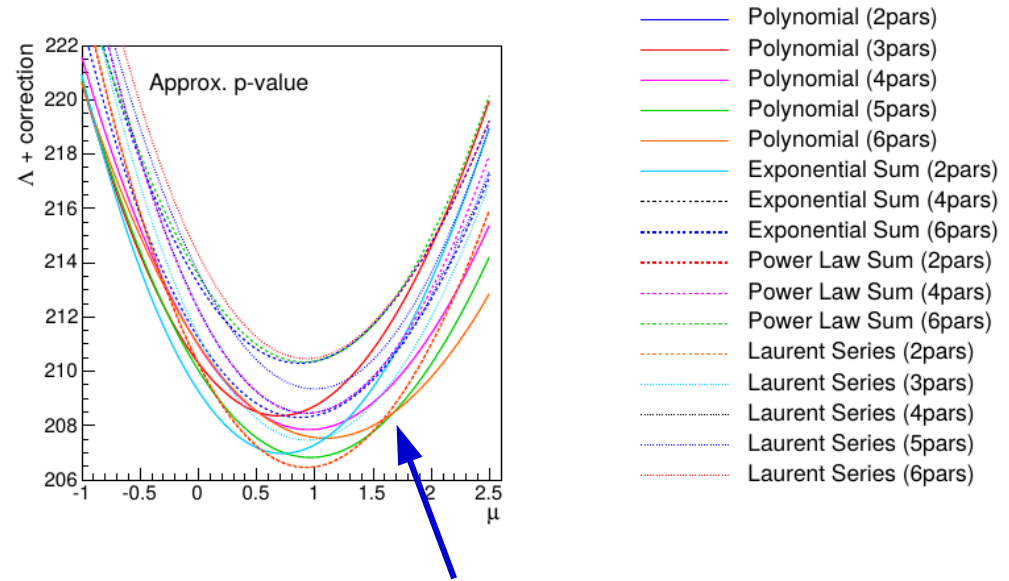
→ Used in the **CMS  $H \rightarrow \gamma\gamma$**  analysis, works well in this context.

## Caveats:

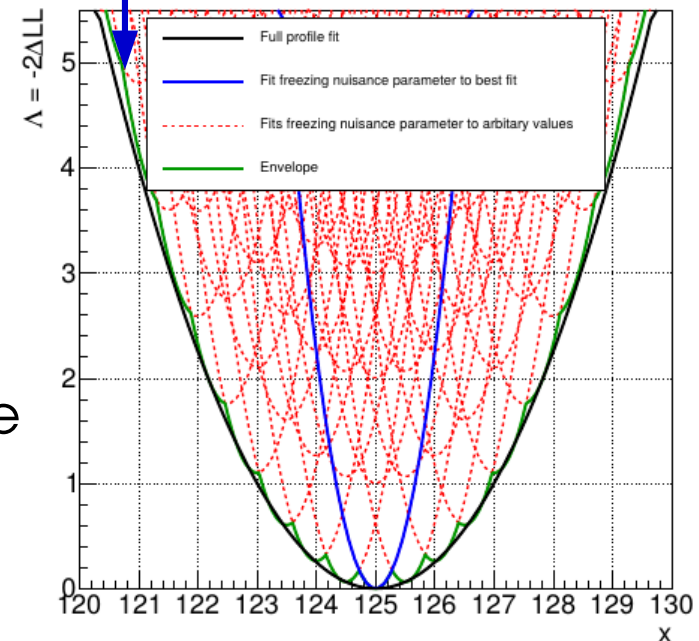
→ for  $N$  categories and  $M$  functional forms,  **$M^N$  possibilities to check** in principle – difficult in practice

→ Need a **well-chosen pool of sensible functions** for the method to work

→ **Large MC samples** for selection and checks



**Take lower envelope of all functions when profiling**



# Gaussian Processes: 1-slide Summary

---

the data are drawn from one

**HUGE**<sup>\*</sup>  
**Gaussian**

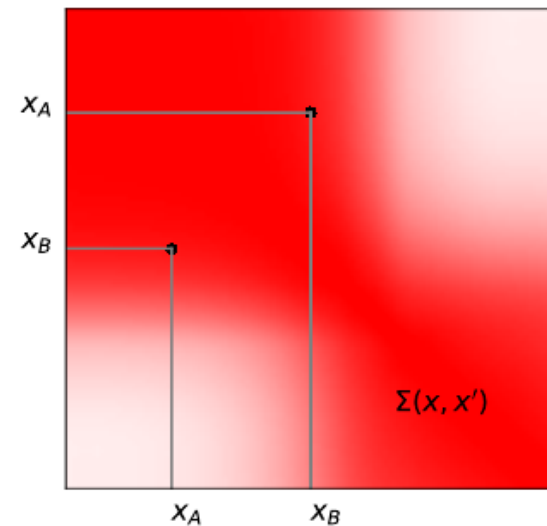
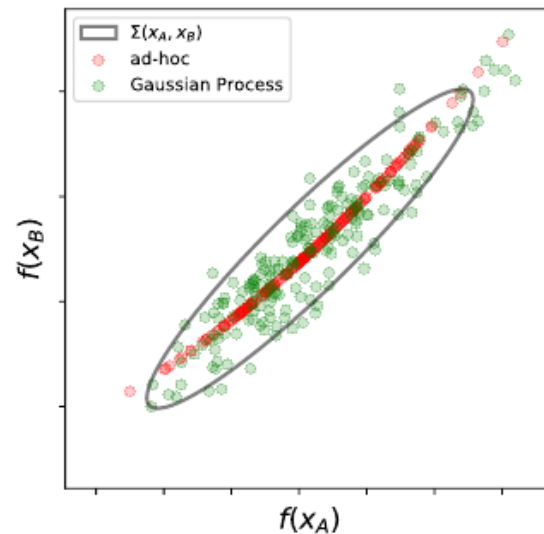
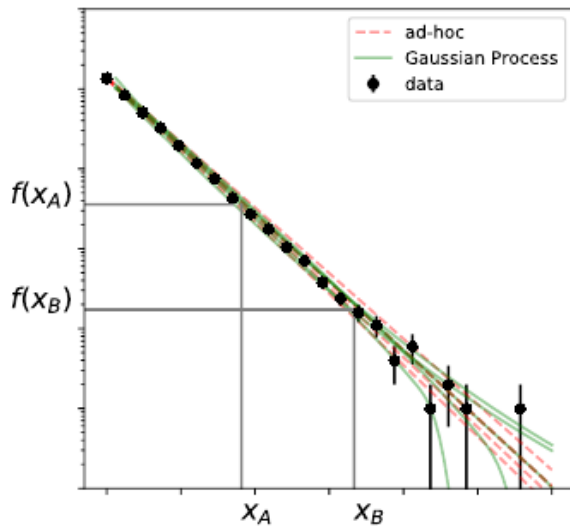
<sup>\*</sup> the dimension is the number of data points.

Image Credits:  
K. Cranmer

# Gaussian Processes: Longer 1-slide Summary

- Describe background distribution through the **correlations between values at different points**.
- More flexible than a functional form
- **Correlation function (Kernel)** can be
  - Defined using a length scale, to ignore narrow peaks
  - Obtained from first principles (e.g. from known JES/PDF effects)

$$K(x_1, x_2) = \exp\left[-\frac{(x_1 - x_2)^2}{2L^2}\right]$$



arXiv:1709.05681

- ⊕ More flexible than functional form, degrees of freedom less ad-hoc
- ⊖ Still need large MC samples to check for signal bias
- ⊖ Mainly for Gaussian processes, not well-adapted to Poisson regime

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# **Statistical Modeling:**

## **II. Systematics**

# Systematics NPs

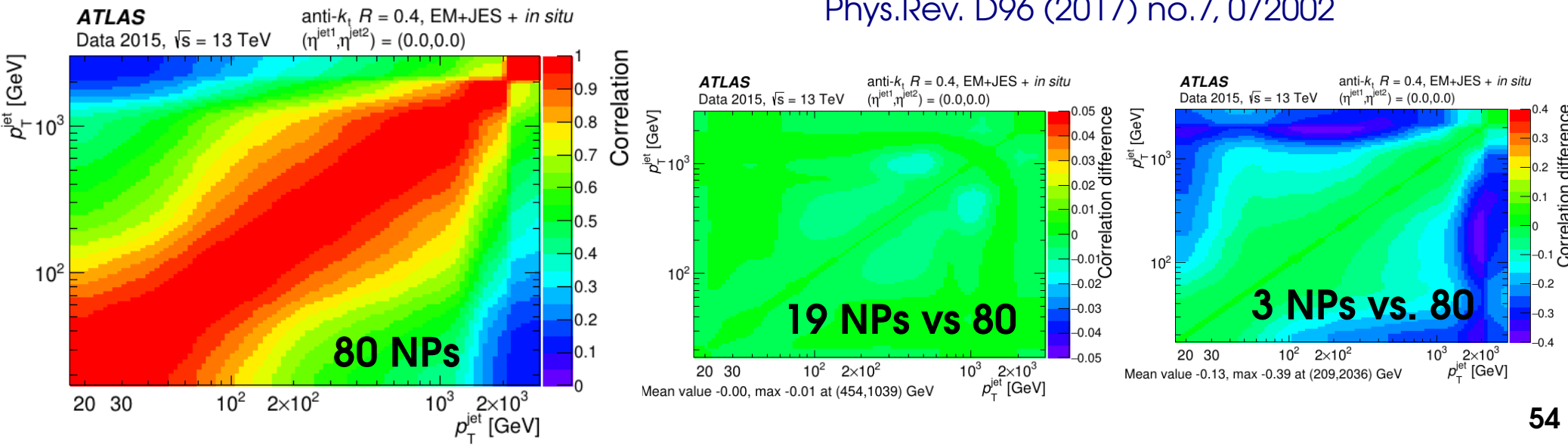
Each systematics NP represent **an independent source of uncertainty**  
 ⇒ Usually constrained by a single 1-D PDF (Gaussian, etc.)

Sometimes multiple parameters **conjointly constrained** by an n-dim. PDF.  
 → multiple measurements constraining multiple NPs

Assume **n-dim Gaussian** PDF: then can **diagonalize the covariance matrix C**  
 and re-express the uncertainties in basis of eigenvector NPs ⇒ **n 1-dim PDFs**

Can also diagonalize to **prune** irrelevant uncertainties: keep NPs with large eigenvalues, combine in quadrature the others

Phys.Rev. D96 (2017) no.7, 072002



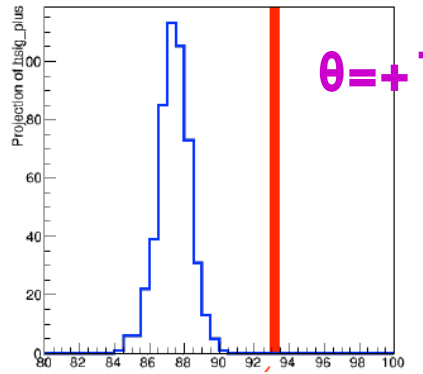
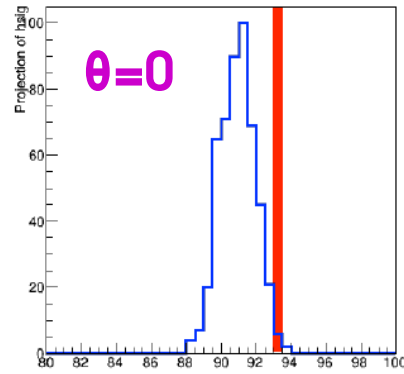
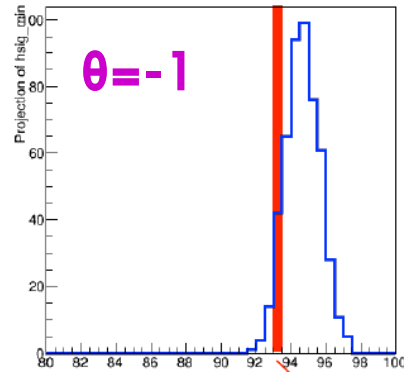
# Systematics : Impact on Model

The effect of **each NP**  $\theta_i$  should be propagated to all the relevant **model parameters**  $X_j$ .

→ **Propagation through MC:**

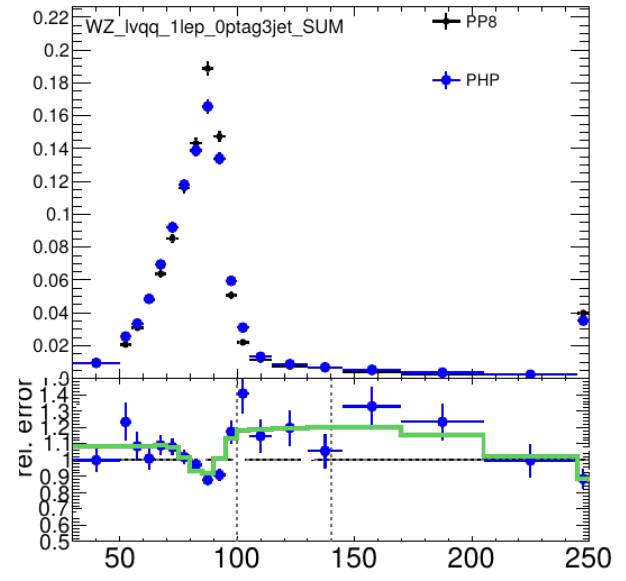
1. Apply  $\pm 1\sigma$  systematic variations in MC,
  - ⇒ obtain shifted values  $X_j^{\pm} = X_j^0 (1 \pm \Delta_{ij})$ .
  - Possibly smooth out MC stats effects

2. Implement systematic in model, e.g. replace or morph shapes:



→ can affect event yields, shapes, etc.

Assumes **Gaussian uncertainties** and **linear impact** on model parameters



Constrained by unit Gaussian

$$X_j \rightarrow X_j^0 (1 + \Delta_{ij} \theta_i)$$

# Systematics : Constraints

Ideally, constraint = **likelihood of auxiliary measurement**

⇒ e.g. Poisson for constraint from counting in a low-stat CR.

Sometimes no clear auxiliary measurement

⇒ Semi-arbitrary “pseudo-measurement” motivated by Central Limit Theorem:

- **Gaussian** for additive corrections
- **Log-normal** for multiplicative corrections

**Gaussian:**

- represent impact as  $X_j \rightarrow X_j^0 (1 + \Delta_{ij} \theta_i)$   
→ or similar morphing for distributions

**Constrained by unit Gaussian**

Can include asymmetric variations  $\Delta^+, \Delta^-$ :  $X_j \rightarrow X_j^0 \left( 1 + \begin{cases} \Delta_{ij}^+ \theta_i & \theta_i > 0 \\ \Delta_{ij}^- \theta_i & \theta_i < 0 \end{cases} \right)$

However discontinuity in derivative at 0, so use smooth interpolation instead, e.g. implementation in `RooStats::HistFactory::FlexibleInterpVar`.



# Systematics : Log-normal Constraint

**Log-normal:**  $x \sim \text{log-normal}$  if  $\log(x)$  is normal  
 → **always**  $> 0$ , useful to avoid numerical issues  
 → **PDF:**

$$P(s; X_0, \kappa) = \frac{1}{x \kappa \sqrt{2\pi}} \exp\left(-\frac{1}{2} \left(\frac{\log(x) - X_0}{\kappa}\right)^2\right)$$

However usually simpler to implement as :

$$X_j \rightarrow X_j^0 \exp(\kappa_{ij} \theta_i)$$

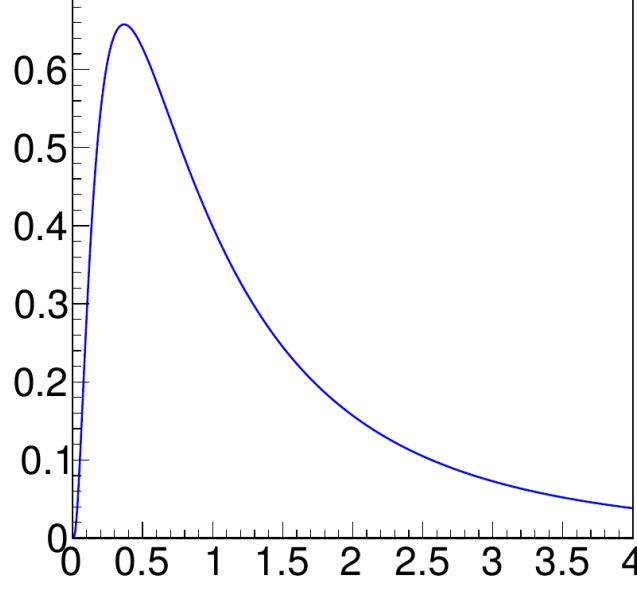
where  $\theta_i$  is constrained by a unit Gaussian as usual

→ Correct form for a multiplicative uncertainty:

$$\log \sqrt[n]{(X_0 k_1)(X_0 k_2) \dots (X_0 k_n)} = \frac{1}{n} \sum_{i=1}^n \log(X_0 k_i) \stackrel{n \rightarrow \infty}{\sim} G(\log X_0, \frac{\text{RMS}(\log(k))}{\sqrt{n}} = \kappa)$$

Similarly to Gaussian → represent  $X = X_0 e^{\kappa\theta} \sim G(\log X_0, \kappa)$  if  $\theta \sim G(0,1)$

**Which  $\kappa$  to use ?**  $\kappa = \text{RMS}(X)$  only at first order. For larger uncertainties,  
 e.g. **Match  $\pm 1\sigma$  variations:**  $X_j(\theta=\pm 1) = X_j^\pm \Rightarrow \kappa_\pm = \pm \log(X_j^\pm / X_j^0)$



Implemented in RooStats::HistFactory::FlexibleInterpVar.

# Systematics : Theory Constraints

---

**Missing high-order terms in perturbative calculations:** evaluate from scale variations – but no underlying random process. Possible constraint shapes:

- **Gaussians** (ATLAS/CMS Higgs analyses, see [Yellow Report 4, I.4.1.d](#))

- Usually several independent “sources” of uncertainty (QCD/EW/resummation)
- ⇒ overall uncertainty may be rather Gaussian
- Numerically well-behaved
- Uncertainties add in quadrature as usual

- **Flat constraints** : “100% confidence” intervals

- no preference for any value in the range
- Need regularization to avoid numerical issues
- uncertainties add linearly

→ For Higgs cross-sections, rather similar results for both cases

# Constraints : Two-point systematics

Sometimes differences between 2 discrete cases → e.g. Pythia vs. Herwig  
Solutions:

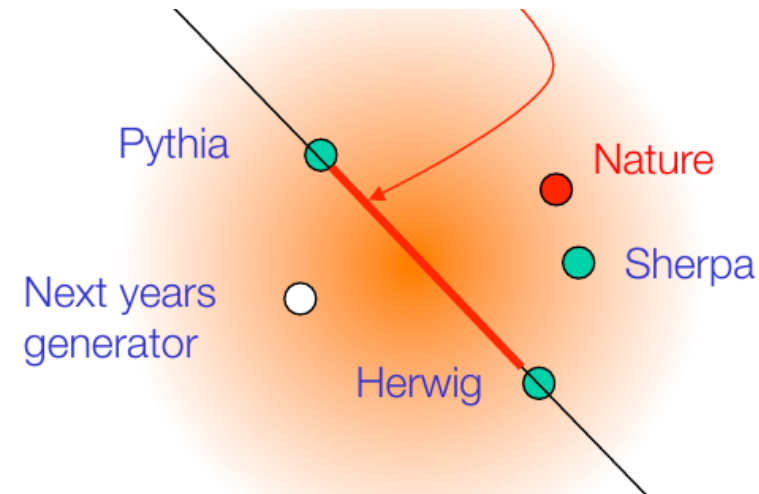
- Results for one case only
- Full results for both cases
- Single result with an uncertainty that covers the difference  
→ **Two-point uncertainty**

Usually implemented as **1D linear interpolations** between the two cases  
→ However cannot guarantee this covers the space of possible configurations

⇒ ***This is not even a pseudo-measurement...***

Ideally, need to define proper uncertainties within a single model, which would cover the other cases  
→ e.g. showering uncertainties within Pythia, covering Herwig

→ **Usually a difficult task**

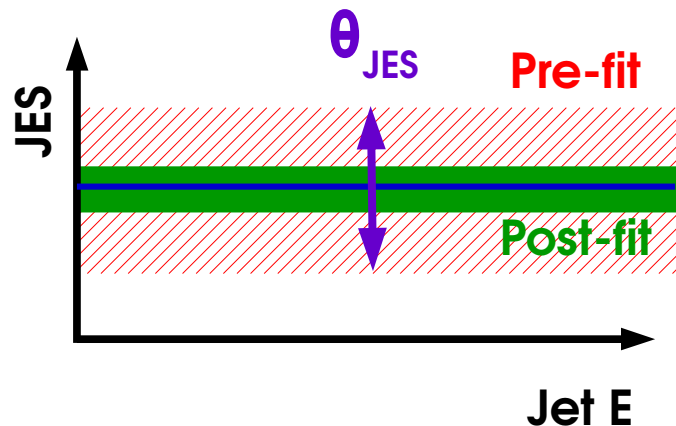


# Profiling Issues

**Too simple modeling** can have unintended effects

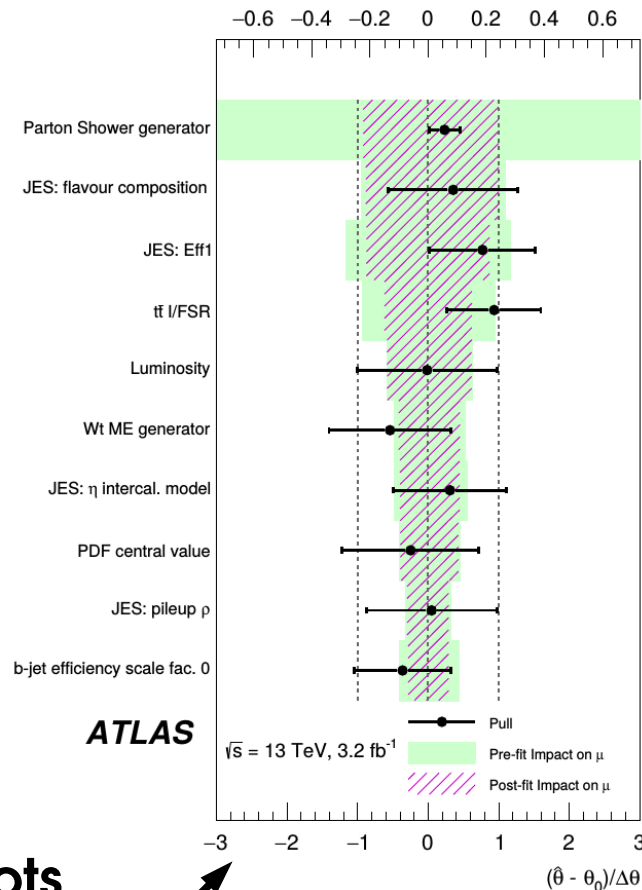
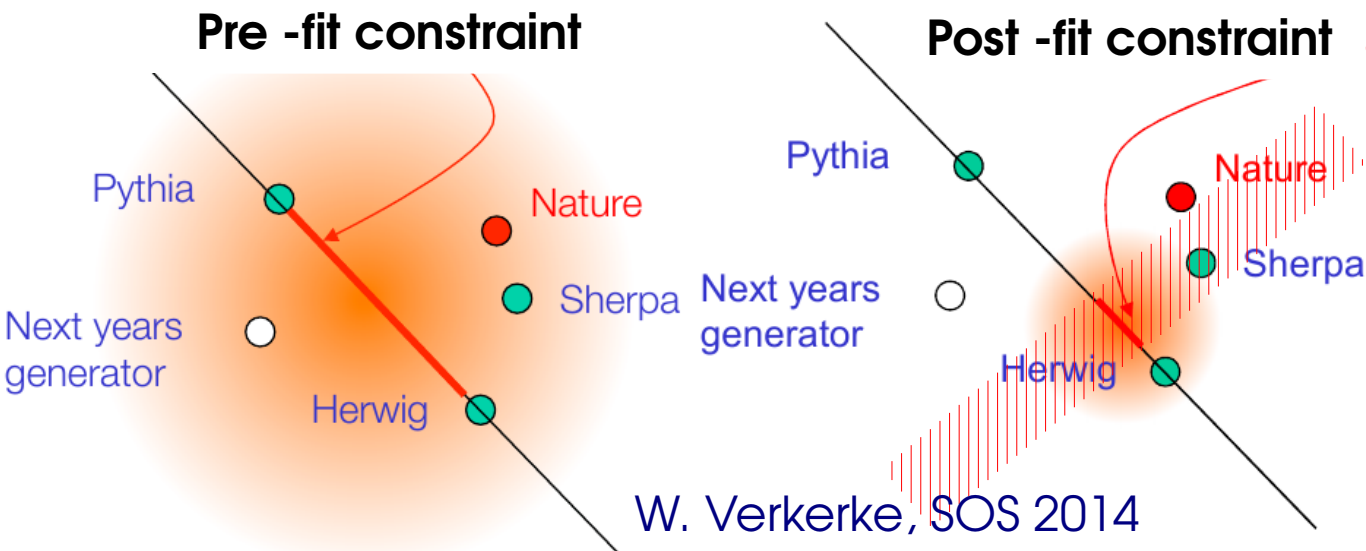
→ e.g. single Jet E scale parameter:

⇒ Low-E jets calibrate high-E jets – intended ?



**Two-point uncertainties:**

→ Interpolation may not cover full configuration space, can lead to too-strong constraints



**NP central values and uncertainties in pull/impact plots provide important “debugging” information for profiling**

# Outline

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Profiling

Look-Elsewhere Effect

Bayesian methods

Statistical modeling in practice

Building binned likelihoods

Choosing PDFs in unbinned likelihoods

Implementing systematics

**BLUE**

---

***BLUE***

# BLUE

Commonly-used ansatz for combination of measurements:

1. **Build a  $\chi^2$ :** (same as  $-2\log L$  for Gaussian L)

$$\chi^2(\mathbf{X}) = \sum_i \left( \mathbf{X}_i^{\text{obs}} - \mathbf{X} \right) \mathbf{C}_{ij}^{-1} \left( \mathbf{X}_j^{\text{obs}} - \mathbf{X} \right)$$

$\mathbf{C}_{ij}$ : covariance matrix of measurements:

$$\mathbf{C} = \begin{bmatrix} \sigma_1^2 & \rho \sigma_1 \sigma_2 & \cdots \\ \rho \sigma_1 \sigma_2 & \sigma_2^2 & \cdots \\ \vdots & \vdots & \ddots \end{bmatrix}$$

$\rho$ : correlation coefficients

2. **Estimate combined X from minimum of  $\chi^2(\mathbf{X})$**

- In the Gaussian case, equivalent to ML solution  $\Rightarrow$  inherits good properties:
  - **Unbiased** :  $\langle \hat{\mathbf{X}} \rangle = \mathbf{X}^*$
  - **Optimal**: minimizes the combined uncertainty
- Solution is a linear combination of the inputs:

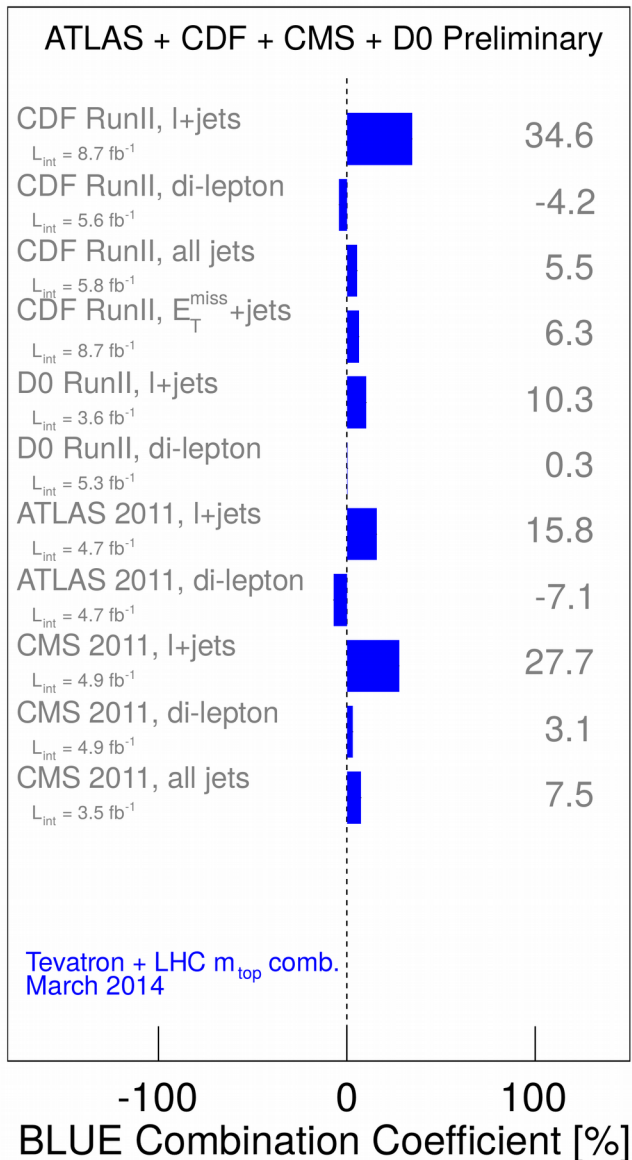
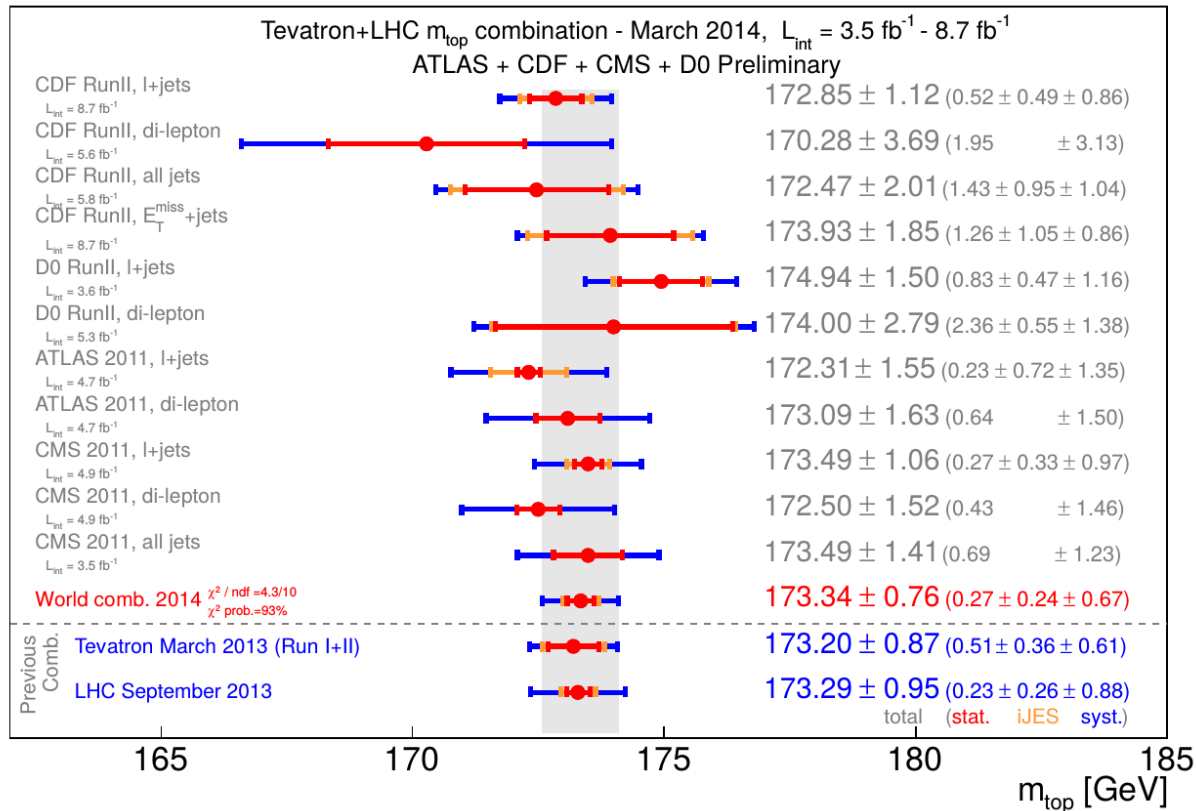
$$\boldsymbol{\lambda} = \frac{\mathbf{C}^{-1} \mathbf{J}}{\mathbf{J}^T \mathbf{C}^{-1} \mathbf{J}}, \quad \mathbf{J} = \begin{pmatrix} 1 \\ 1 \\ \vdots \end{pmatrix}$$

$\lambda_i$  = combination weight of measurement i

$$\hat{\mathbf{X}} = \sum_i \lambda_i \mathbf{X}^{\text{obs}, i}$$

$\Rightarrow$  “**Best Linear Unbiased Estimator**” (**BLUE**)

## Example: World $m_{\text{top}}$ combination



**Limitation:** relies on **Gaussian assumptions** (satisfied in this case!)

Negative weights possible! (for large correlations, see [Eur. Phys. J. C 74 \(2014\), 2717](#))



# BLUE and PLR

**PLR Computation:** 2 measurements  
+ 1 auxiliary measurement

$$\begin{aligned} X_1 &= X + \Delta_1 \theta \sim G(X^*, \sigma_1) \\ X_2 &= X + \Delta_2 \theta \sim G(X^*, \sigma_2) \\ \theta &\sim G(0, 1) \end{aligned}$$

**Single measurement:**  $\lambda(X, \theta) = \frac{1}{\sigma_1^2} (X + \Delta_1 \theta - X_1^{\text{obs}})^2 + (\theta - \theta^{\text{obs}})^2$

**MLEs:** 
$$\begin{cases} \hat{\theta} = \theta^{\text{obs}} \\ \hat{X} = X_1^{\text{obs}} - \Delta_1 \theta^{\text{obs}} \end{cases}$$

**PLR:** 
$$\lambda(X) = \frac{(X - \hat{X})^2}{\sigma_{1, \text{tot}}^2} \quad \sigma_{1, \text{tot}}^2 = \sigma_1^2 + \Delta_1^2$$

**Combination:** 
$$\lambda(X, \theta) = \frac{1}{\sigma_1^2} (X + \Delta_1 \theta - X_1^{\text{obs}})^2 + \frac{1}{\sigma_2^2} (X + \Delta_2 \theta - X_2^{\text{obs}})^2 + (\theta - \theta^{\text{obs}})^2$$

**MLE:** 
$$\hat{X} = \lambda_1 X_1^{\text{obs}} + \lambda_2 X_2^{\text{obs}} + \lambda_\theta \theta^{\text{obs}} \quad \lambda_{1(2)} = \frac{\sigma_{2(1), \text{tot}}^2 - \Delta_1 \Delta_2}{\sigma_{1, \text{tot}}^2 + \sigma_{2, \text{tot}}^2 - 2\Delta_1 \Delta_2}$$

**PLR:** 
$$\lambda(X) = \frac{(X - \hat{X})^2}{\sigma_{X, \text{tot}}^2} \quad \sigma_{X, \text{tot}}^2 = \frac{\sigma_{1, \text{tot}}^2 \sigma_{2, \text{tot}}^2 - \Delta_1^2 \Delta_2^2}{\sigma_{1, \text{tot}}^2 + \sigma_{2, \text{tot}}^2 - 2\Delta_1 \Delta_2}$$

**BLUE computation:** measurements  $X_1$  and  $X_2$  with uncorrelated statistical uncertainties  $\sigma_1$  and  $\sigma_2$ , correlated systematics  $\Delta_1$  and  $\Delta_2$ .

**Single measurement:** stat uncertainty  $\sigma_1$ , systematic  $\Delta_1$

- Uncorrelated uncertainties
  - Assume everything is Gaussian
- ⇒ Uncertainties add

in quadrature:

$$\sigma_{1, \text{tot}}^2 = \sigma_1^2 + \Delta_1^2$$

**Combination:**

$$C = \begin{bmatrix} \sigma_{1, \text{tot}}^2 & \rho \sigma_{1, \text{tot}} \sigma_{2, \text{tot}} \\ \rho \sigma_{1, \text{tot}} \sigma_{2, \text{tot}} & \sigma_{2, \text{tot}}^2 \end{bmatrix} \quad \rho = \frac{\Delta_1 \Delta_2}{\sigma_{1, \text{tot}} \sigma_{2, \text{tot}}}$$

**BLUE weights**

$$\hat{X} = \lambda_1 X_1^{\text{obs}} + \lambda_2 X_2^{\text{obs}}$$

$$\lambda_{1(2)} = \frac{\sigma_{2(1), \text{tot}}^2 - \rho \sigma_{1, \text{tot}} \sigma_{2, \text{tot}}}{\sigma_{1, \text{tot}}^2 + \sigma_{2, \text{tot}}^2 - 2\rho \sigma_{1, \text{tot}} \sigma_{2, \text{tot}}}$$

Propagate uncertainties from C:

$$\sigma_{X, \text{tot}}^2 = \frac{\sigma_{1, \text{tot}}^2 \sigma_{2, \text{tot}}^2 (1 - \rho^2)}{\sigma_{1, \text{tot}}^2 + \sigma_{2, \text{tot}}^2 - 2\rho \sigma_{1, \text{tot}} \sigma_{2, \text{tot}}}$$

# Negative BLUE Weights

Occasionally, negative BLUE weights:

Can happen if  $\rho \sim 1$ :

$$\lambda_2 = \frac{\sigma_{1, \text{tot}} (\sigma_{1, \text{tot}} - \rho \sigma_{2, \text{tot}})}{\sigma_{1, \text{tot}}^2 + \sigma_{2, \text{tot}}^2 - 2\rho \sigma_{1, \text{tot}} \sigma_{2, \text{tot}}} < 0 \text{ for } \rho > \frac{\sigma_{1, \text{tot}}}{\sigma_{2, \text{tot}}}$$

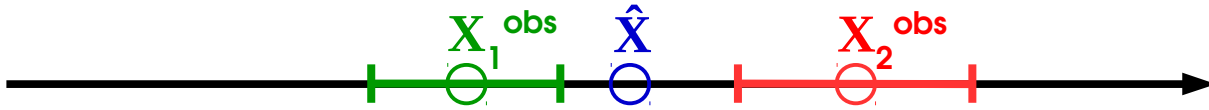
Not intuitive! (Can also have  $\lambda_2 = 0$  for  $\sigma_{1, \text{tot}} = \rho \sigma_{2, \text{tot}}$ ...)

Can be explained in the PLR picture:

$$X_1 = X + \Delta \theta$$

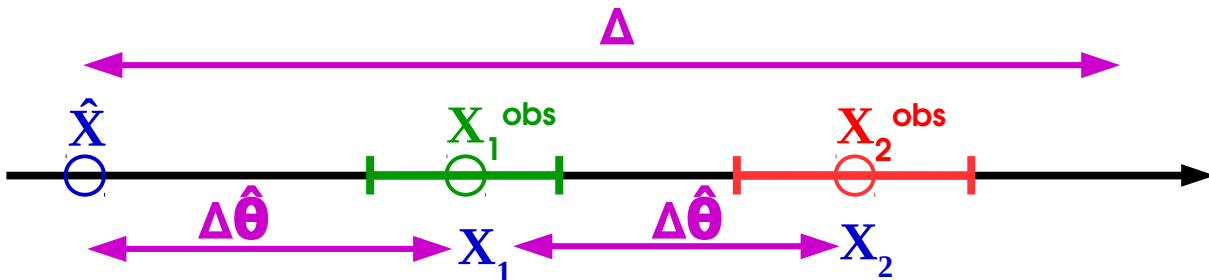
$$X_2 = X + 2\Delta \theta$$

Without correlated systematics ( $\Delta = 0$ ):



$$\lambda_{1(2)} = \frac{\sigma_{2(1)}^2}{\sigma_1^2 + \sigma_2^2} > 0$$

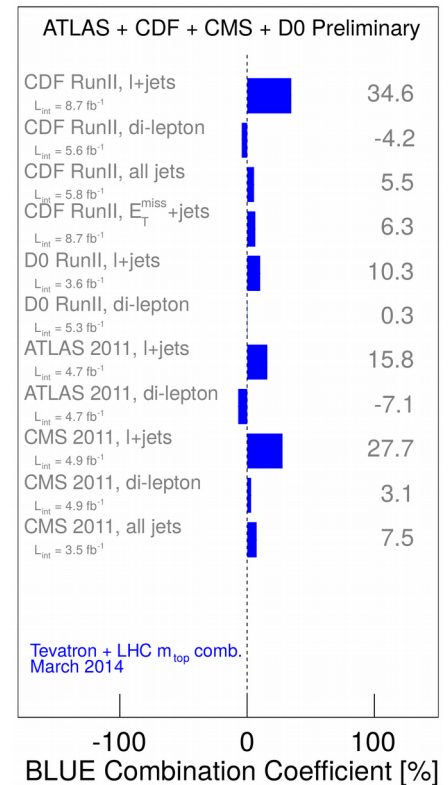
With large correlated systematics ( $\Delta \gg \sigma_{1,2}$ )



$\hat{\theta}$  value makes  $X_1$  and  $X_2$  match observations, small pull on  $\theta$  if  $\Delta$  is large

$$\lambda_1 < 0$$

$\rho \sim 1 \Rightarrow \theta$  measurement is important  $\Rightarrow$  possibly very different MLE than  $X_1 \oplus X_2 \dots$



# Uncertainty Decomposition

Often useful to break down uncertainties into components (stat + syst, etc.)

**PLR approach:** perform measurement twice

1. With all uncertainties included  
→ **nominal uncertainty**  $\sigma_{\text{total}}$
2. Removing some uncertainties  
(e.g. all syst uncertainties) →  $\sigma_{\text{no-syst}}$

⇒ Subtract in quadrature:

$$\sigma_{\text{syst}} = \sqrt{\sigma_{\text{total}}^2 - \sigma_{\text{no-syst}}^2}$$

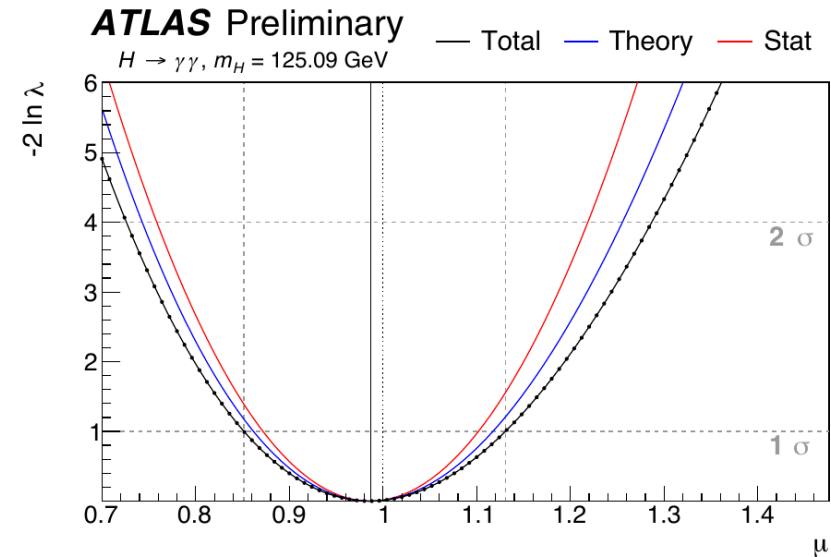
**BLUE-based approach:**

1. Propagate each source of uncertainty (stat & syst) to the observables
2. Propagate through to the measurement using the BLUE weights

$$\hat{X} = \sum_i \lambda_i X^{\text{obs},i}$$

**The two methods are not completely equivalent** (recently discovered!)

→ In the BLUE case, weights still computed including systematics effects



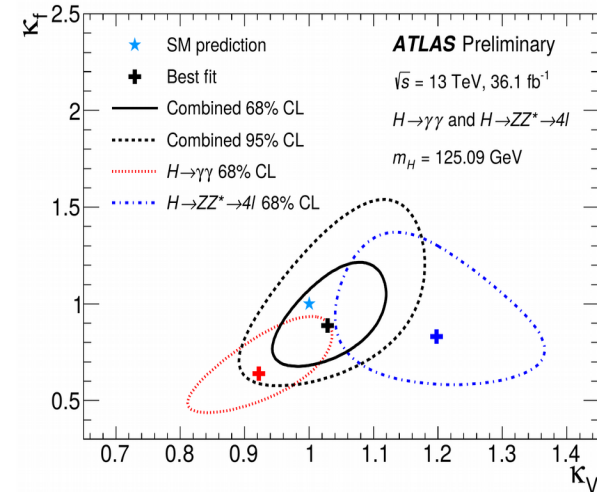
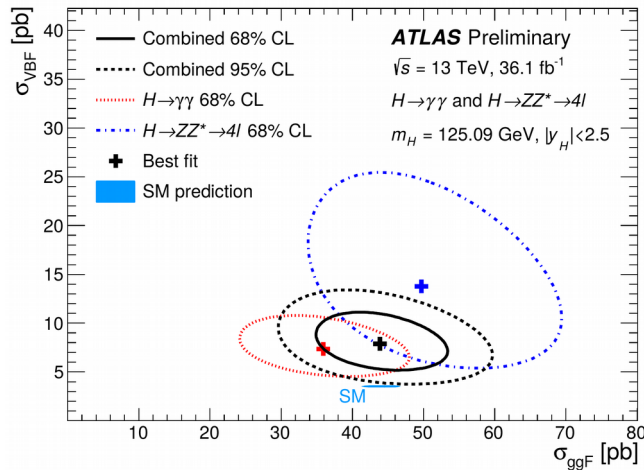
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# Presentation of Results

# Presentation of Results

Measurements often recast to constrain a particular theory model.

→ Ideally, by **reparameterizing the likelihood** and repeating the measurement



⇒ **Done by experiments for selected benchmark models**

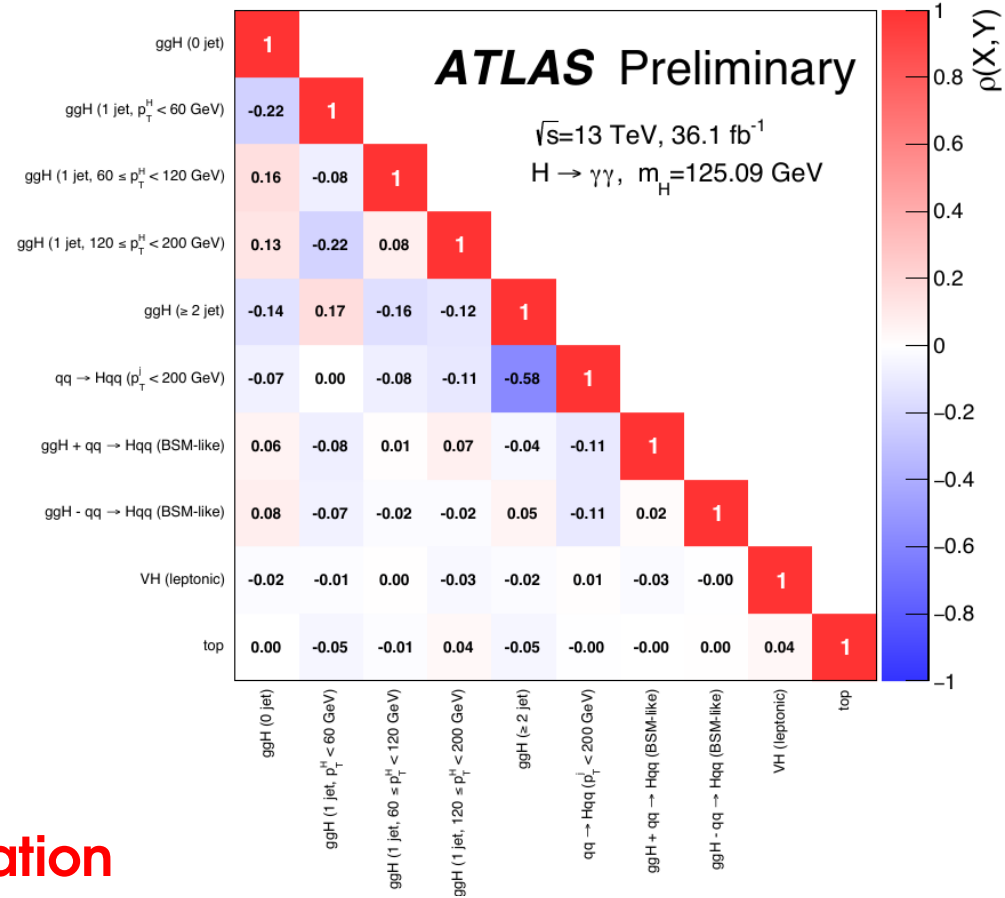
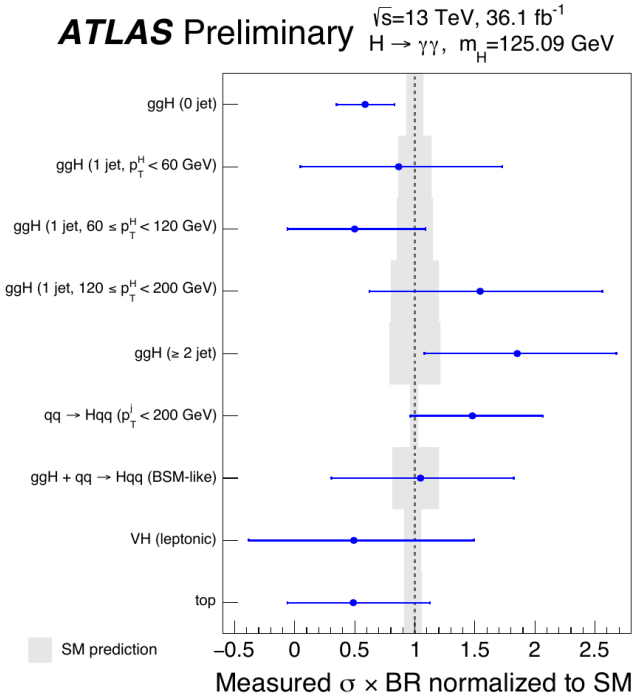
→ However, **often too complex to implement widely:**

- Full likelihood typically not published
- theorists typically do not want to deal with 4000 NPs...

→ **Other approaches:** e.g. reimplementing the analysis in a public fast-simulation framework (e.g. SUSY searches). However clear accuracy limitations

# Presentation of Results

→ **Current solution**: publish covariance matrices in **HEPData**, together with the individual measurements



- **Only valid in the Gaussian approximation**
- To go further, need some form of **simplified likelihoods**
- **Profile likelihood** – function of POI only (NPs profiled out)
- **Additional terms** for non-Gaussian effects
- Significantly more complex (many dimensions!)
- Will be needed eventually as measurements become syst-dominated

# Conclusion

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- Significant evolution in the statistical methods used in HEP
- Variety of methods, adapted to various situations and target results
- Allow to
  - model the statistical process with high precision in difficult situations (large systematics, small signals)
  - make optimal use of available information
- Implemented in standard RooFit/RooStat toolkits within the ROOT framework, as well as other tools (BAT)
- Improvement and uniformization efforts are still ongoing
- Still many open questions and areas that could use improvement  
→ e.g. how to present results with all available information to the “outside”



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# Extra Slides

# Uncertainty decomposition

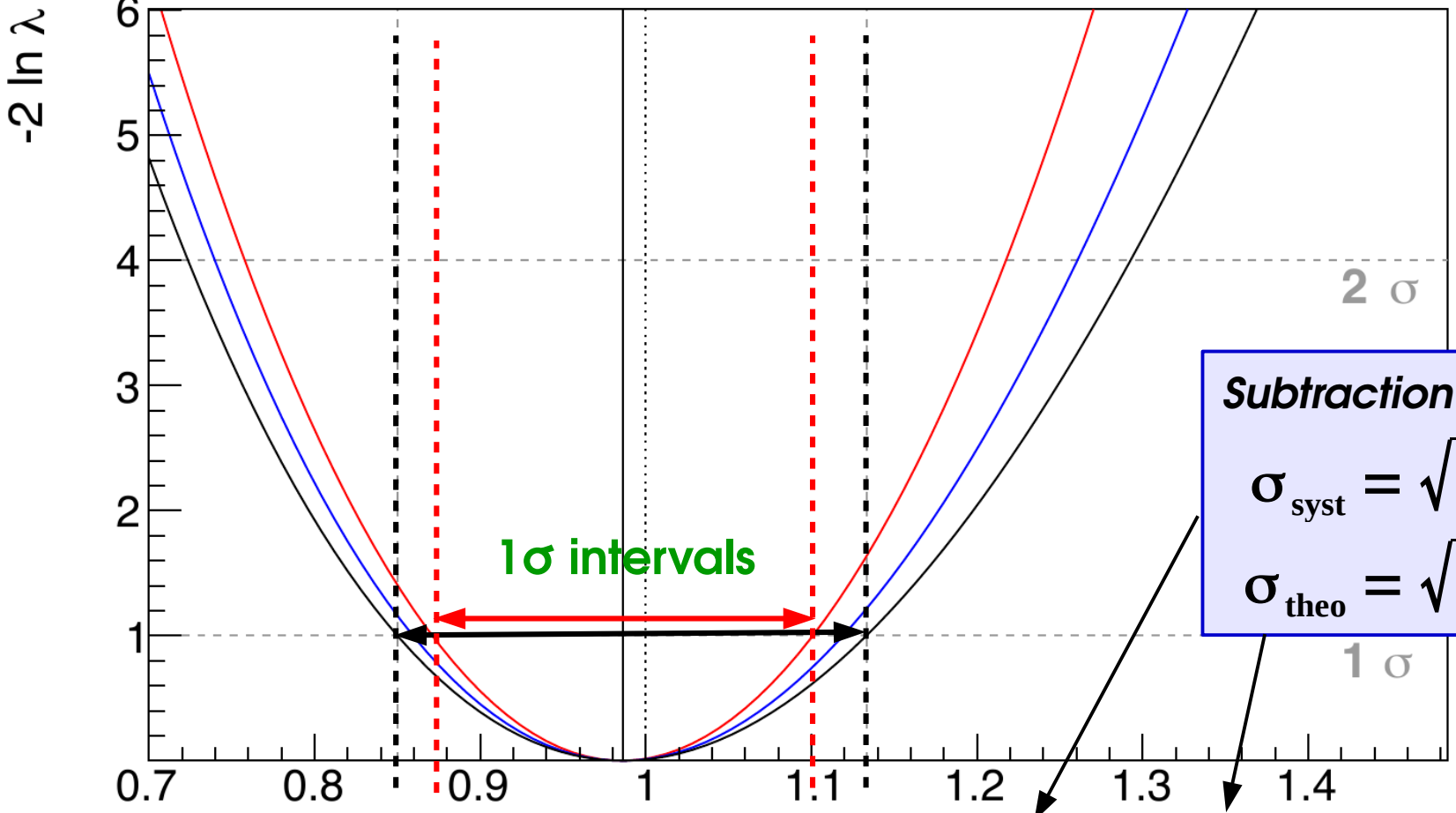
All systematics NPs fixed to 0 : statistical uncertainty only

exp. syst. NPs fixed to 0 : stat+theory uncertainty

**ATLAS**

$H \rightarrow \gamma\gamma, m_H = 125.09 \text{ GeV}$

— Total    — Theory    — Stat



**Subtraction in quadrature**

$$\sigma_{\text{syst}} = \sqrt{\sigma_{\text{total}}^2 - \sigma_{\text{stat}}^2}$$

$$\sigma_{\text{theo}} = \sqrt{\sigma_{\text{stat+theo}}^2 - \sigma_{\text{stat}}^2}$$

$$\mu = 0.99 \pm 0.12 \text{ (stat)} \pm 0.06 \text{ (syst)} \pm 0.06 \text{ (theo)}^{\mu}$$

# Gaussian Profiling

Gaussian measurement with 1 POI  $\mu$  and 1 NP  $\theta$ :

$$L(\mu, \theta; \hat{\mu}, \hat{\theta}) = \exp \left[ -\frac{1}{2} \begin{pmatrix} \mu - \hat{\mu} \\ \theta - \hat{\theta} \end{pmatrix}^T C^{-1} \begin{pmatrix} \mu - \hat{\mu} \\ \theta - \hat{\theta} \end{pmatrix} \right] \quad C = \begin{bmatrix} \sigma_\mu^2 & \gamma \sigma_\mu \sigma_\theta \\ \gamma \sigma_\mu \sigma_\theta & \sigma_\theta^2 \end{bmatrix}$$

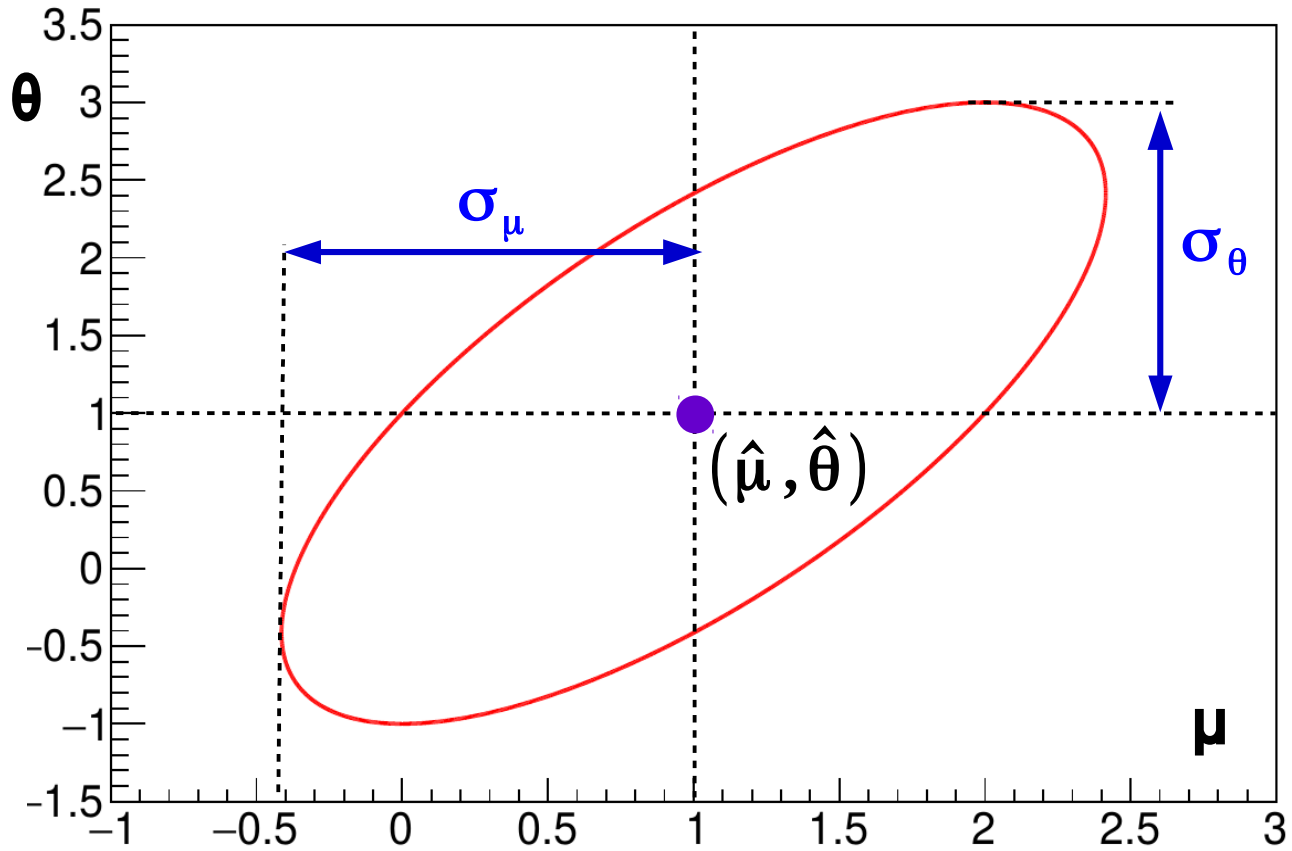
“data”

→  $\lambda(\mu, \theta)$  defines an **ellipse**:

$$\lambda(\mu, \theta; \hat{\mu}, \hat{\theta}) = F_{\mu\mu}(\mu - \hat{\mu})^2 + 2F_{\mu\theta}(\mu - \hat{\mu})(\theta - \hat{\theta}) + F_{\theta\theta}(\theta - \hat{\theta})^2 \quad F \equiv C^{-1} = \begin{bmatrix} F_{\mu\mu} & F_{\mu\theta} \\ F_{\mu\theta} & F_{\theta\theta} \end{bmatrix}$$

### Uncertainty on $\mu$ :

- From  $C$ , with  $\theta$  included:  $\sigma_\mu$



# Gaussian Profiling

$$C = \begin{bmatrix} \sigma_\mu^2 & \gamma \sigma_\mu \sigma_\theta \\ \gamma \sigma_\mu \sigma_\theta & \sigma_\theta^2 \end{bmatrix}$$

$$F = \begin{bmatrix} F_{\mu\mu} & F_{\mu\theta} \\ F_{\mu\theta} & F_{\theta\theta} \end{bmatrix}$$

$$\lambda(\mu, \theta; \hat{\mu}, \hat{\theta}) = F_{\mu\mu}(\mu - \hat{\mu})^2 + 2F_{\mu\theta}(\mu - \hat{\mu})(\theta - \hat{\theta}) + F_{\theta\theta}(\theta - \hat{\theta})^2$$

Profiled  $\theta$  (minimize  $\lambda$  at fixed  $\mu$ ) :

$$\hat{\theta}(\mu) = \hat{\theta} - F_{\theta\theta}^{-1} F_{\theta\mu}(\mu - \hat{\mu})$$

Profile likelihood ratio:

$$\lambda(\mu, \hat{\theta}(\mu); \hat{\mu}, \hat{\theta}) = (F_{\mu\mu} - F_{\mu\theta} F_{\theta\theta}^{-1} F_{\theta\mu})(\mu - \hat{\mu})^2 = C_{\mu\mu}^{-1}(\mu - \hat{\mu})^2 = \left(\frac{\mu - \hat{\mu}}{\sigma_\mu}\right)^2$$

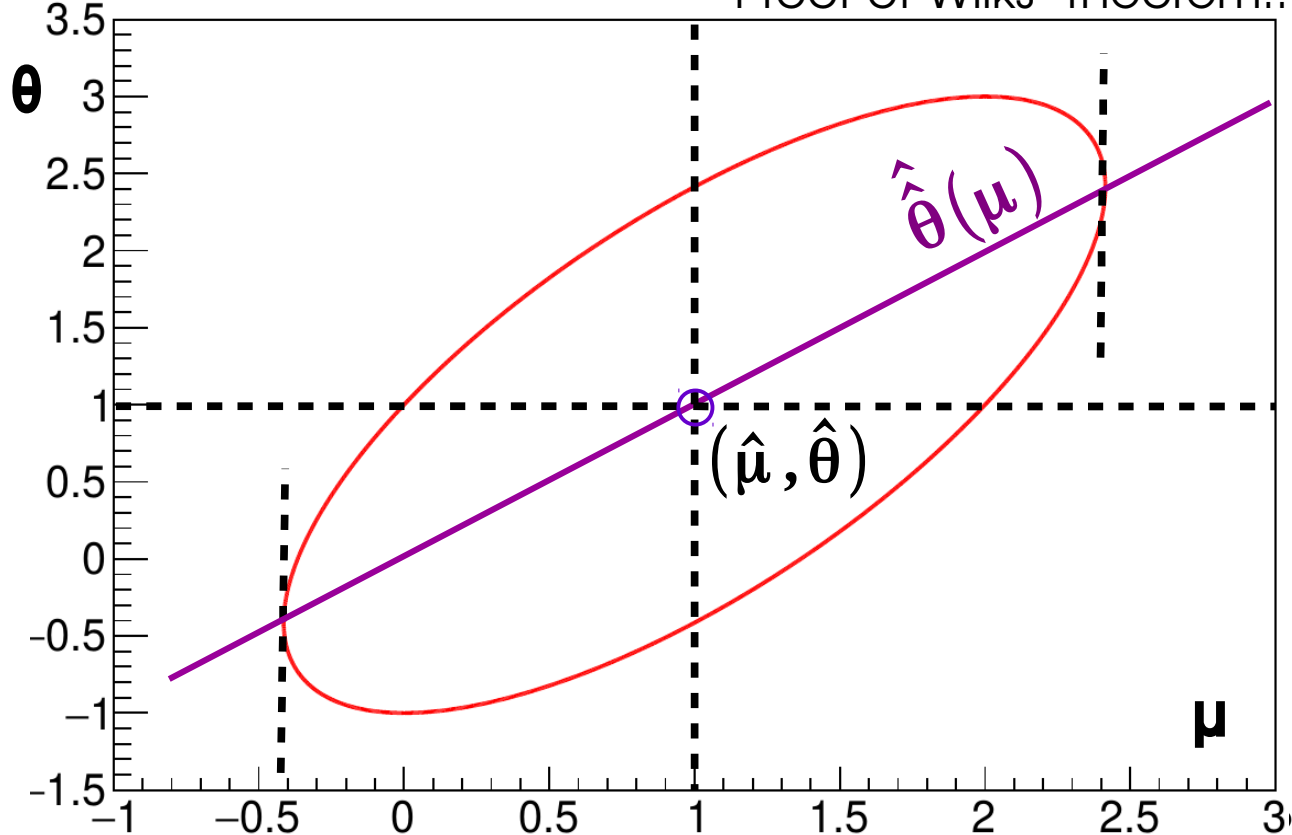
$F_{\mu\mu} \neq C_{\mu\mu}^{-1} !!$

Proof of Wilks' theorem...

## Uncertainty on $\mu$ :

- From C:  $\sigma_\mu$
- From PLR:  $\sigma_\mu$

Profiled  $\theta$  **crosses ellipse at vertical tangents** by definition (L is lower at other points on the tangent)



# Gaussian Profiling

$$\lambda(\mu, \theta; \hat{\mu}, \hat{\theta}) = F_{\mu\mu}(\mu - \hat{\mu})^2 + 2F_{\mu\theta}(\mu - \hat{\mu})(\theta - \hat{\theta}) + F_{\theta\theta}(\theta - \hat{\theta})^2$$

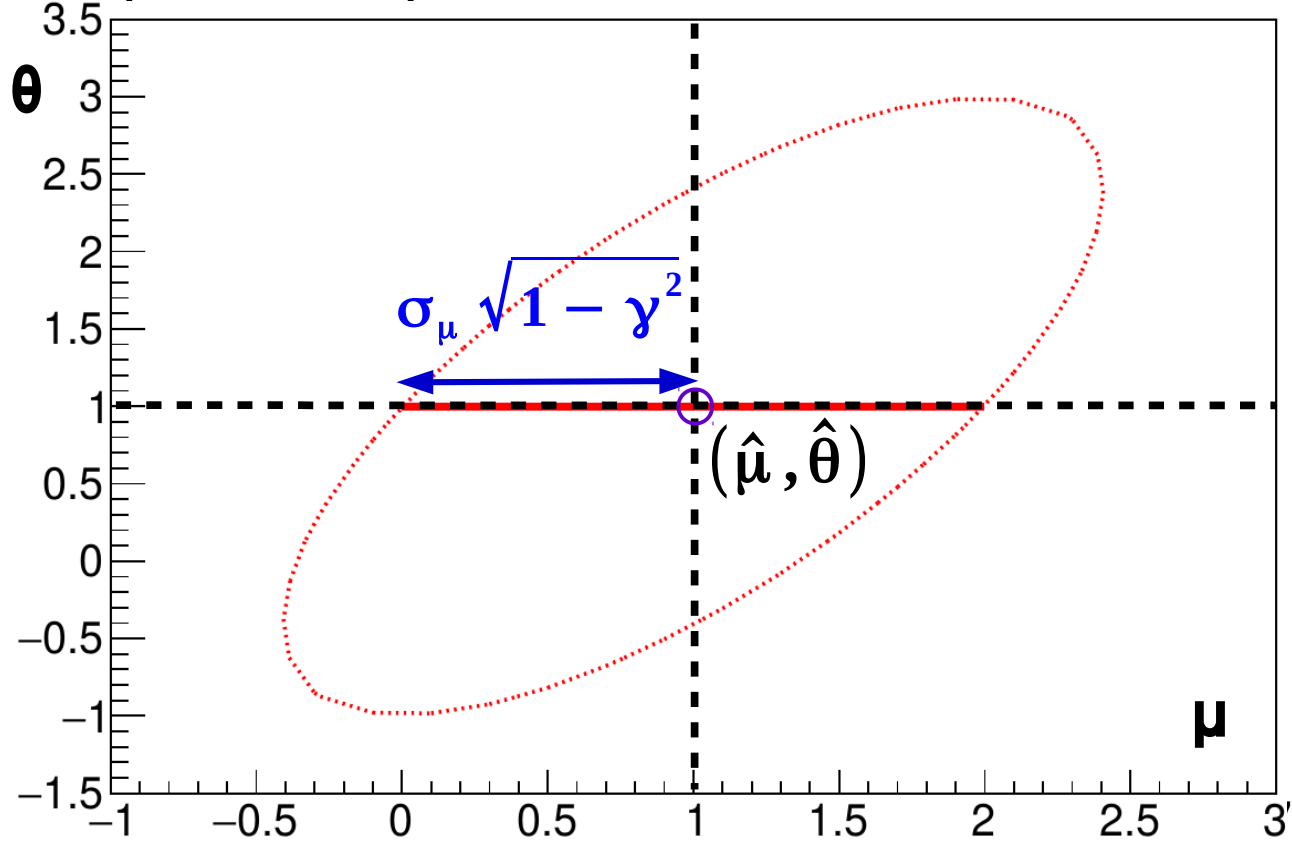
$$F \equiv C^{-1} = \frac{1}{1 - \gamma^2} \begin{bmatrix} \frac{1}{\sigma_\mu^2} & \frac{\gamma}{\sigma_\mu \sigma_\theta} \\ \frac{\gamma}{\sigma_\mu \sigma_\theta} & \frac{1}{\sigma_\theta^2} \end{bmatrix}$$

→ For fixed  $\theta = \hat{\theta}$ ,  $\lambda(\mu)$  defines an interval:

$$\lambda(\mu, \theta = \hat{\theta}; \hat{\mu}, \hat{\theta}) = F_{\mu\mu}(\mu - \hat{\mu})^2 = \left( \frac{\mu - \hat{\mu}}{\sigma_\mu \sqrt{1 - \gamma^2}} \right)^2$$

## Uncertainty on $\mu$ :

- From C:  $\sigma_\mu$
- From PLR:  $\sigma_\mu$
- From  $\lambda(\mu)$ :  $\sigma_\mu \sqrt{1 - \gamma^2}$



# Gaussian Profiling

$$\lambda(\mu, \theta; \hat{\mu}, \hat{\theta}) = F_{\mu\mu}(\mu - \hat{\mu})^2 + 2F_{\mu\theta}(\mu - \hat{\mu})(\theta - \hat{\theta}) + F_{\theta\theta}(\theta - \hat{\theta})^2$$

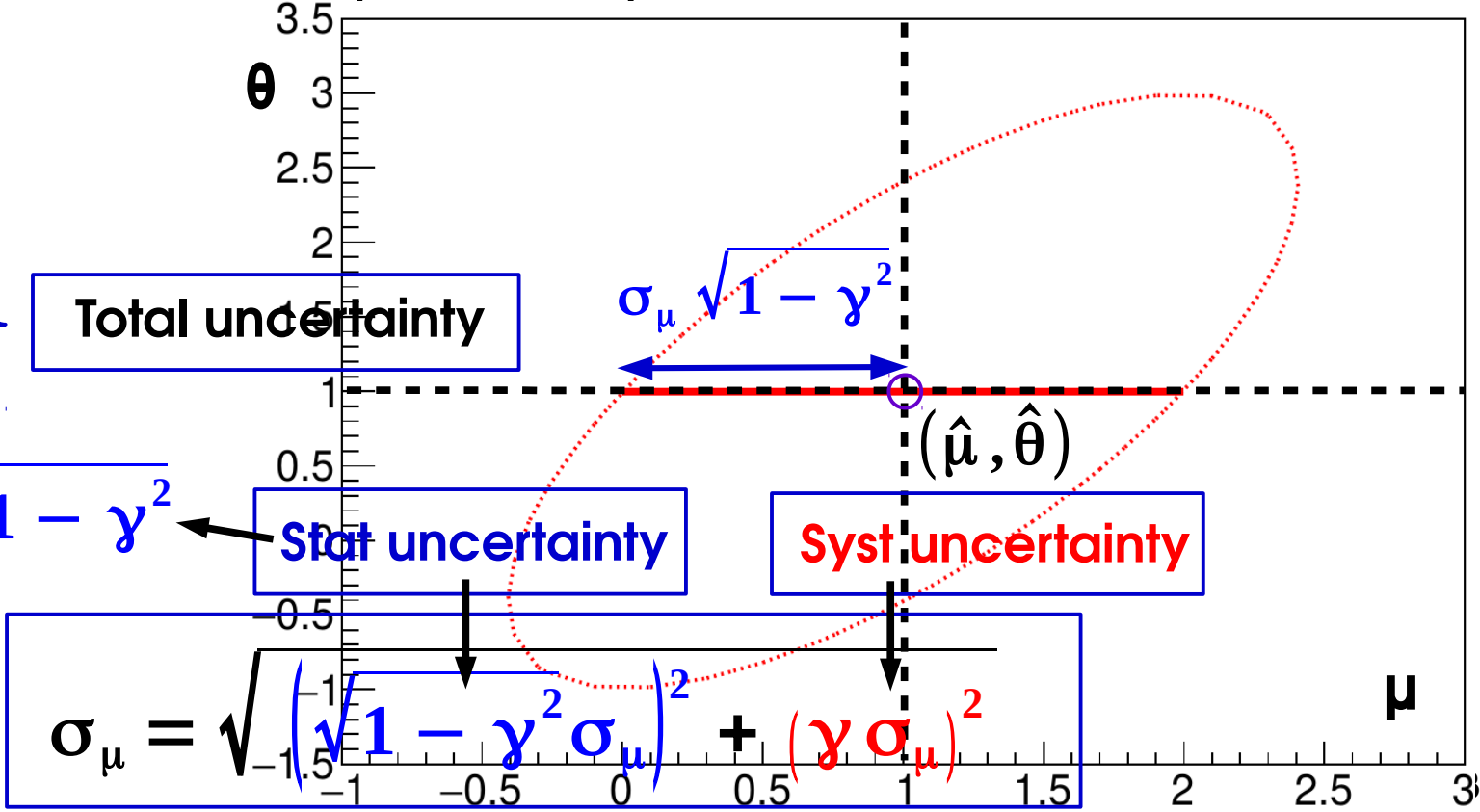
$$F \equiv C^{-1} = \frac{1}{1 - \gamma^2} \begin{bmatrix} \frac{1}{\sigma_\mu^2} & \frac{\gamma}{\sigma_\mu \sigma_\theta} \\ \frac{\gamma}{\sigma_\mu \sigma_\theta} & \frac{1}{\sigma_\theta^2} \end{bmatrix}$$

→ For fixed  $\theta = \hat{\theta}$ ,  $\lambda(\mu)$  defines an interval:

$$\lambda(\mu, \theta = \hat{\theta}; \hat{\mu}, \hat{\theta}) = F_{\mu\mu}(\mu - \hat{\mu})^2 = \left( \frac{\mu - \hat{\mu}}{\sigma_\mu \sqrt{1 - \gamma^2}} \right)^2$$

## Uncertainty on $\mu$ :

- From C:  $\sigma_\mu$
- From PLR:  $\sigma_\mu$
- From  $\lambda(\mu)$ :  $\sigma_\mu \sqrt{1 - \gamma^2}$



# Comparison with LEP/TeVatron definitions

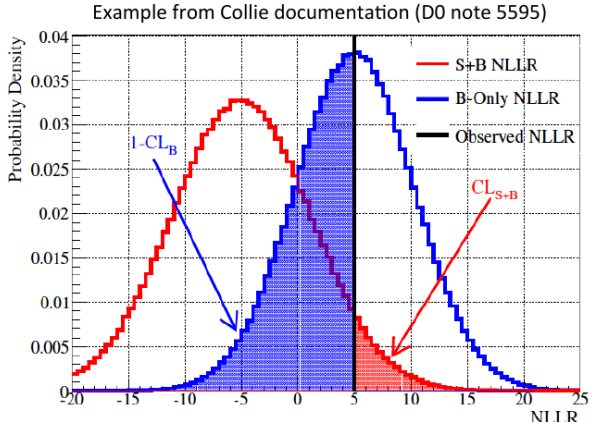
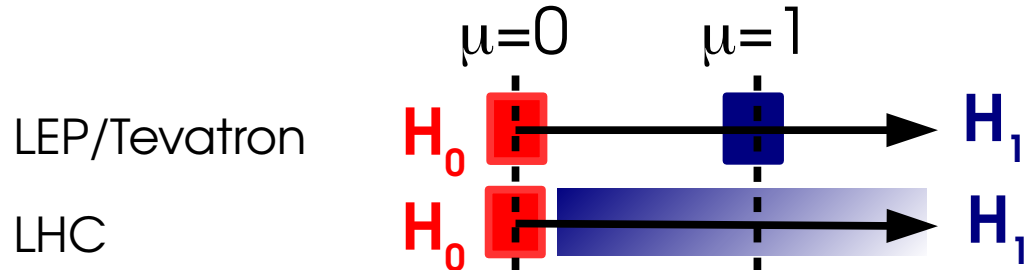
Likelihood ratios are not a new idea:

- **LEP**: Simple LR with NPs from MC
  - Compare  $\mu=0$  and  $\mu=1$
- **TeVatron**: PLR with profiled NPs

$$q_{LEP} = -2 \log \frac{L(\mu=0, \tilde{\theta})}{L(\mu=1, \tilde{\theta})}$$

$$q_{TeVatron} = -2 \log \frac{L(\mu=0, \hat{\theta}_0)}{L(\mu=1, \hat{\theta}_1)}$$

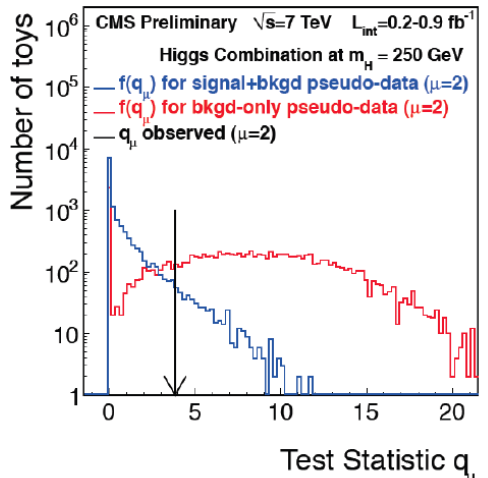
Both compare to  $\mu=1$  instead of best-fit  $\hat{\mu}$



→ Asymptotically:

- **LEP/TeVatron**:  $q$  linear in  $\mu \Rightarrow \sim \text{Gaussian}$
- **LHC**:  $q$  quadratic in  $\mu \Rightarrow \sim \chi^2$

→ Still use TeVatron-style for discrete cases



# Spin/Parity Measurements

Phys. Rev. D 92 (2015) 012004

