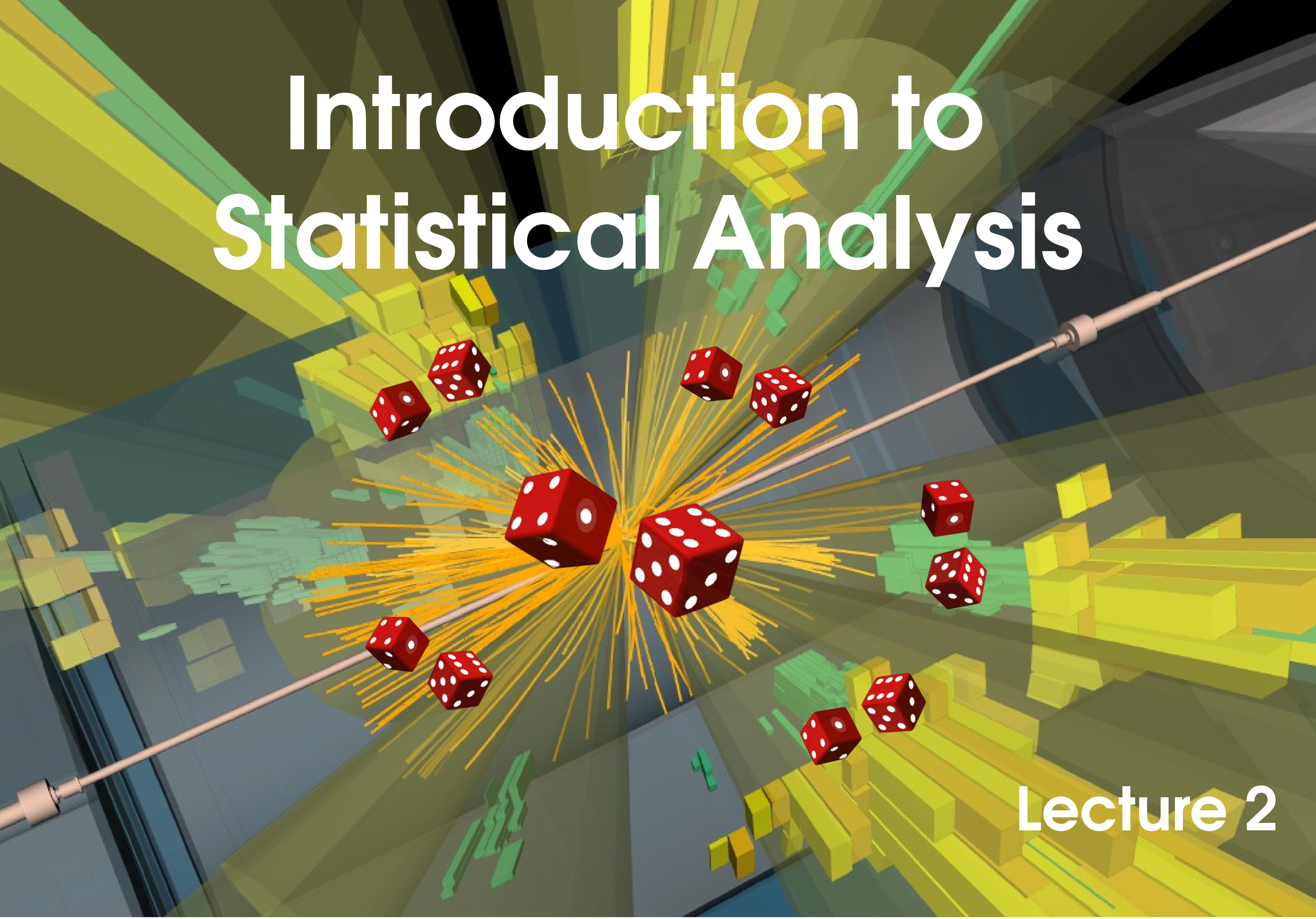
# Introduction to Statistical Analysis



## Lecture 2

Nicolas Berger (LAPP Annecy)

# Outline

Previously in these lectures

- Statistical modeling
- Estimating parameters
- Testing for discovery
- Confidence intervals

Today

- Upper limits
- Expected results
- Reparameterization and presentation of results
- Profiling

# Highlights : Discovery

Given a statistical model P(data; μ), define likelihood **L(μ) = P(data; μ)**

**To estimate a parameter**, use the value **$\hat{\mu}$** that maximizes L(μ) → best-fit value

**To decide between hypotheses** $H_0$ and $H_1$, use the **likelihood ratio** $\dfrac{L(H_0)}{L(H_1)}$

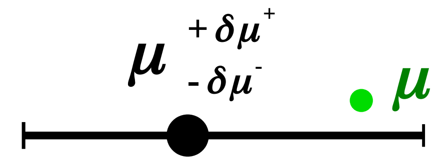
To test for **discovery**, use $q_0 = -2\log\dfrac{L(S=0)}{L(\hat{S})}$ $\quad \hat{S} \geq 0$

For large enough datasets (n >~ 5), $Z = \sqrt{q_0}$

For a **Gaussian** measurement, $Z = \dfrac{\hat{S}}{\sqrt{B}}$

For a **Poisson** measurement, $Z = \sqrt{2\left[(\hat{S}+B)\log\left(1+\dfrac{\hat{S}}{B}\right) - \hat{S}\right]}$

# Highlights: Confidence intervals



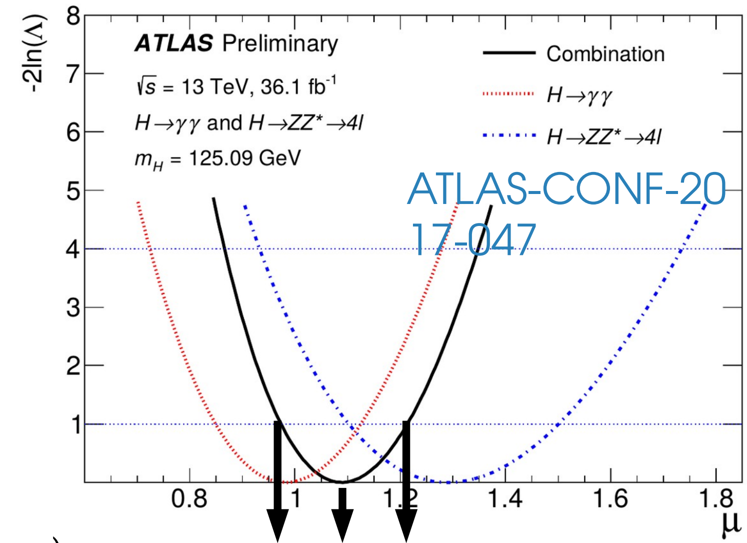

Contain the true value with given probability

To obtain, **compute the log-likelihood ratio** as a function of $\mu_0$.

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

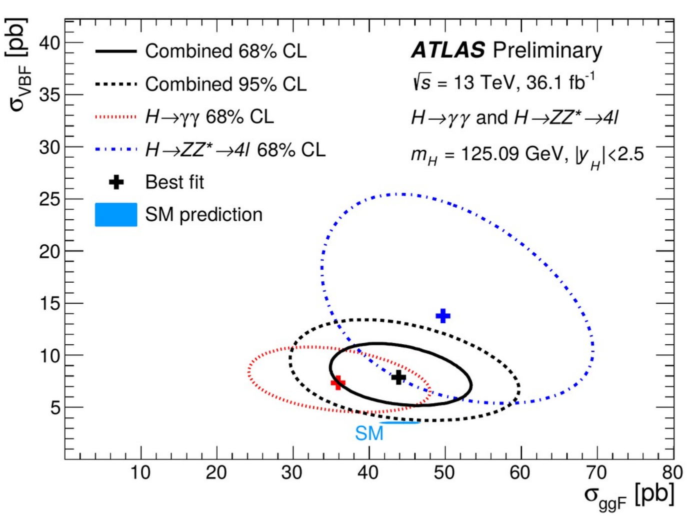
**Interval endpoints** = $\mu^\pm$ for which $t_{\mu^\pm} = 1$

**Gaussian case** : $\hat{\mu} \pm \sigma$

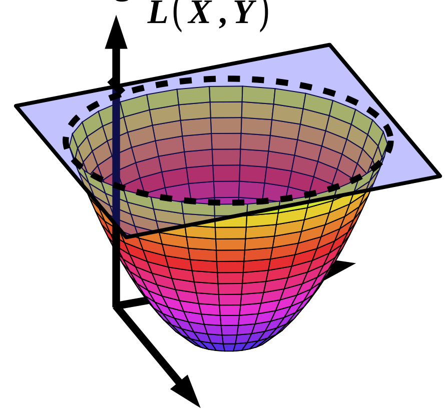



$\mu = 1.09 \pm 0.12$

Works also to obtain **contours in 2D**:




$$t = -2\log\frac{L(X_0, Y_0)}{L(\hat{X}, \hat{Y})}$$



# Outline

Computing statistical results

Confidence intervals

Upper limits on signal yields

Expected Limits

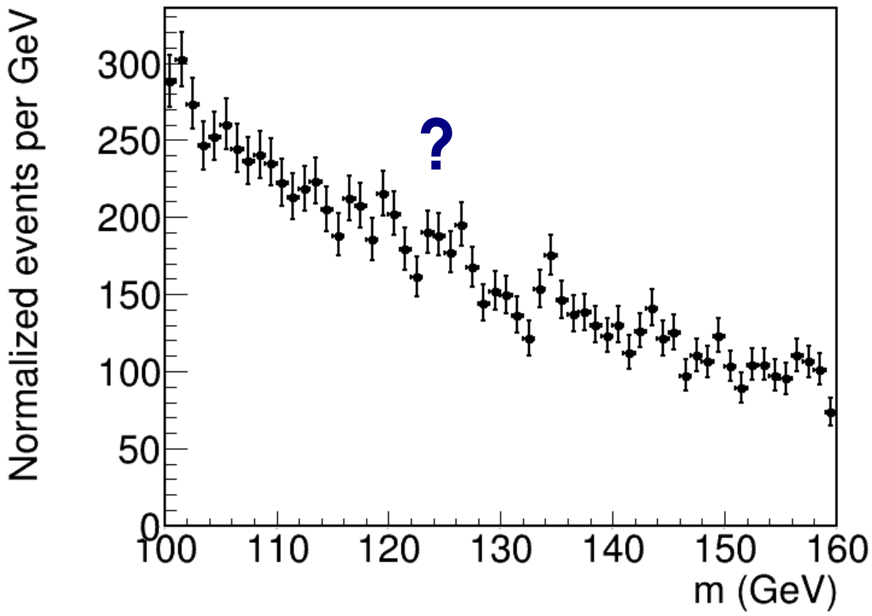
# Hypothesis tests for Limits

If no signal in data, testing for discovery not very relevant (report 0.2σ excess ?)

→ More interesting to **exclude large signals**

⇛ **Upper limits on signal yield**

→ Typically report **95% CL** upper limit (p-value = 5%) : "$S < S_0$ @ 95% CL"



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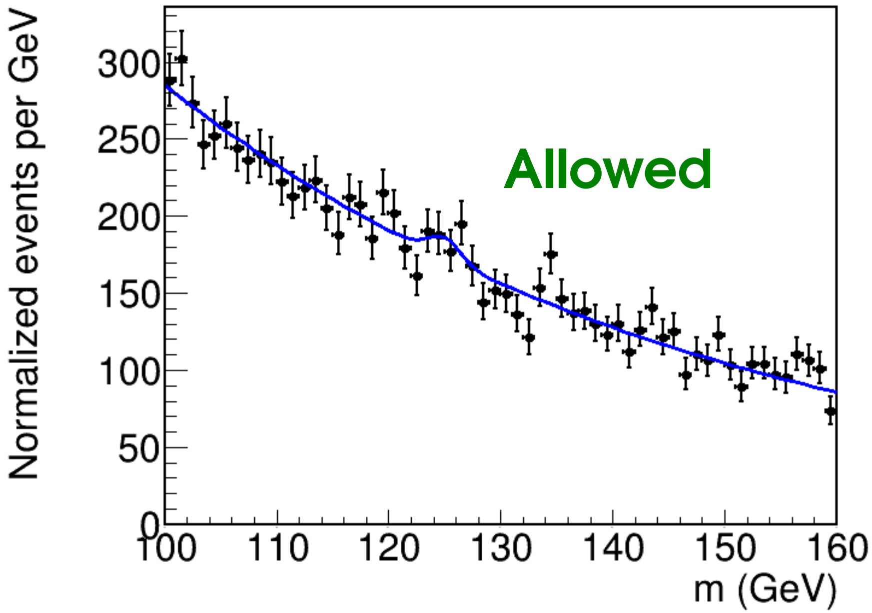

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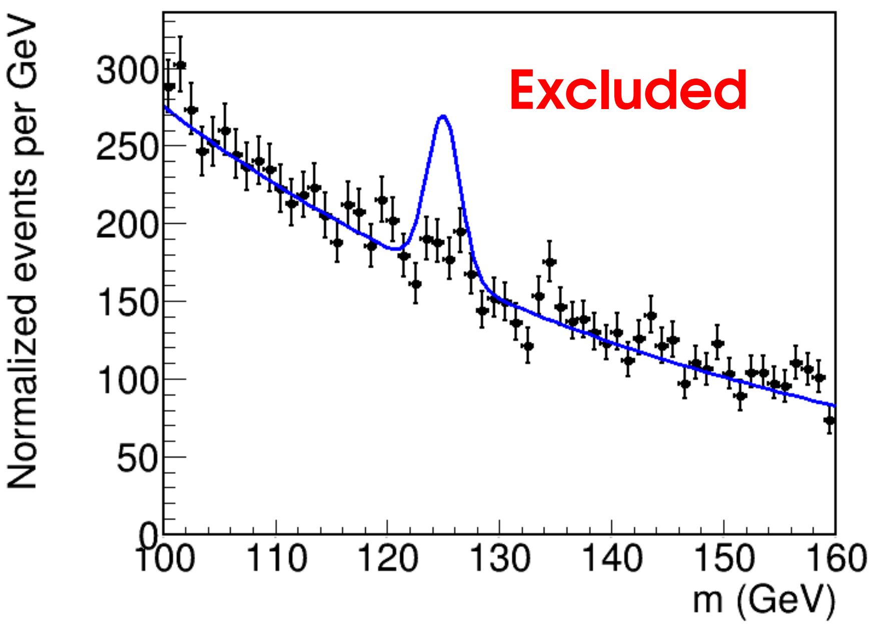

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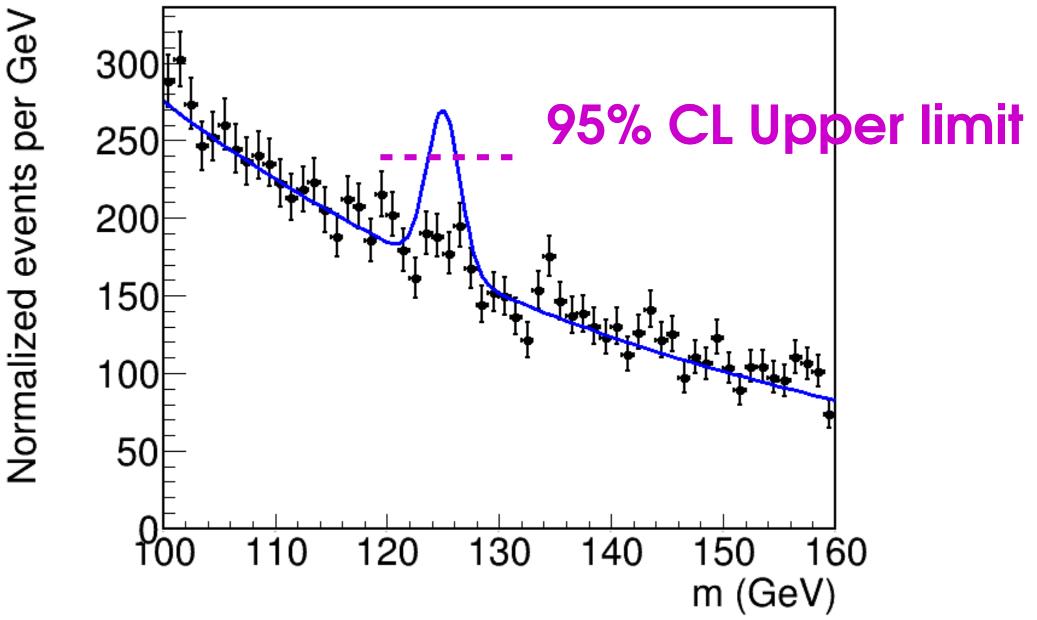

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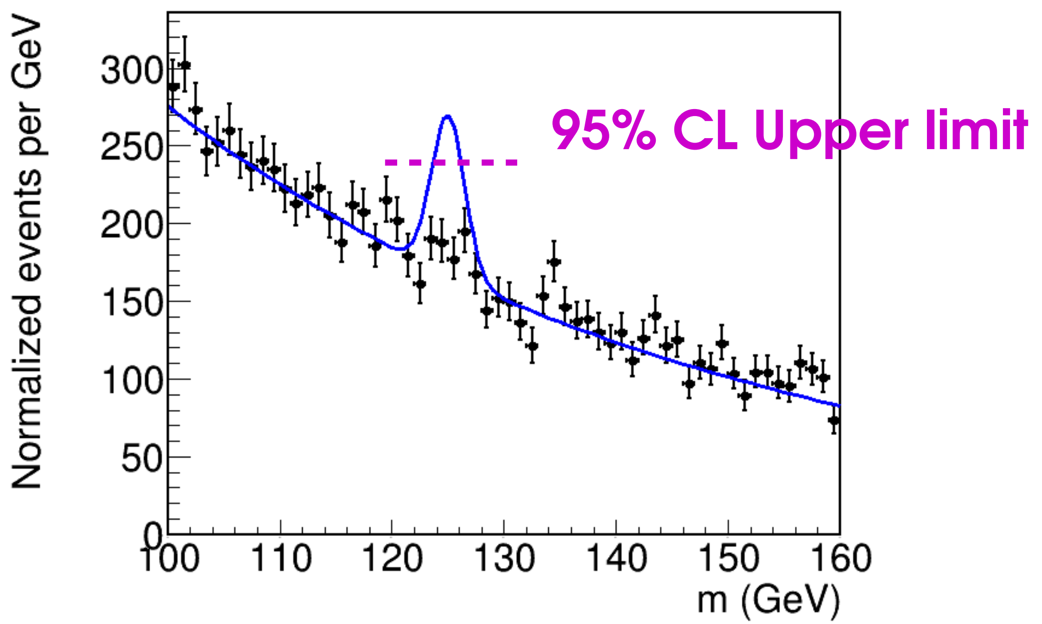
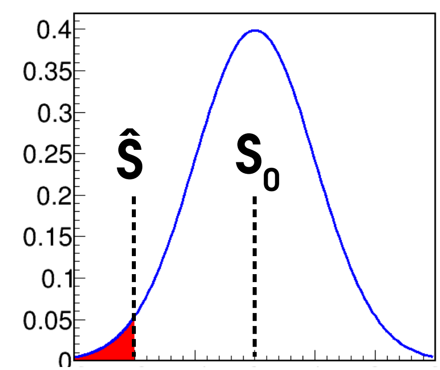
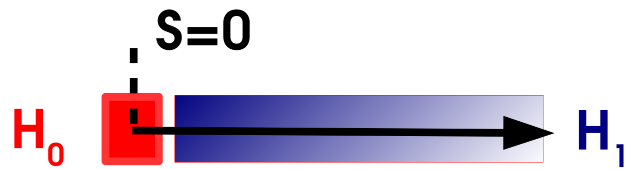


# Test Statistic for Limit-Setting

**Discovery :**

- $H_0 : S = 0$
- $H_1 : S > 0$




$$q_0 = -2\log\frac{L(S=0)}{L(\hat{S})}$$

**Compare**

- Likelihood of $H_0$
- Likelihood of $H_1$

$(\hat{S} > 0)$

---

**Limit-setting**

- $H_0 : S = S_0$
- $H_1 : S < S_0$


$$q_{S_0} = -2\log\frac{L(S=S_0)}{L(\hat{S})}$$

**Compare**

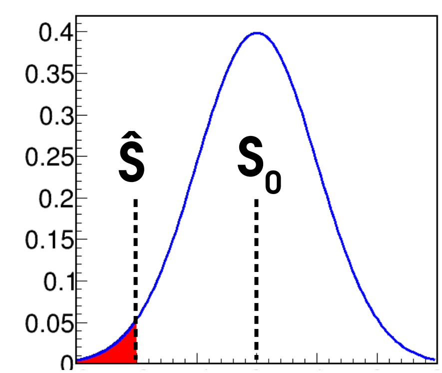
- Likelihood of $H_0$
- Likelihood of $H_1$

$(\hat{S} < S_0)$

Same as $q_0$ :

→ large values ⇒ good rejection of $H_0$.

**Asymptotic case**: p-value $\quad p_{S_0} = 1 - \Phi\left(\sqrt{q_{S_0}}\right)$



# *Inversion* : Getting the limit for a given CL

**Procedure:**

→ Compute $q_{S0}$ for some $S_0$, get the **exclusion p-value $p_{S0}$**.

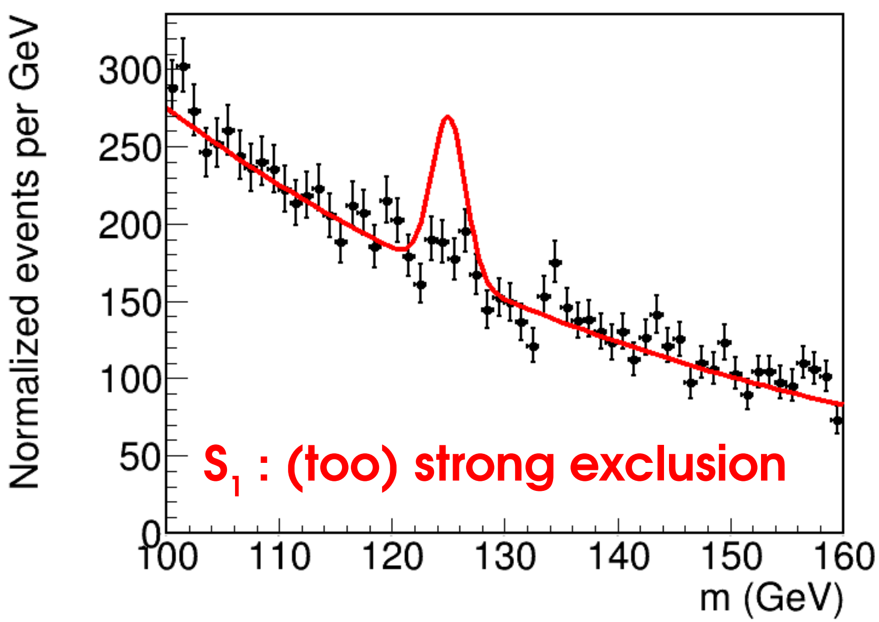
**→ Adjust $S_0$ until 95% CL exclusion ($p_{S0}$ = 5%) is reached**

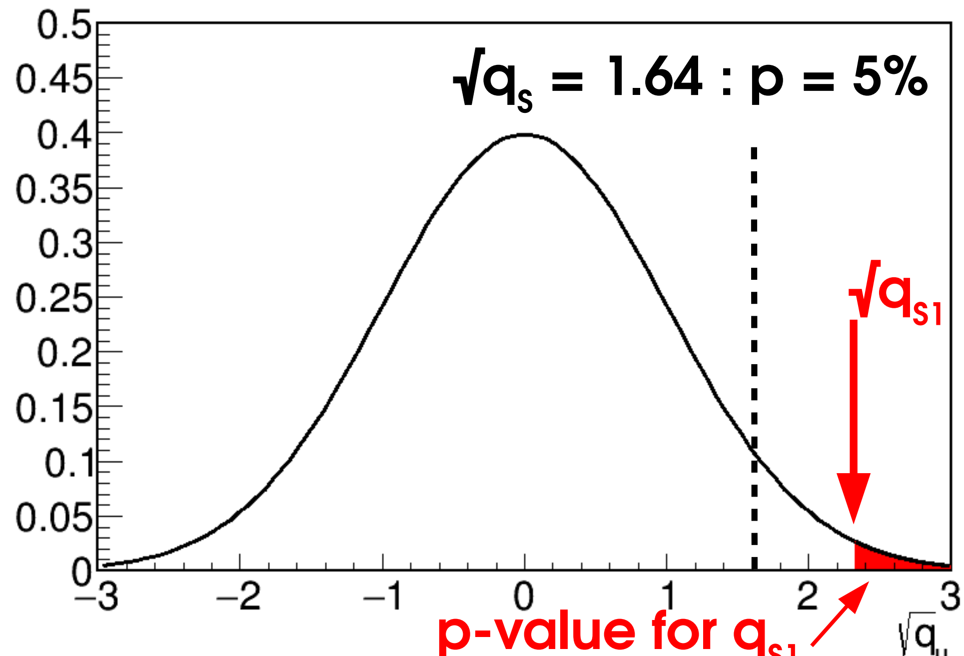
**Asymptotic case: need $\sqrt{q_{S0}}$ = 1.64**

**Asymptotics**

$$\sqrt{q_{S_0}} = \Phi^{-1}(1 - p_0)$$

| CL | Region |
|---|---|
| 90% | $\sqrt{q_S} > 1.28$ |
| 95% | $\sqrt{q_S} > 1.64$ |
| 99% | $\sqrt{q_S} > 2.33$ |



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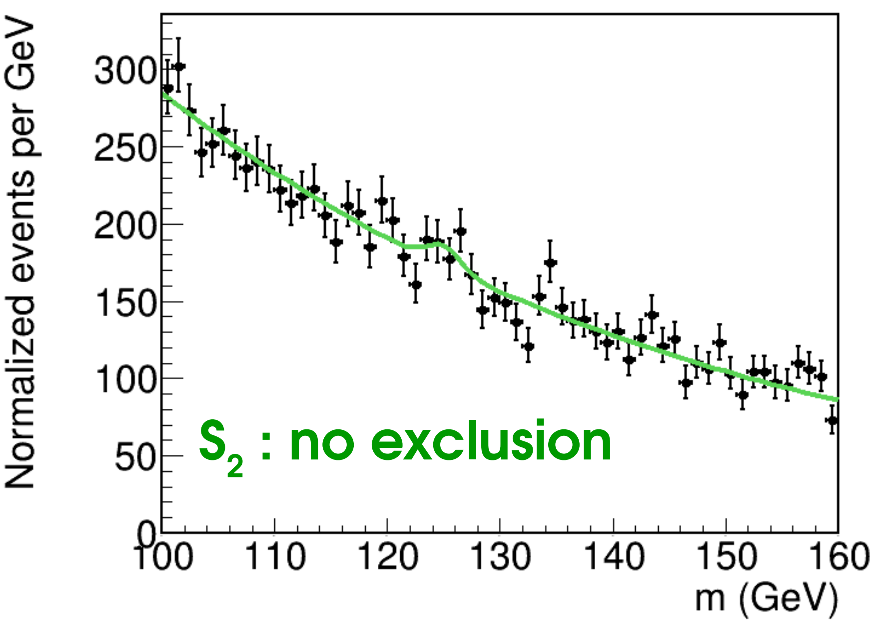


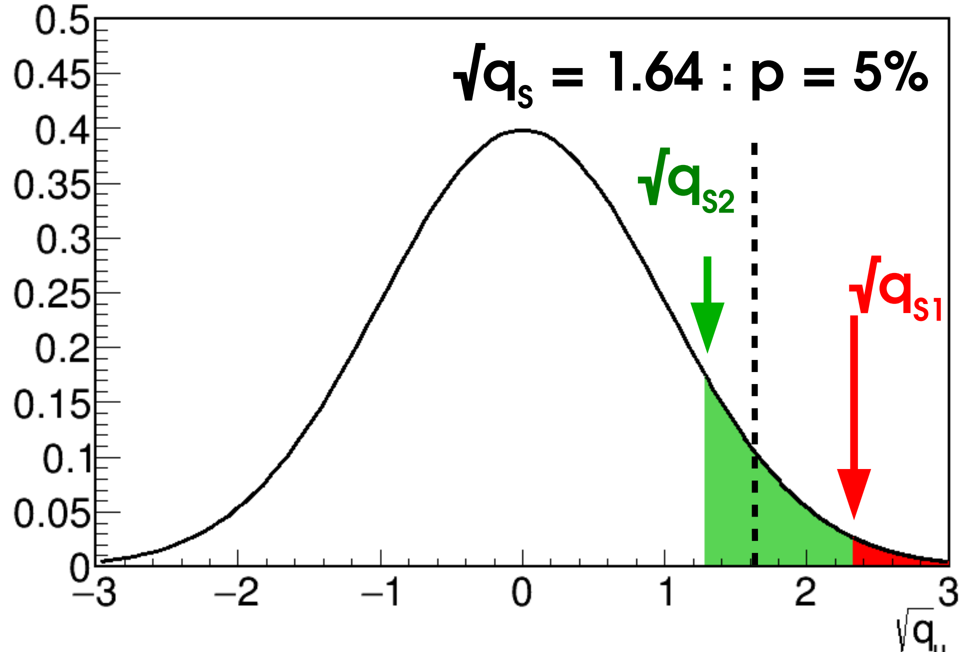

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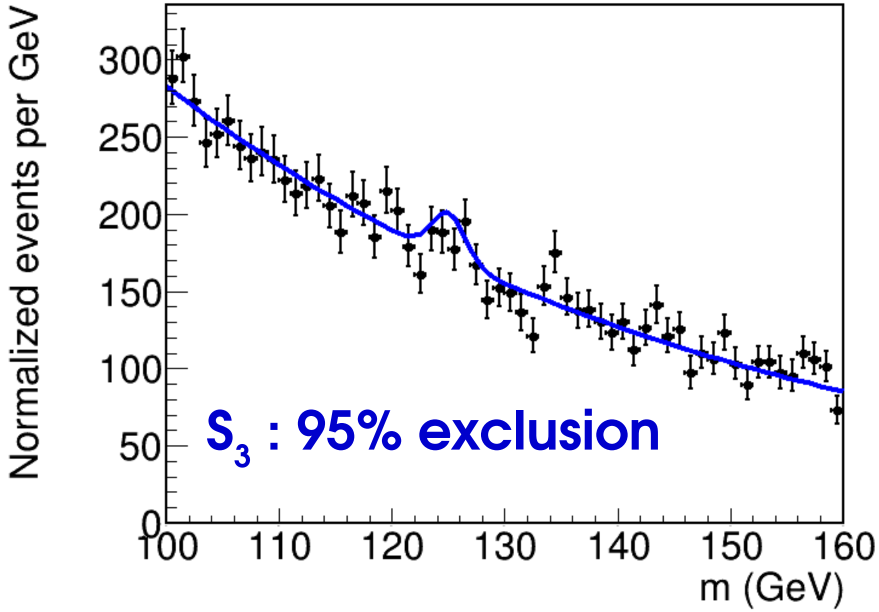
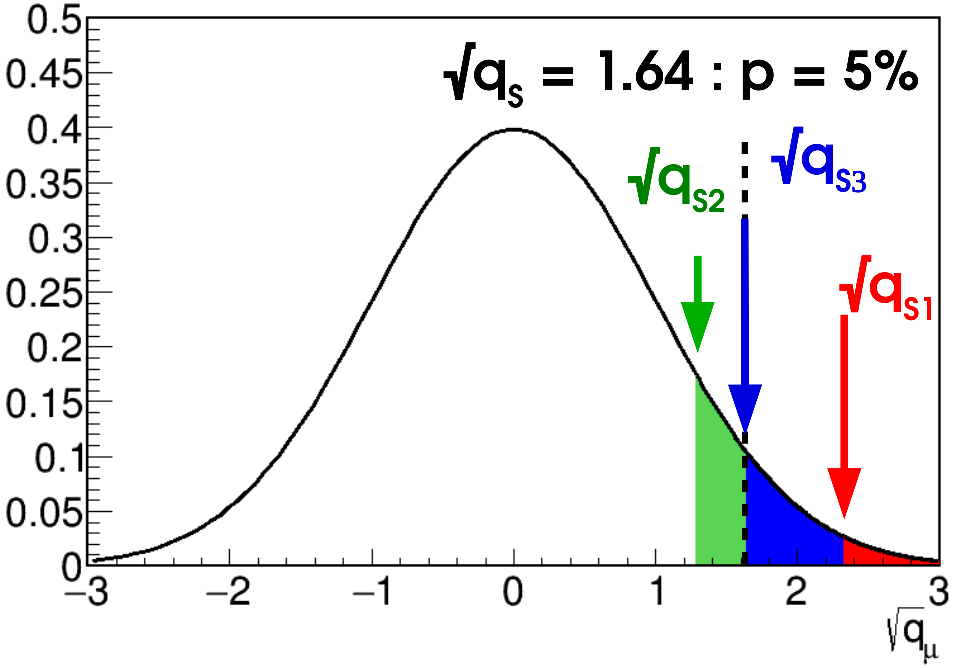
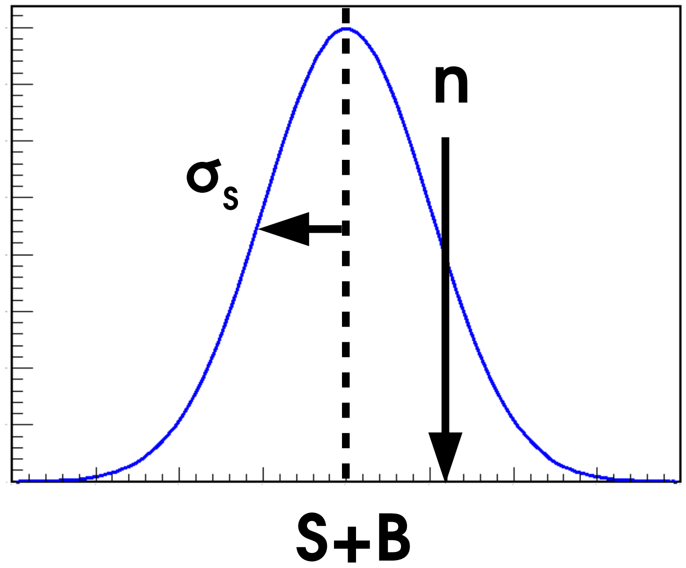


# Homework 4: Gaussian Example




Usual Gaussian counting example with known B:

$$L(S;n) = e^{-\frac{1}{2}\left(\frac{n-(S+B)}{\sigma_S}\right)^2}$$

$\sigma_S \sim \sqrt{B}$ for small S

**Reminder:** Significance: $Z = \hat{S}/\sigma_S$

→ Compute $q_{S0}$

→ Compute the 95% CL upper limit on S, $S_{up}$, by solving $\sqrt{q_{S0}} = 1.64$.

**Solution**: $S_{up} = \hat{S} + 1.64\,\sigma_S$ at 95 % CL

# Upper Limit Pathologies

**Upper limit**: $S_{up} \sim \hat{S} + 1.64\,\sigma_S$.

**Problem**: for negative $\hat{S}$, get **very** good observed limit.

→ For $\hat{S}$ sufficiently negative, even $S_{up} < 0$ !

How can this be ?

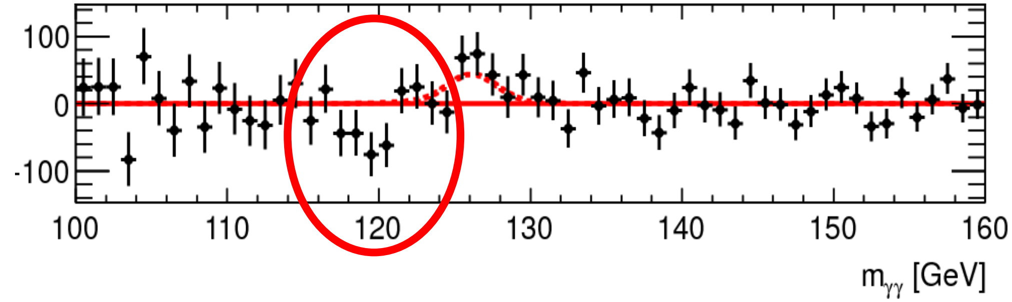
→ **Background modeling issue ?...** Or:

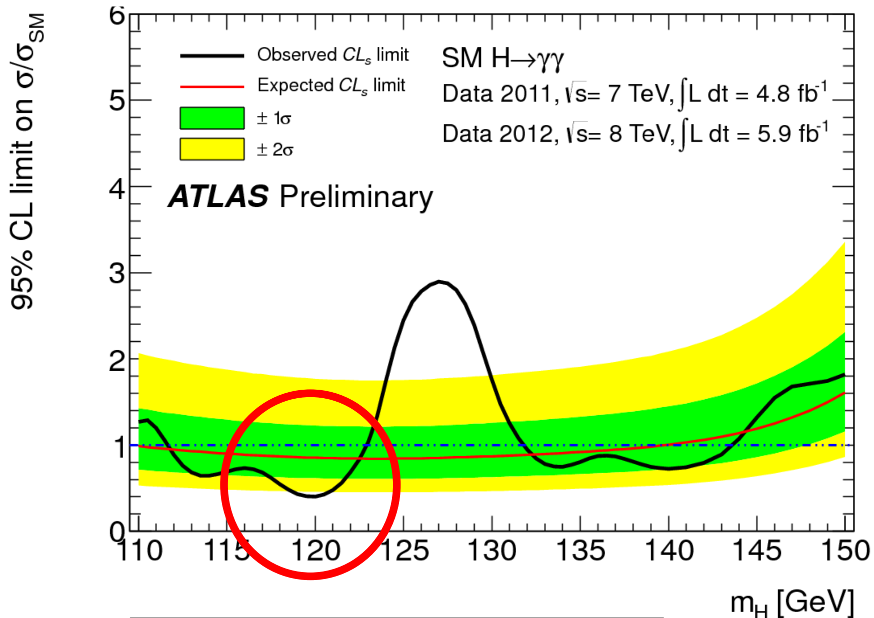
→ This is a **95%** limit ⇒ **5% of the time, the limit wrongly excludes the true value,** *e.g.* $S^*=0$.

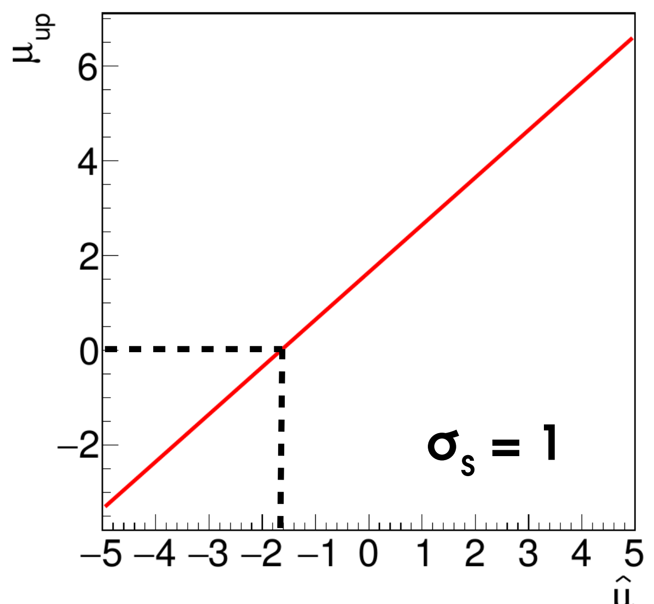
**Options**

→ **live with it**: sometimes report limit < 0

→ **Special procedure to avoid these cases,** since if we assume S must be >0, we know a priori this is just a fluctuation.



# $CL_s$

A. Read, J.Phys. G28 (2002) 2693-2704

Usual solution in HEP : **$CL_s$**.

→ Compute modified p-value

$$p_{CL_s} = \frac{p_{S_0}}{(1 - p_B)}$$

The usual p-value under $H(S=S_0)$ (=5%)

The p-value computed under $H(S=0)$

⇒ **Rescale** exclusion at $S_0$ by exclusion at S=0.

→ Somewhat ad-hoc, but good properties...

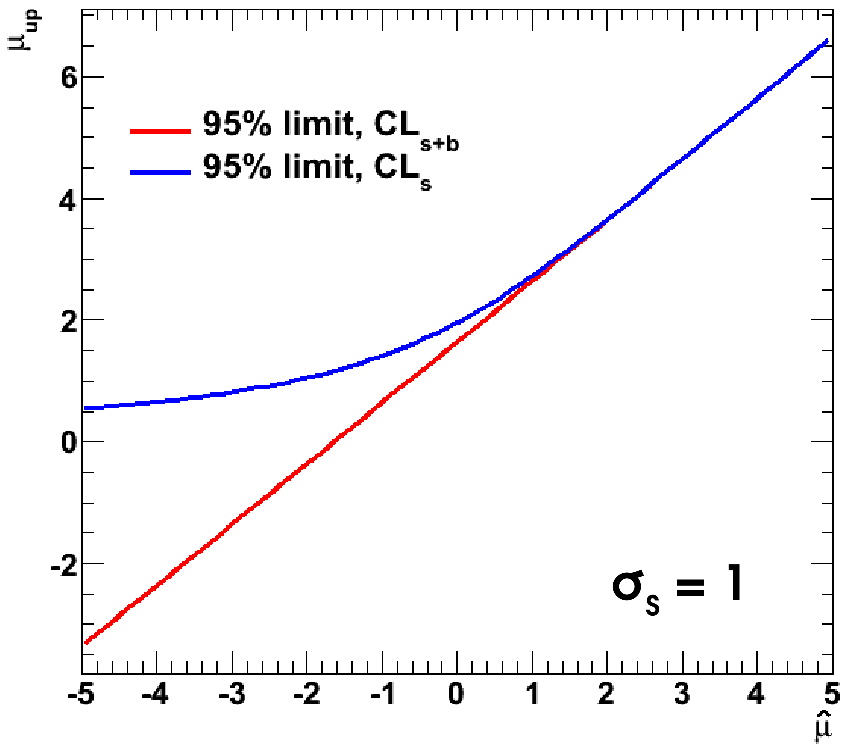
**$\hat{S}$ compatible with 0** : $p_B \sim O(1)$

$p_{CLs}$ ~ **$p_{S0}$ ~ 5%, no change**.

**Far-negative $\hat{S}$** : $1 - p_B \ll 1$

**$p_{CLs} \sim p_{S0}/(1-p_B) \gg 5\%$**

→ lower exclusion ⇒ higher limit,
usually >0 as desired




**Drawback**: ***overcoverage***

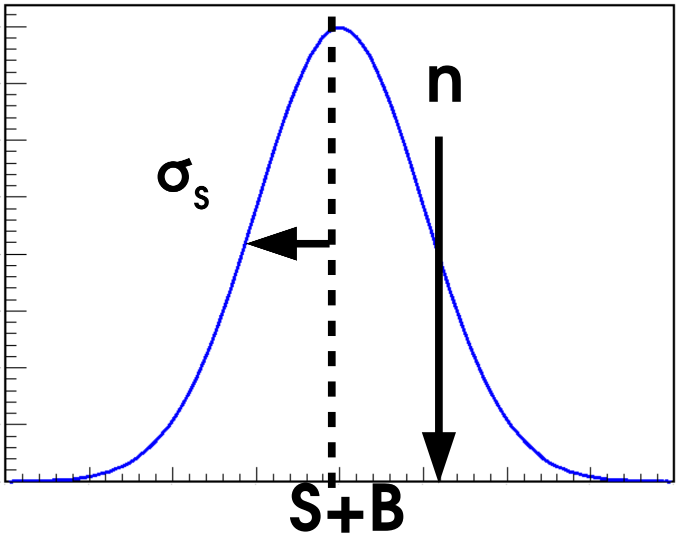
→ limit is claimed to be 95% CL, but actually >95% CL for small $1-p_B$.

# Homework 5: $CL_s$ : Gaussian Case

Usual Gaussian counting example with known B:

$$L(S;n) = e^{-\frac{1}{2}\left(\frac{n-(S+B)}{\sigma_S}\right)^2}$$

$\sigma_S \sim \sqrt{B}$ for small S




**Reminder**

$CL_{s+b}$ limit: $S_{up} = \hat{S} + 1.64\,\sigma_S$ at 95 % CL

**$CL_s$ upper limit** :

→ Compute $p_{S0}$ (same as for CLs+b)

→ Compute $1-p_B$ (hard!)

**Solution:** $$S_{up} = \hat{S} + \left[\Phi^{-1}\left(1 - 0.05\,\Phi\left(\hat{S}/\sigma_S\right)\right)\right]\sigma_S \text{ at } 95\% \text{ CL}$$

for $\hat{S} \sim 0$, $S_{up} = \hat{S} + 1.96\,\sigma_S$ at 95 % CL

# Homework 6: $CL_s$ Rule of Thumb for $n_{obs}$=0

Same exercise, for the Poisson case with $n_{obs} = 0$. Perform an exact computation of the 95% CLs upper limit based on the definition of the p-value:

**p-value** : *sum probabilities of cases at least as extreme as the data*

**Hint**: for $n_{obs}=0$, there are no "more extreme" cases (cannot have n<0 !), so

$p_{S0}$ = Poisson(n=0 | $S_0$+B) and 1 - $p_B$ = Poisson(n=0 | B)

$$S_{up}(n_{obs}=0) = \log(20) = 2.996 \approx 3$$

**Solution**:

**⇒ Rule of thumb: when $n_{obs}$ = 0, the 95% $CL_s$ limit is 3 events (for any B)**

# Outline

Computing statistical results

- Discovery
- Confidence intervals
- Upper limits

Reparameterization and presentation of results

Expected results

Profiling

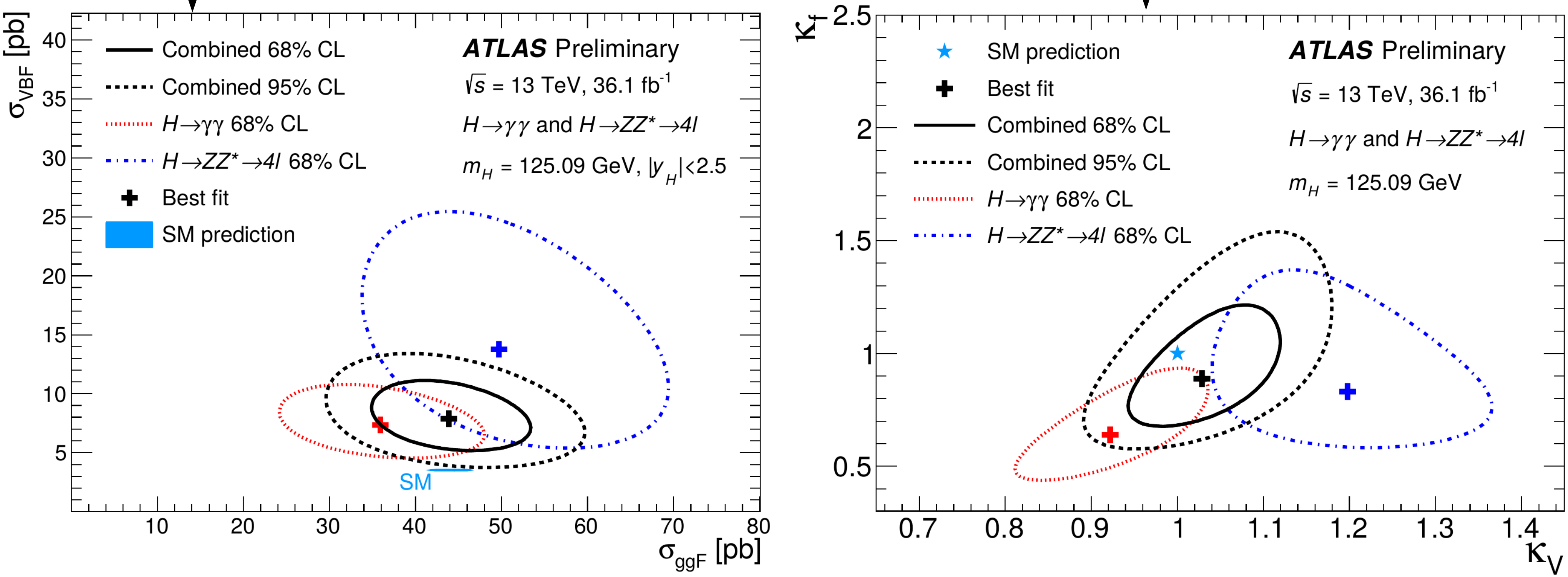
# Reparameterization

Start with basic measurement in terms of e.g. **σ×B**

→ How to measure derived quantities (couplings, parameters in some theory model, etc.) ? → **just reparameterize the likelihood:**

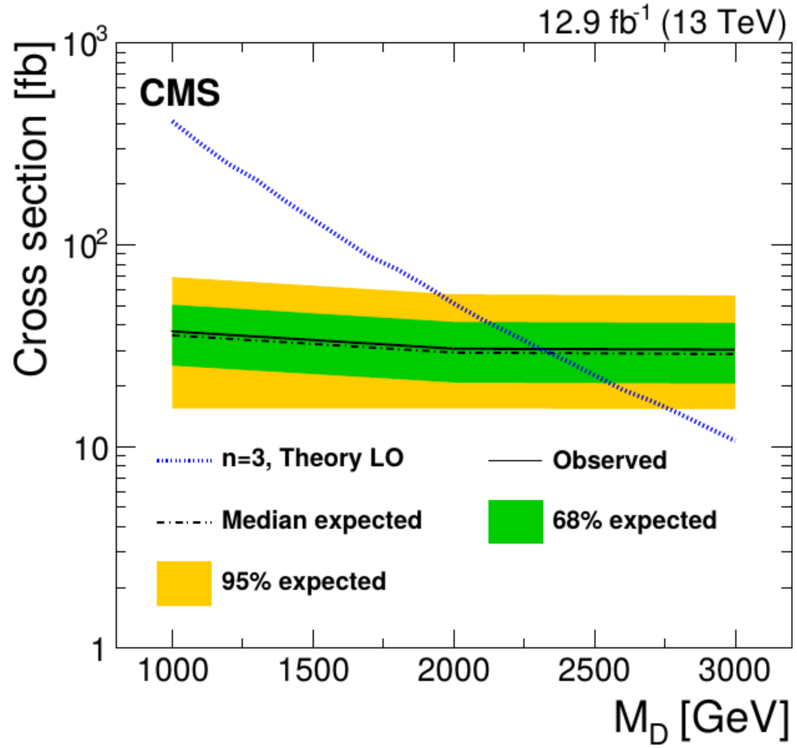
*e.g.* Higgs couplings: $\sigma_{ggF}$, $\sigma_{VBF}$ sensitive to Higgs coupling modifiers $\kappa_V$, $\kappa_F$.

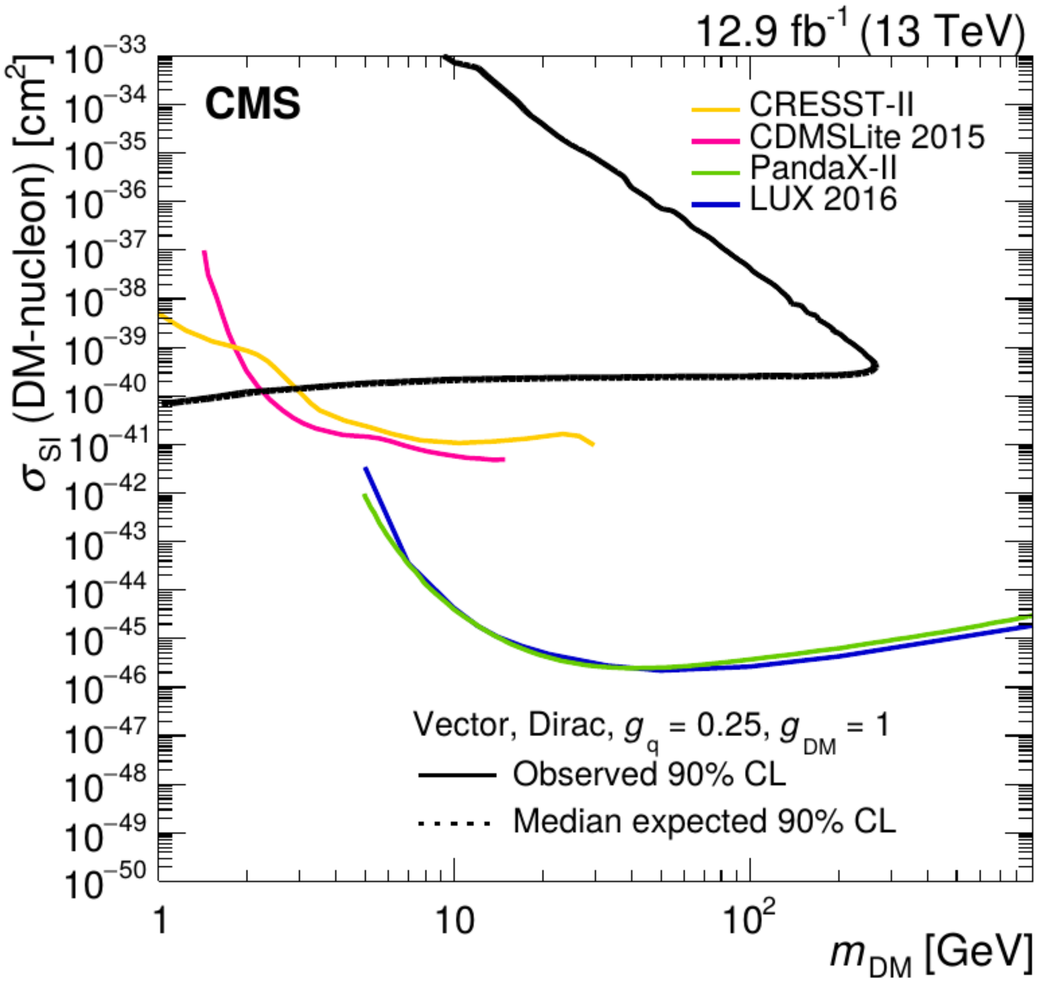
$$L(\sigma_{ggF},\sigma_{VBF}) \xrightarrow[\sigma_{VBF}\to\sigma_{VBF}(\kappa_V,\kappa_F)]{\sigma_{ggF}\to\sigma_{ggF}(\kappa_V,\kappa_F)} L(\sigma_{ggF}(\kappa_V,\kappa_F),\sigma_{VBF}(\kappa_V,\kappa_F)) \equiv L'(\kappa_V,\kappa_F)$$

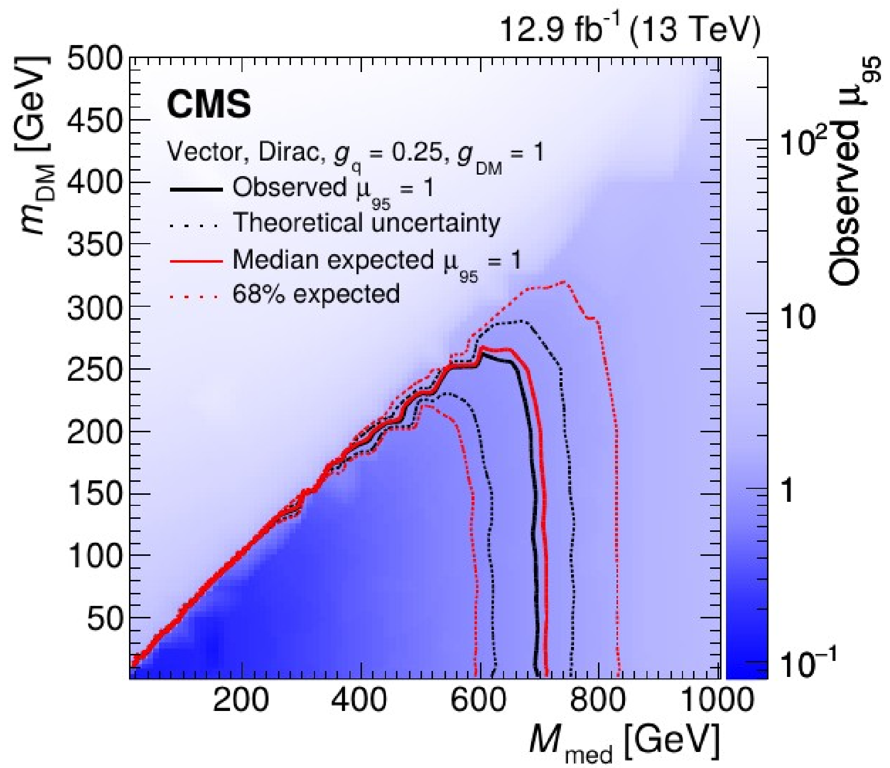


# Reparameterization: Limits

CMS Run 2 Monophoton Search: measured **$N_s$** in a counting experiment reparameterized according to various DM models



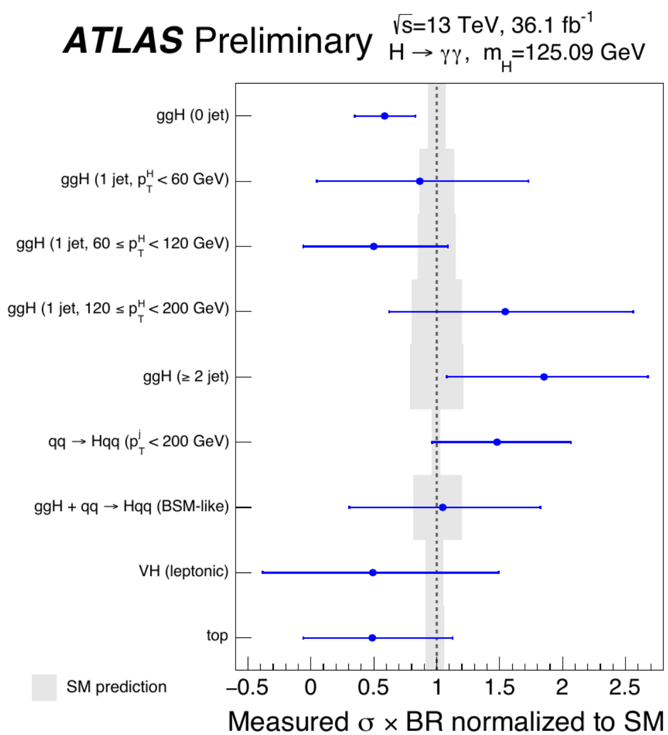



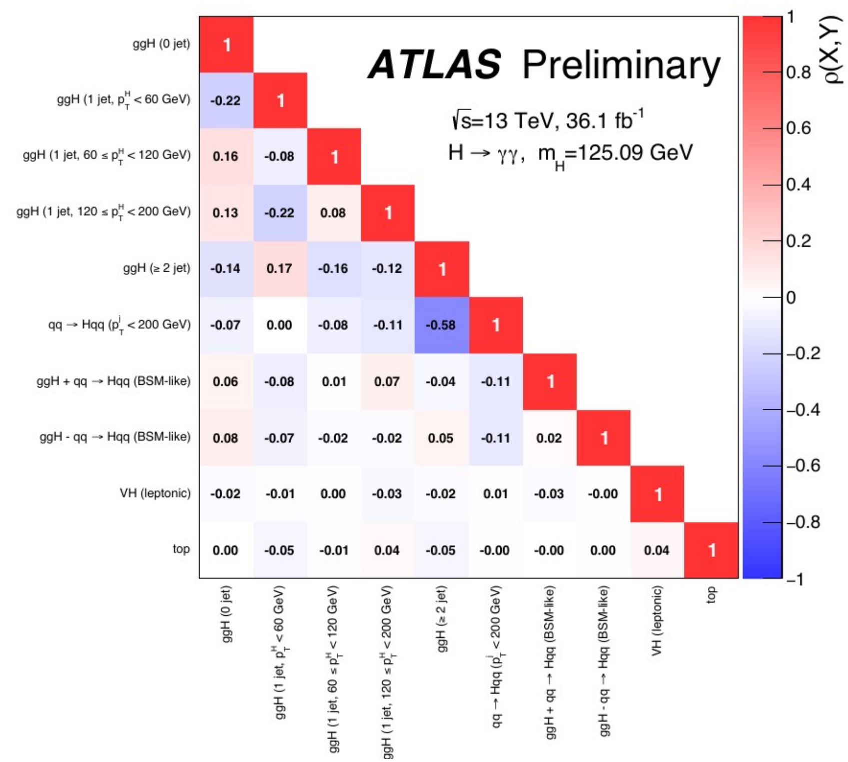



# Presentation of Results

→ Cannot test every model : need to make enough information public so that others (theorists) are able to do it independently

⇒ **Gaussian case**: sufficient to provide measurements + covariance matrix
→ For example using the HEPData repository.




**Non-Gaussian case**: not so simple, but can publish full likelihood (e.g. here)

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- Discovery
- Confidence intervals
- Upper limits

Reparameterization and presentation of results

Expected results

Profiling

# Generating Pseudo-data

Model describes the distribution of the observable: **P(data; parameters)**

⇒ Possible outcomes of the experiment, for given parameter values

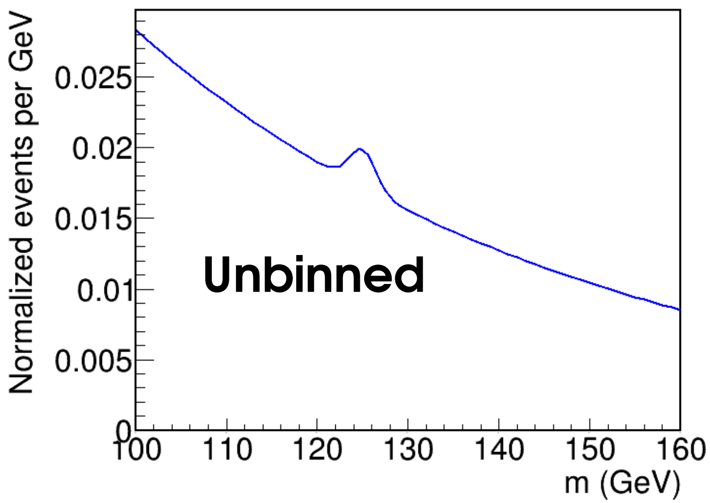
Can draw random events according to PDF : **generate** ***pseudo-data***

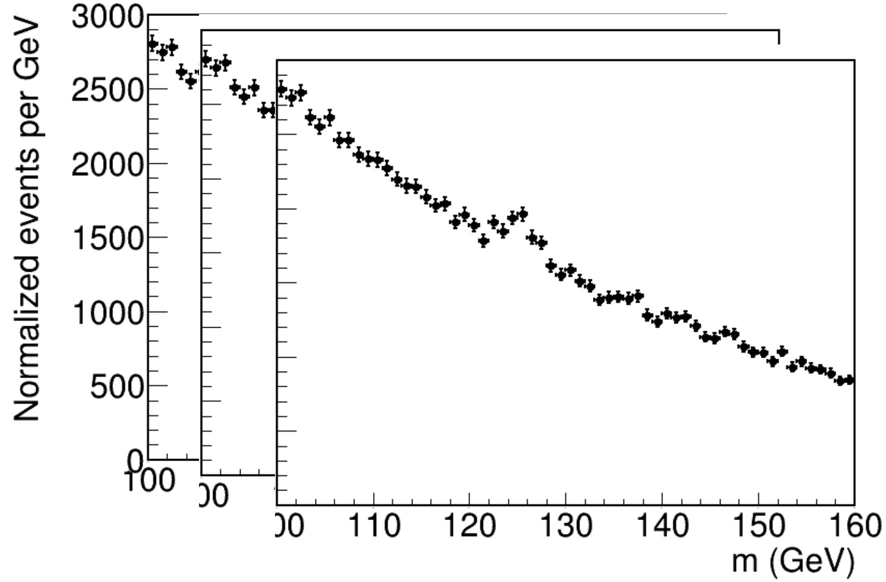
$$P(\lambda=5)$$

**2, 5, 3, 7, 4, 9, ....**

Each entry = separate "experiment"

**Generate**



# Expected Limits: Toys

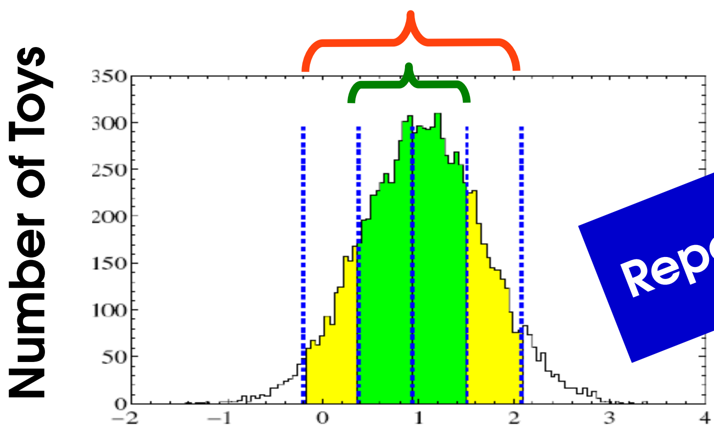
***Expected* results**: median outcome under a given hypothesis
→ usually B-only for searches, but other choices possible.

Two main ways to compute:

**→ Pseudo-experiments (*toys*):**

- Generate a pseudo-dataset in B-only hypothesis
- Compute limit
- Repeat and histogram the results
- Central value = median, bands based on quantiles

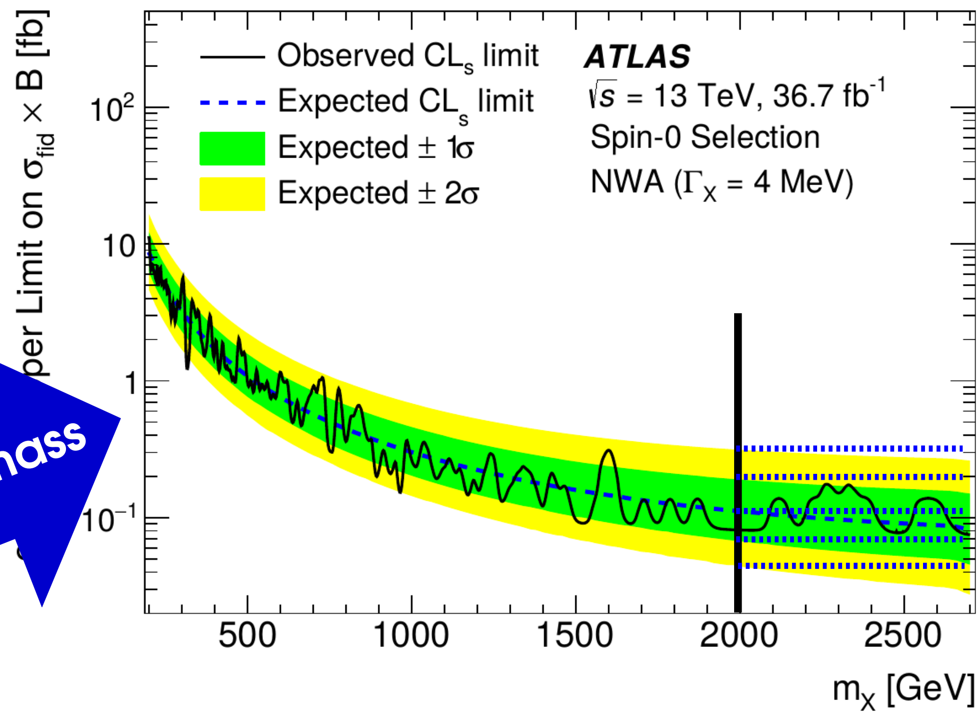
**68% of toys** **95% of toys**




Eur.Phys.J.C71:1554,2011

Repeat for each mass

Phys. Lett. B 775 (2017) 105



# Expected Limits: Asimov Datasets

***Expected* results**: median outcome under a given hypothesis
→ usually B-only for searches, but other choices possible.

Two main ways to compute:

Strictly speaking, Asimov dataset if

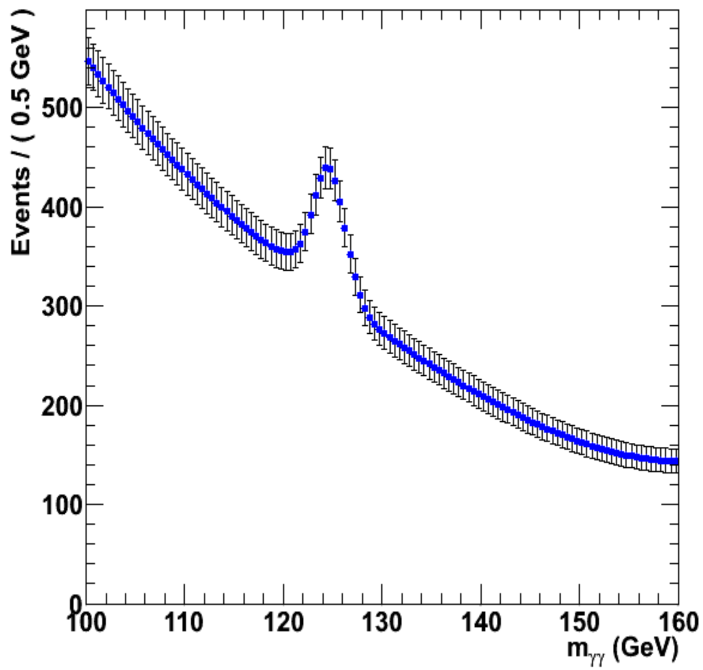
**$\hat{X} = X_0$ for all parameters $X$,**

where $X_0$ is the generation value

**→ *Asimov Datasets***

- Generate a "perfect dataset" – *e.g.* for binned data, set bin contents carefully, no fluctuations.
- Gives the median result immediately:
  **median(toy results) ↔ result(median dataset)**
- Get bands from asymptotic formulas:
  Band width

$$\sigma^2_{S_0,A} = \frac{S_0^2}{q_{S_0}(\text{Asimov})}$$



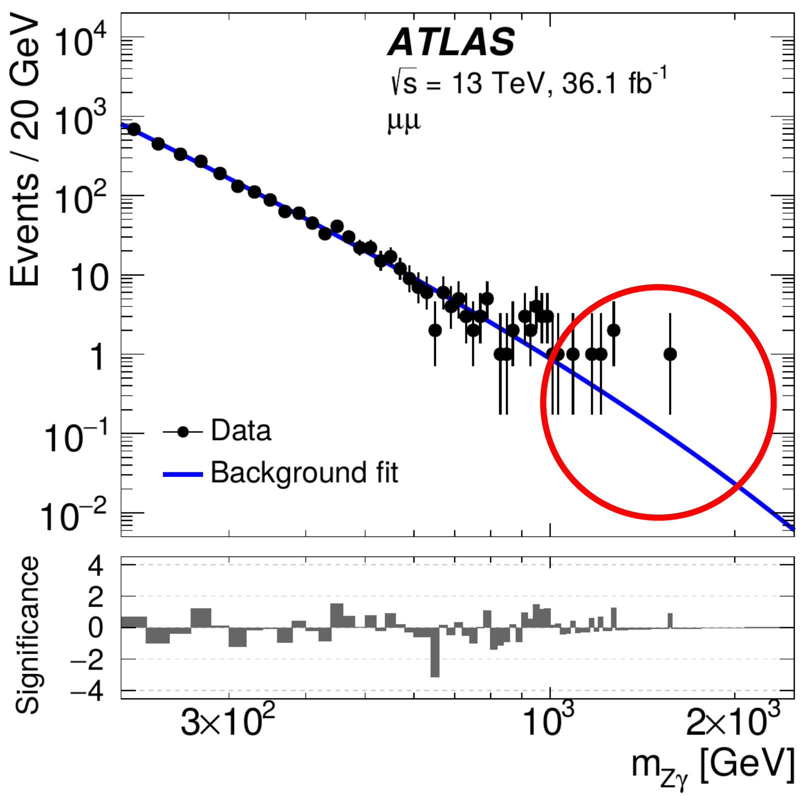

⊕ **Much faster (1 "toy")**

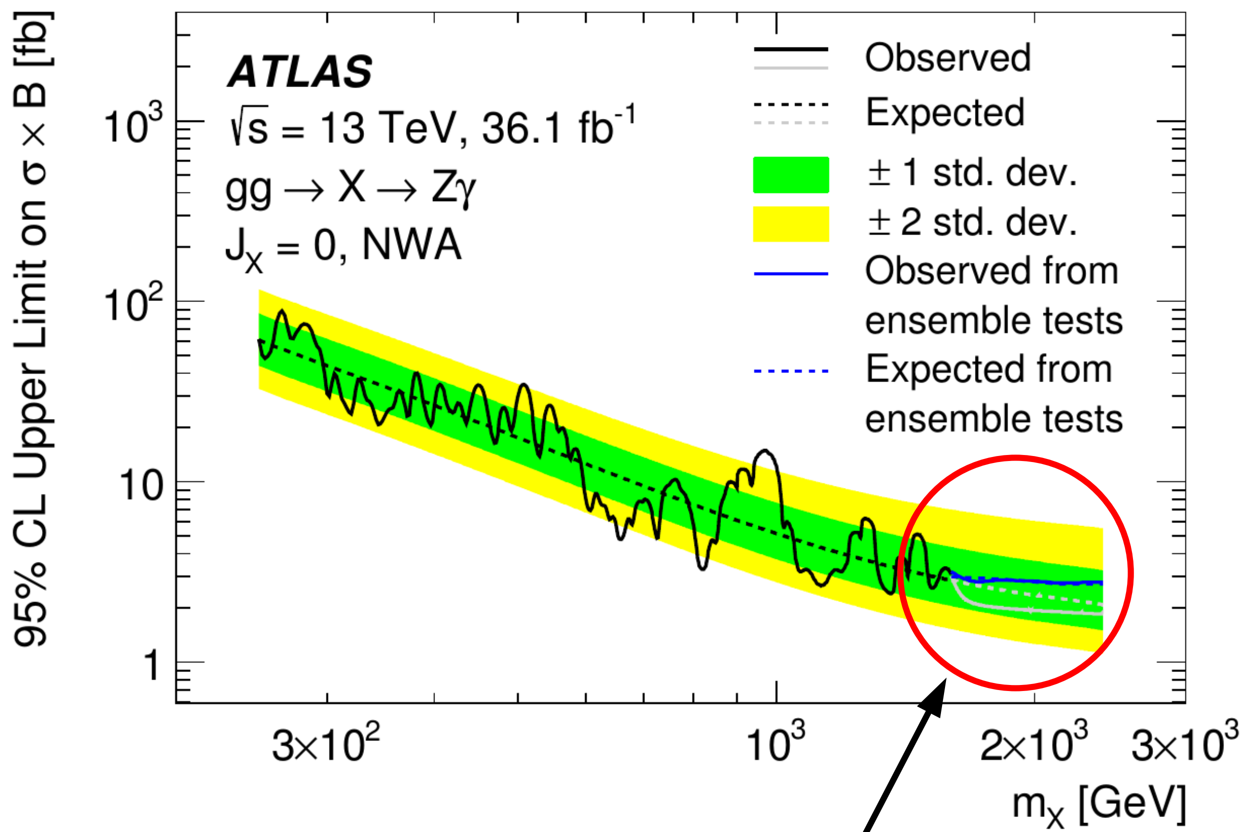
⊖ **Relies on Gaussian approximation**

# Toys: Example

JHEP 10 (2017) 112

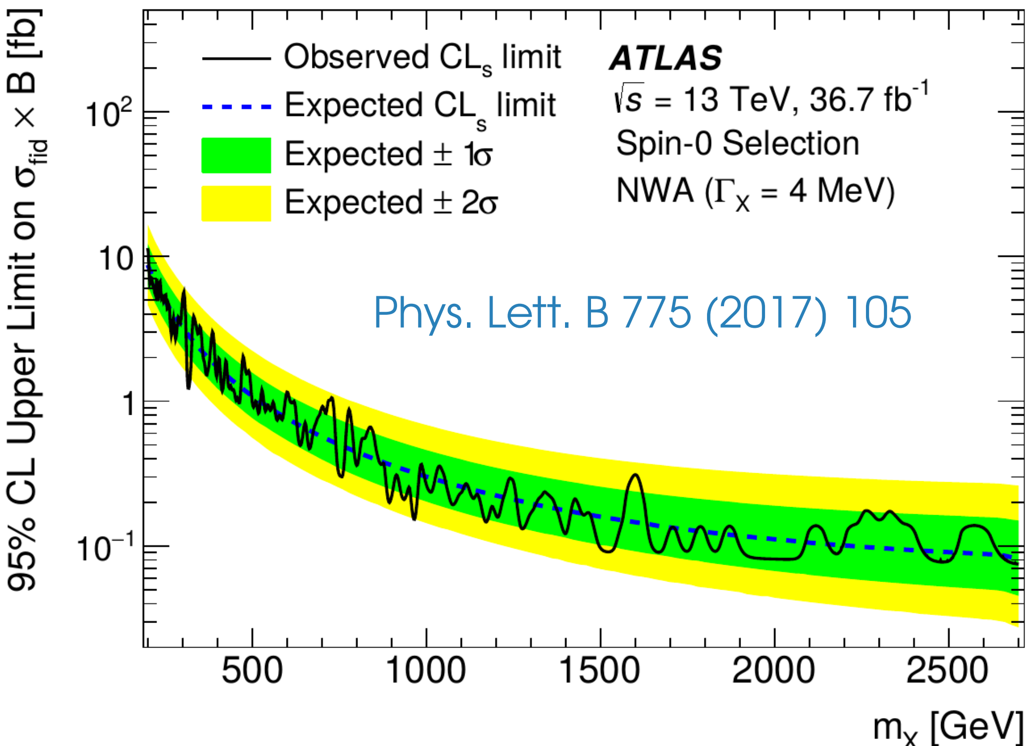
ATLAS $X \to Z\gamma$ Search: covers 200 GeV < $m_X$ < 2.5 TeV
→ for $m_X$ > 1.6 TeV, low event counts ⇒ derive results from toys



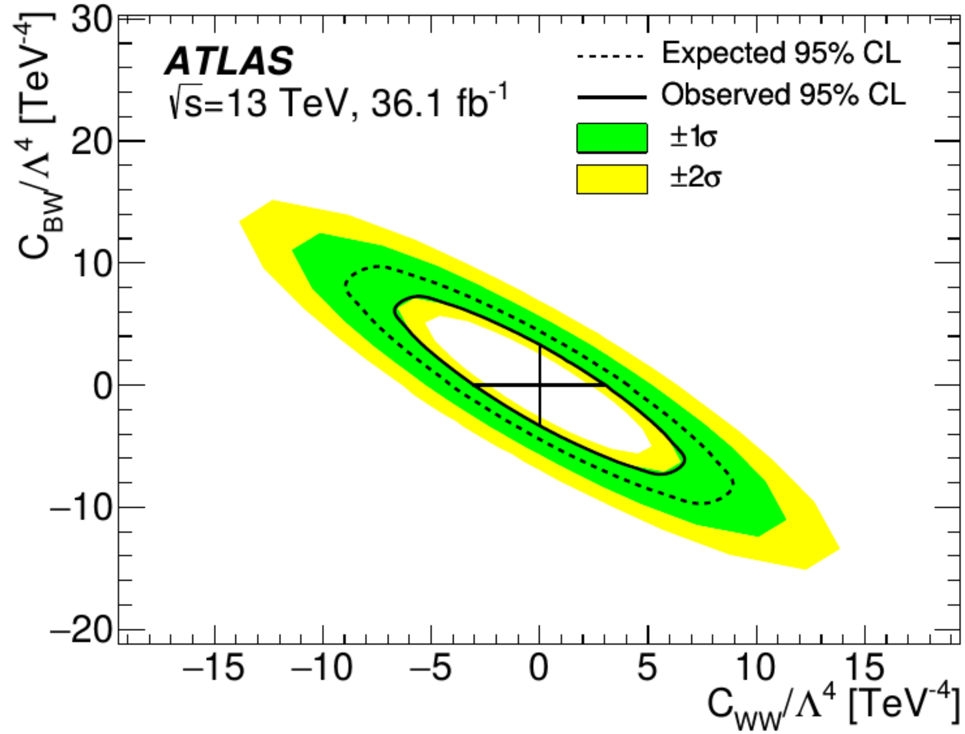



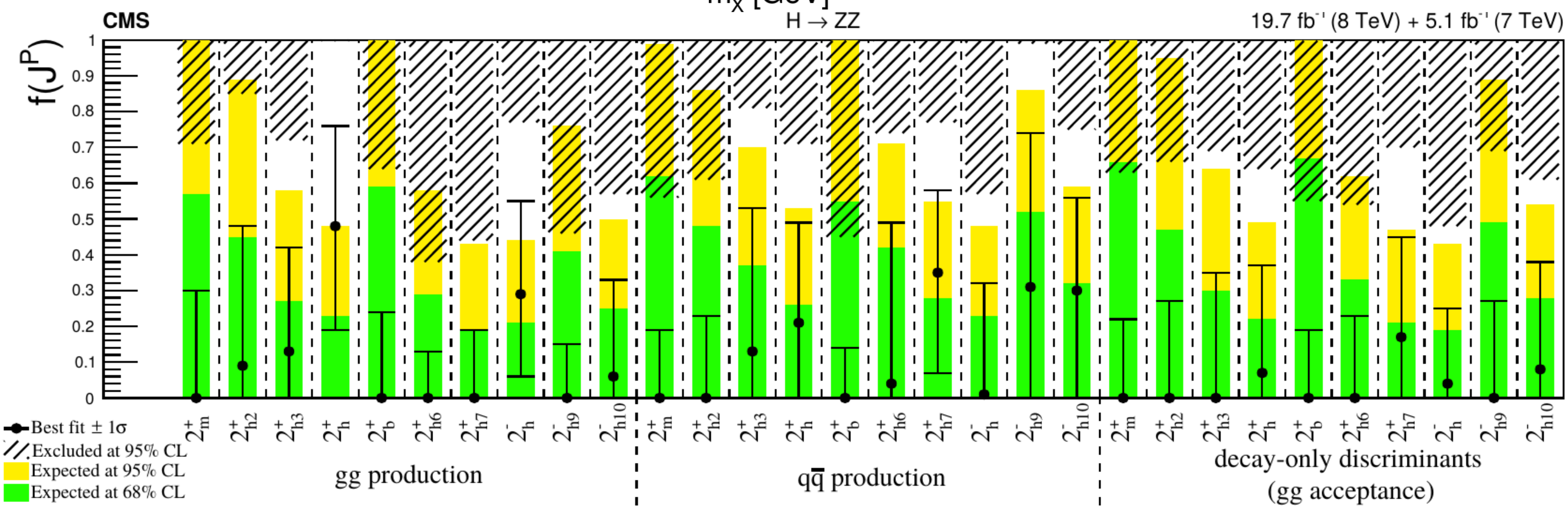

Asimov results (in gray) give optimistic result compared to toys (**in blue**)

# Upper Limit Examples




ATLAS 2015-2016 4l aTGC Search

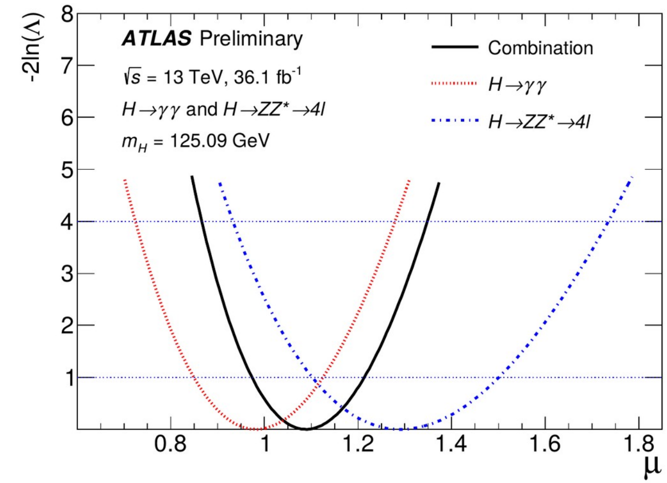



Phys. Rev. D 92 (2015) 012004

# Takeaways

**Confidence intervals**: use $$t_{\mu_0} = -2\log\frac{L(\mu=\mu_0)}{L(\hat{\mu})}$$



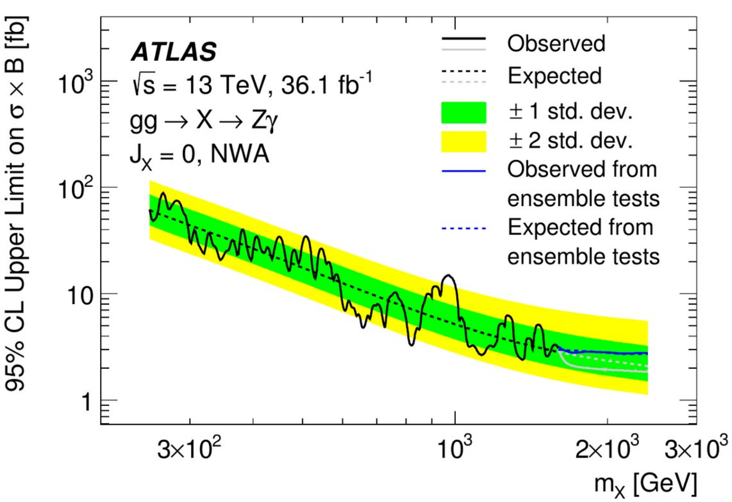

→ Crossings with $t_{\mu 0} = Z^2$ for $\pm Z\sigma$ intervals (in 1D)

**Gaussian regime**: $\mu = \hat{\mu} \pm \sigma_\mu$ (1σ interval)

**Limits** : use LR-based test statistic: $$q_{S_0} = -2\log\frac{L(S=S_0)}{L(\hat{S})} \quad S_0 \geq \hat{S}$$

→ Use **$CL_s$ procedure** to avoid negative limits

**Poisson regime**, n=0 : **$S_{up}$ = 3 events**



# Outline

Computing statistical results

- Discovery
- Confidence intervals
- Upper limits

Reparameterization and presentation of results

Expected results

Profiling

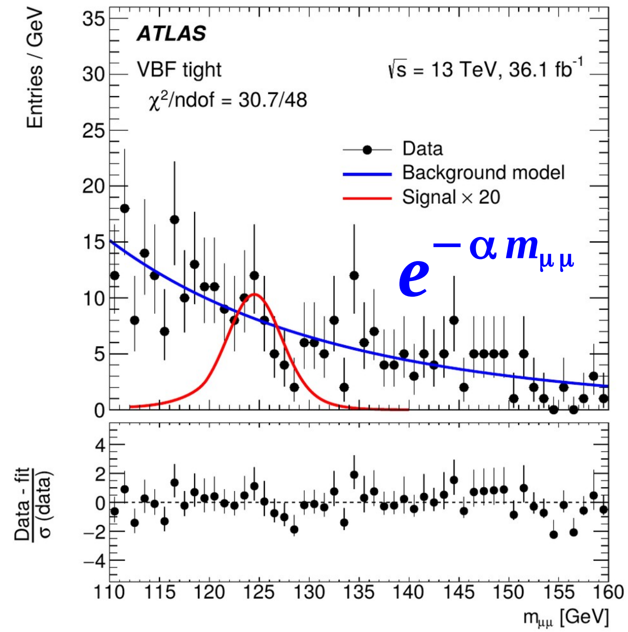
# Nuisances and Systematics

Phys. Rev. Lett. 119 (2017) 051802

Likelihood typically includes

- **Parameters of interest** (POIs) : **S**, **σ×B**, **$m_W$**, ...
- **Nuisance parameters** (NPs) : other parameters needed to define the model

  → Ideally, **constrained by data** like the POI




**What about systematics ?**

= what we don't know about the random processs

⇒ **Parameterize using additional NPs**

⇒ Add constraints in the likelihood

$$L(\mu, \theta; \text{data}) = L_{\text{measurement}}(\mu, \theta; \text{data})\ C(\theta)$$

**POI** **Systematics NP** **Measurement Likelihood** **NP Constraint term**

"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 ?*

C(θ) represents extra knowledge about the NP

# Frequentist Systematics

**Prototype**: NP measured in a separate ***auxiliary* experiment**
e.g. luminosity measurement

→ Build the combined likelihood of the main+auxiliary measurements

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

Independent measurements:
⇒ just a product

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

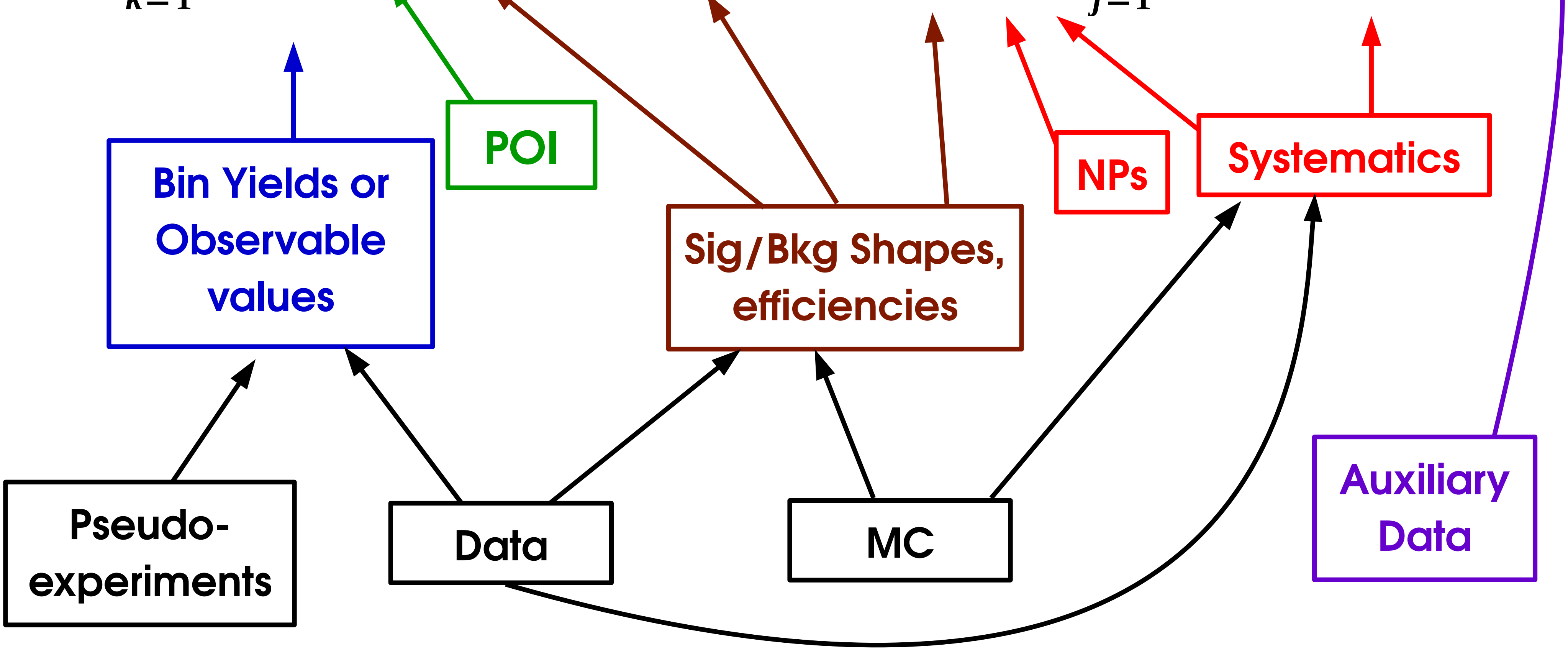
In the combined likelihood, **systematic NPs are constrained**
→ now same as e.g. NPs constrained in sidebands.

→ 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)

$$L\left(\mu, \{\theta_j\}_{j=1\ldots n_{NP}}; \{n_i^{(k)}\}_{i=1\ldots n_{data}^{(k)}}^{k=1\ldots n_{cat}}, \{\theta_j^{obs}\}_{j=1..n_{NP}}\right) =$$

$$\prod_{k=1}^{n_{cat}} P\left[n_i; \overbrace{\mu\, \epsilon_{i,k}(\vec{\theta})\; N_{S,i,k}(\vec{\theta}) + B_{i,k}(\vec{\theta})}^{\text{Expected bin yield}}\right] \prod_{j=1}^{n_{syst}} G(\theta_j^{obs}; \theta_j; 1)$$




× number of categories!

# Reminder: Wilks' Theorem

Cowan, Cranmer, Gross & Vitells
Eur.Phys.J.C71:1554,2011

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

→ Assume **Gaussian regime** (e.g. large $n_{evts}$, Central-limit theorem) : then:

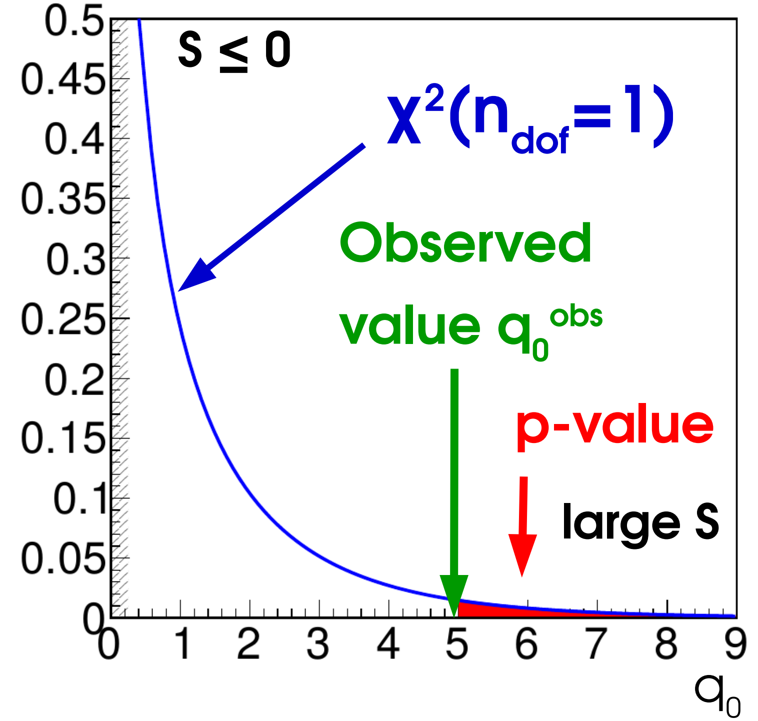
***Wilk's Theorem:*** **$t_{S0}$ is distributed as a $\chi^2$**

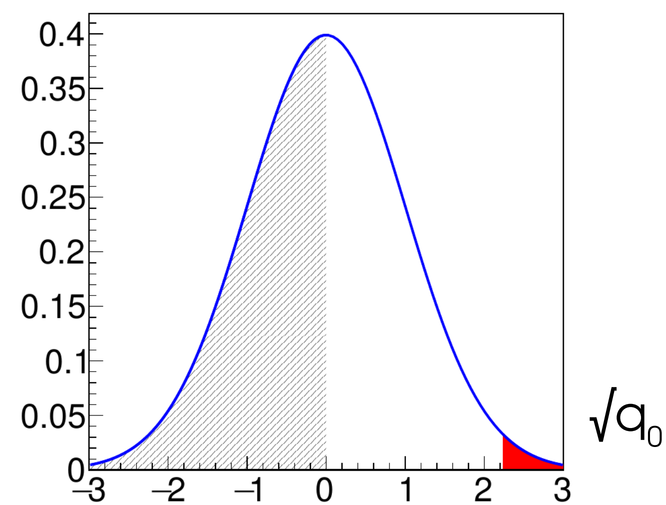
under $H_{S0}(S=S_0)$:

$$f\left(t_{S_0} \mid S=S_0\right) = f_{\chi^2(n_{dof}=1)}\left(t_{S_0}\right)$$

⇒ The significance is:

$$Z = \sqrt{q_0}$$



# Profiling

How to deal with nuisance parameters in likelihood ratios ?

→ **Let the data choose ⇒ use the best-fit values (*Profiling*)**

⇒ **Profile Likelihood Ratio** (PLR)

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

$\hat{\hat{\theta}}(S_0)$ best-fit value for $S=S_0$ (conditional MLE)

$\hat{\theta}$ overall best-fit value (unconditional MLE)

***Wilks' Theorem*: same properties as plain likelihood ratio**

$$f\left(t_{S_0} \mid S=S_0\right) = f_{\chi^2(n_{dof}=1)}\left(t_{S_0}\right)$$

***also with NPs present***

→ Profiling "builds in" the effect of the NPs

**⇒ Can use $t_{S0}$ to compute limits, significance, etc. in the same way as before**

# Homework 7: Gaussian Profiling

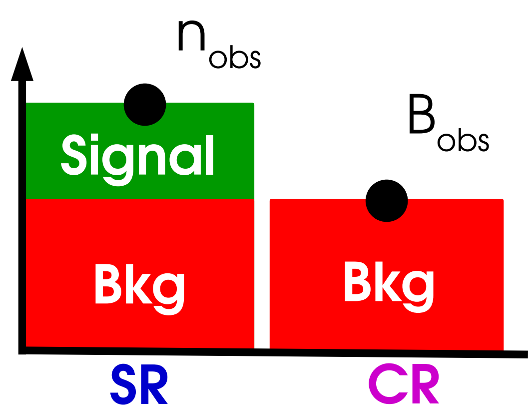
Counting experiment with background uncertainty: **n = S + B** :

→ **Signal region (SR)**: $n_{obs} \sim G(S + B, \sigma_{stat})$

→ **Control region (CR)**: $B_{obs} \sim G(B, \sigma_{bkg})$

$$L(S, B) = G(n_{obs}; S + B, \sigma_{stat})\, G(B_{obs}; B, \sigma_{bkg})$$

**Recall:** Signal region only (fixed B): $t_S = \left(\frac{S - n_{obs}}{\sigma_{stat}}\right)^2$ $\quad S = (n_{obs} - B) \pm \sigma_{stat}$




→ Compute the best-fit (MLEs) for S and B

→ Show that the conditional MLE for B is

$$\hat{\hat{B}}(S) = B_{obs} + \frac{\sigma_{bkg}^2}{\sigma_{stat}^2 + \sigma_{bkg}^2}(\hat{S} - S)$$

→ Compute the profile likelihood $t_S$

→ Compute the 1σ confidence interval on S

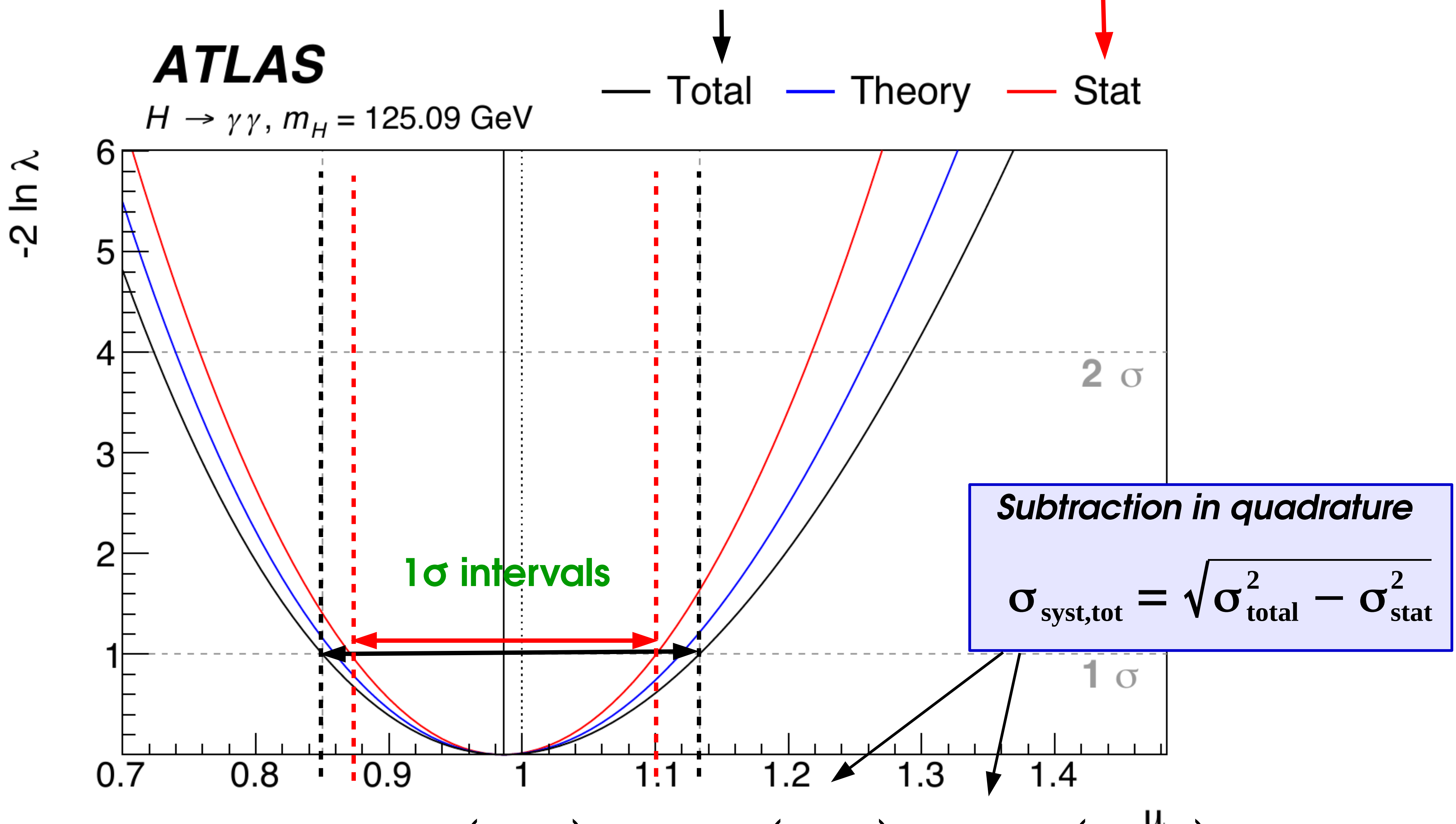
$$S = (n_{obs} - B_{obs}) \pm \sqrt{\sigma_{stat}^2 + \sigma_{bkg}^2} \qquad \sigma_S = \sqrt{\sigma_{stat}^2 + \sigma_{bkg}^2}$$

**Stat uncertainty (on n) and systematic (on B) add in quadrature**

# Uncertainty decomposition

All systematics NPs excluded : statistical uncertainty only

All systematics NPs included: stat+syst uncertaintes




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

# Pull/Impact plots

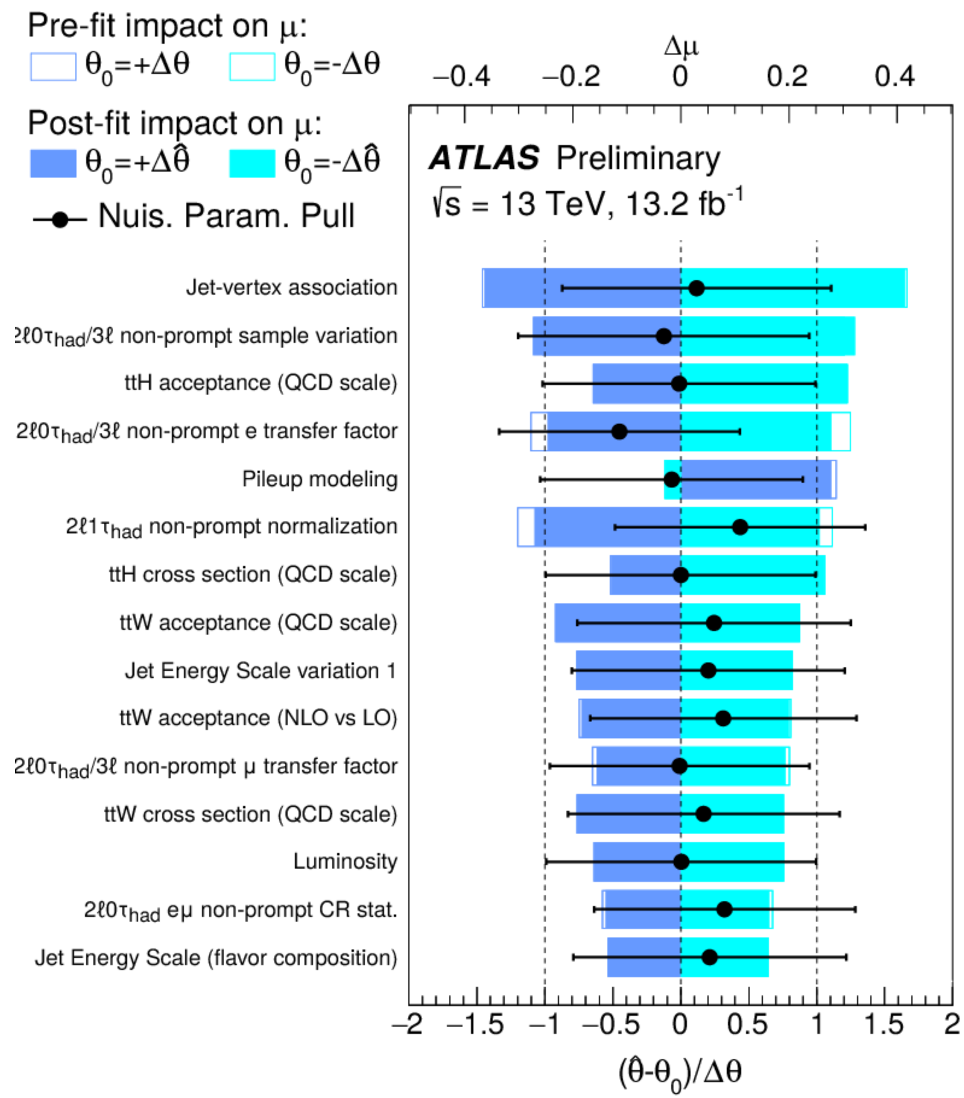
ATLAS-CONF-2016-058

Systematics are described by NPs included in the fit. Define **pull** as

$$\left(\hat{\theta} - \theta_0\right) / \sigma_\theta$$

Nominally:

- **pull = 0** : i.e. the pre-fit expectation
- **pull uncertainty = 1** : from the Gaussian




However fit results may be different:

- **Central value ≠ 0**: some data feature differs from MC expectation ⇒ Need investigation if large
- **Uncertainty < 1** : effect is *constrained* by the data ⇒ Needs checking if this legitimate or a modeling issue
- 

→ **Impact on result** of ±1σ shift of NP allows to gauge which NPs matter most .

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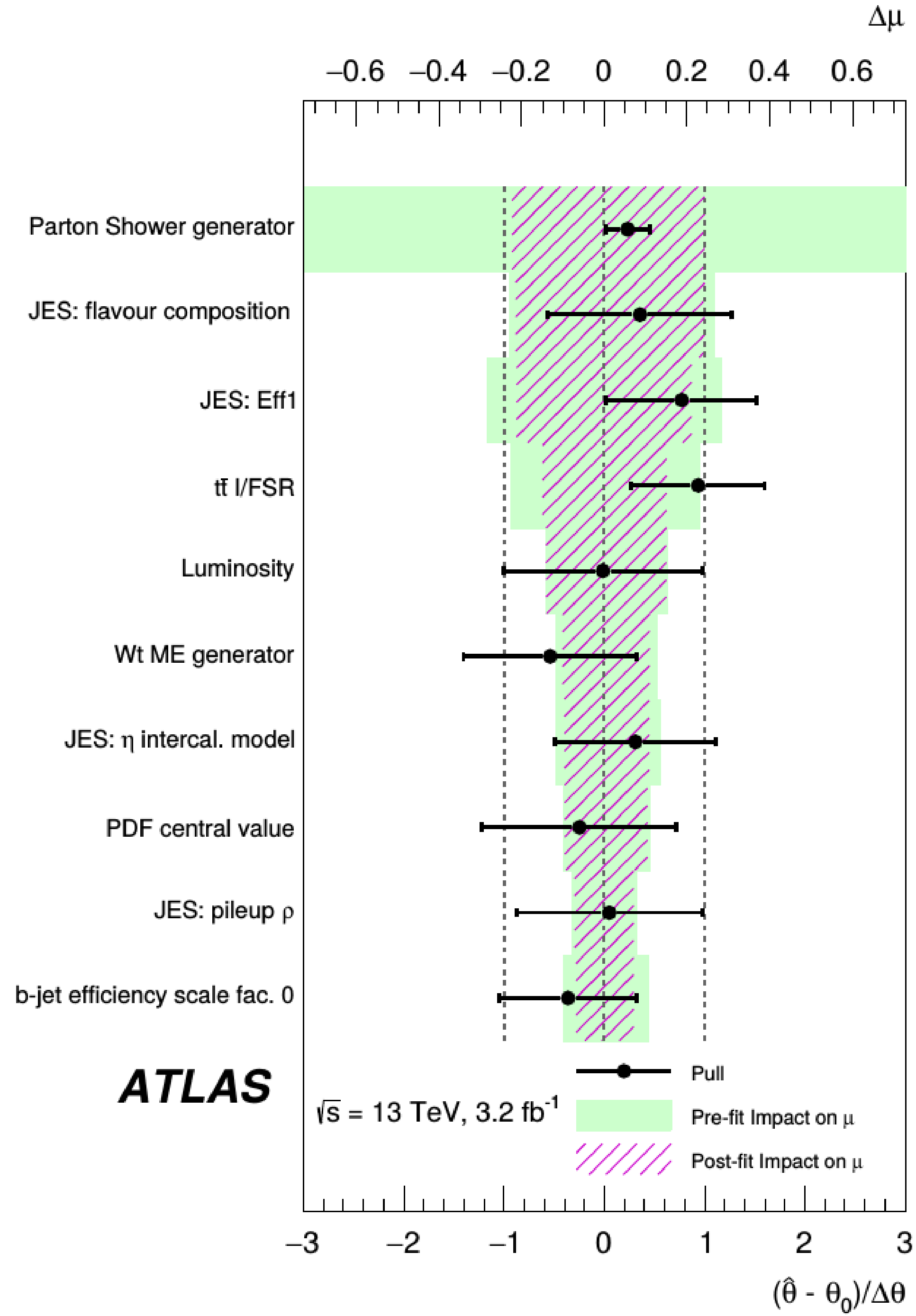
- 

→ **Impact on result** of $\pm 1\sigma$ shift of NP allows to gauge which NPs matter most .

13 TeV single-t XS (arXiv:1612.07231)



# Profiling Takeaways

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

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

Allows to include systematics as uncertainties on nuisance parameters.

Profiling systematics includes their effect into the total uncertainty.

Gaussian:

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

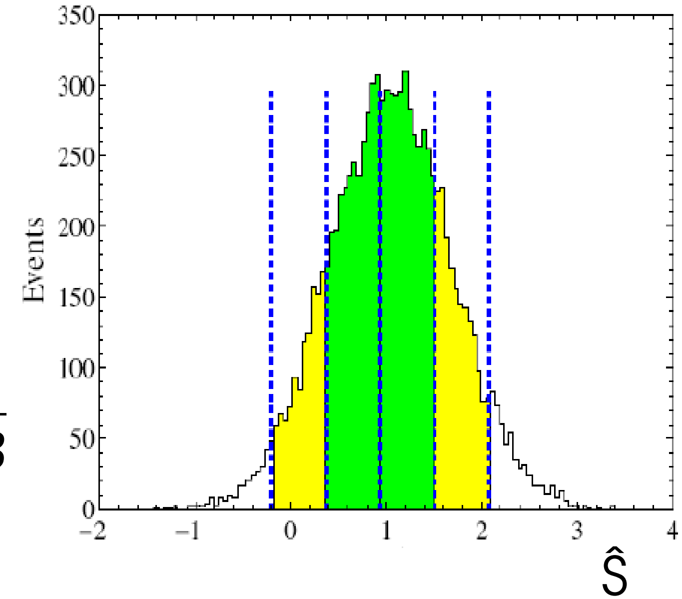
Guaranteed to work well as long as everything is Gaussian, but typically also robust against non-Gaussian behavior.

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

# Extra Slides

# CL$_s$ : Gaussian Bands

Eur.Phys.J.C71:1554,2011




Usual Gaussian counting example with known B:

95% CL$_s$ upper limit on S:

$$S_{up} = \hat{S} + \left[\Phi^{-1}\left(1 - 0.05\ \Phi\left(\hat{S}/\sigma_S\right)\right)\right]\sigma_S$$

with

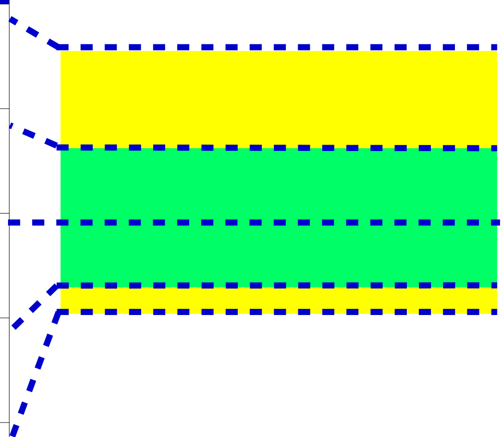
$$\sigma_S = \sqrt{B}$$

Compute expected bands for S=0:

→ **Asimov dataset ⇔ $\hat{S} = 0$** : $S^0_{up,exp} = 1.96\ \sigma_S$

→ **$\pm$ n$\sigma$ bands**: $S^{\pm n}_{up,exp} = \left(\pm n + \left[1 - \Phi^{-1}\left(0.05\ \Phi(\mp n)\right)\right]\right)\sigma_S$

| n | $S_{exp}^{\pm n}$ / $\sqrt{B}$ |
|---|---|
| +2 | 3.66 |
| +1 | 2.72 |
| 0 | 1.96 |
| -1 | 1.41 |
| -2 | 1.05 |



**CLs** :

- Positive bands somewhat reduced,
- Negative ones more so

Band width from $\sigma^2_{S,A} = \dfrac{S^2}{q_S(\text{Asimov})}$ depends on S, for non-Gaussian cases,different values for each band...

# Comparison with LEP/TeVatron definitions

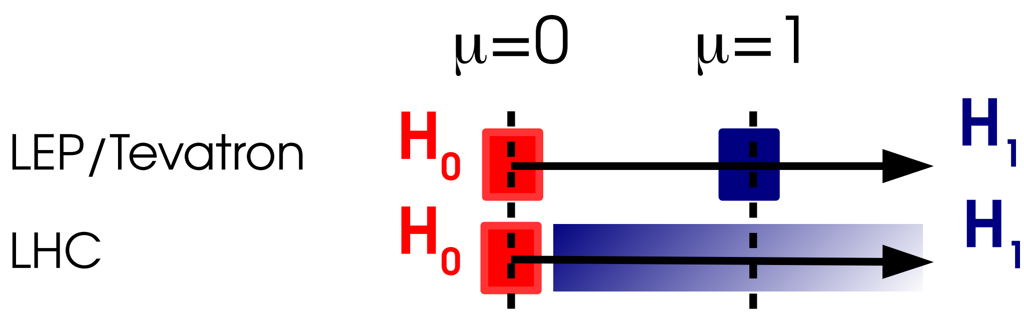
Likelihood ratios are not a new idea:

- **LEP**: Simple LR with NPs from MC
  - Compare μ=0 and μ=1
- **Tevatron**: PLR with profiled NPs

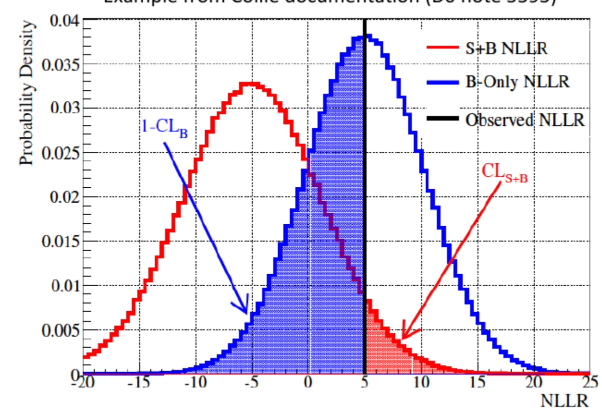
$$q_{LEP} = -2\log \frac{L(\mu=0, \tilde{\theta})}{L(\mu=1, \tilde{\theta})}$$

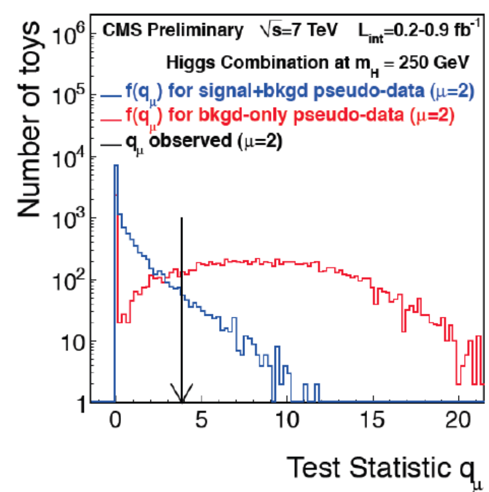
$$q_{Tevatron} = -2\log \frac{L(\mu=0, \hat{\hat{\theta}}_0)}{L(\mu=1, \hat{\hat{\theta}}_1)}$$

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




Example from Collie documentation (D0 note 5595)



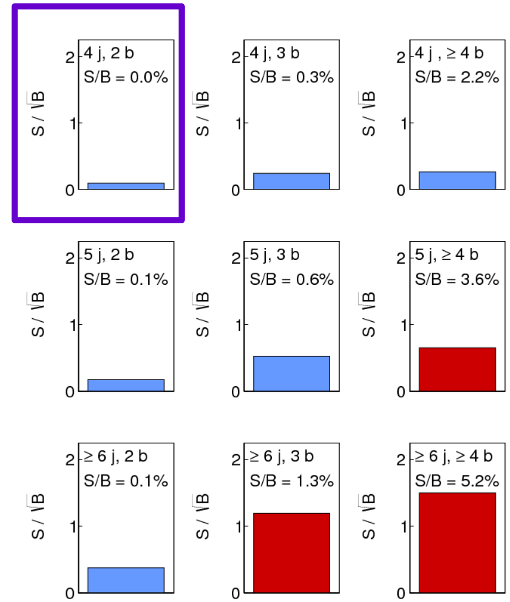

→ Asymptotically:

- **LEP/Tevaton**: q linear in μ ⇒ **~Gaussian**
- **LHC**: q quadratic in μ ⇒ **~χ2**

→ Still use TeVatron-style for discrete cases

Andrey Korytov, EPS 2011

# Profiling Example: ttH→bb

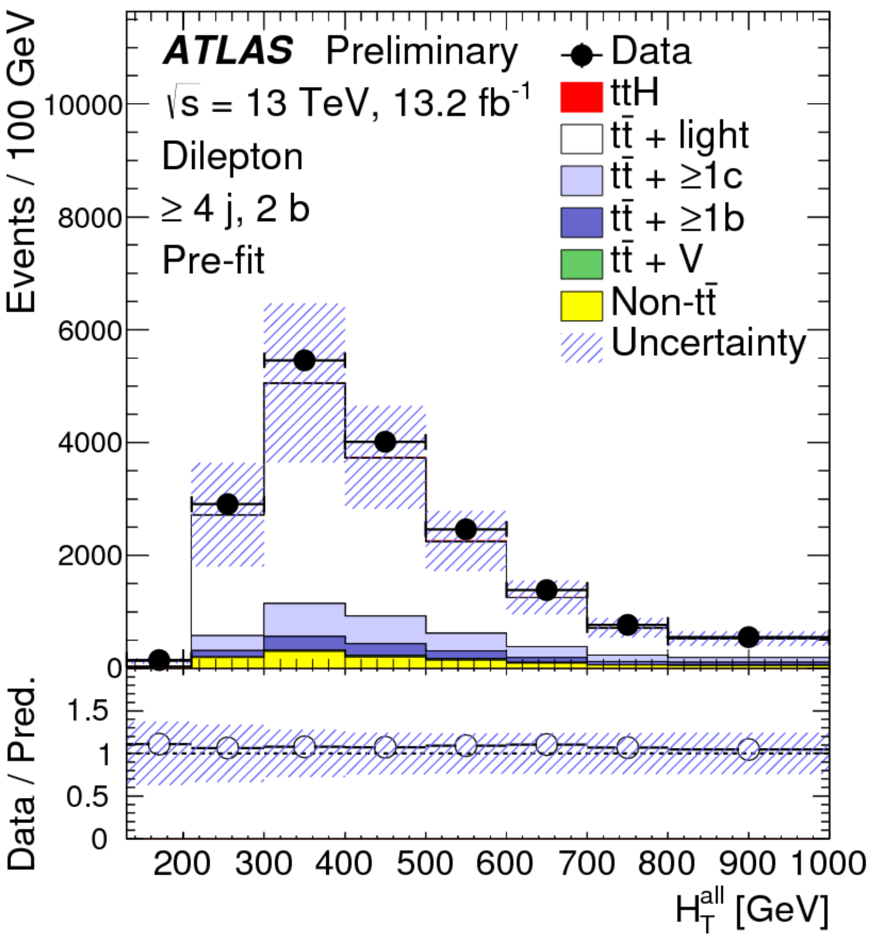


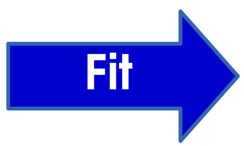

Analysis uses low-S/B categories to constrain backgrounds.

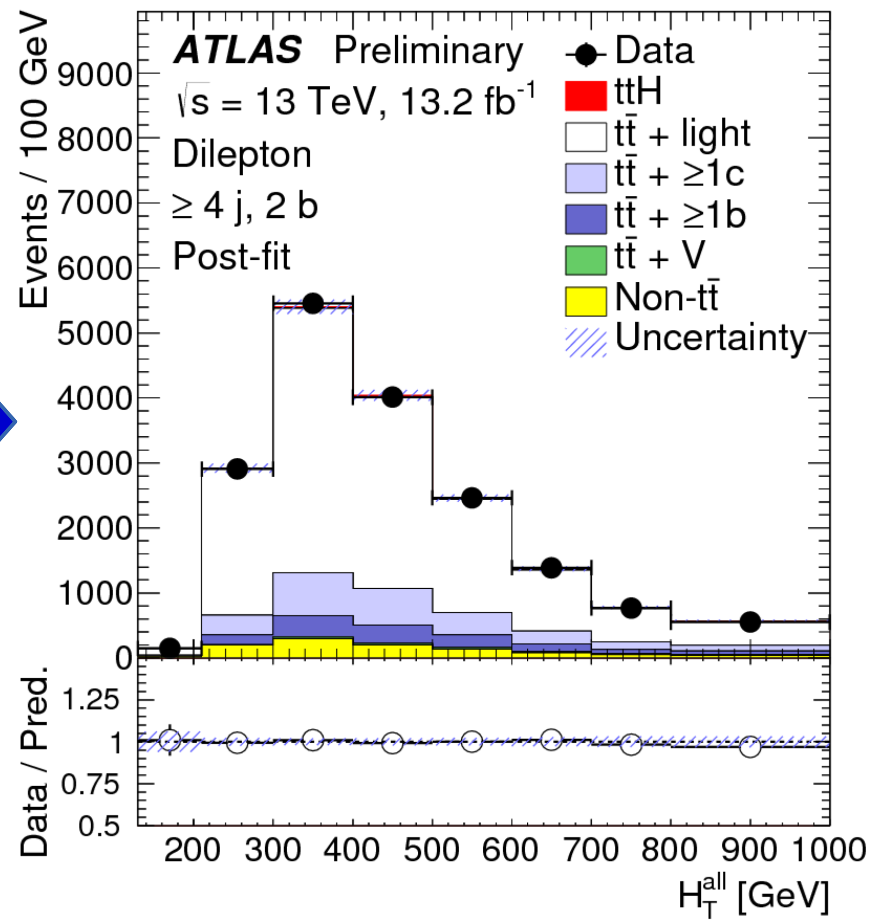
→ **Reduction in large uncertainties on tt bkg**

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

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

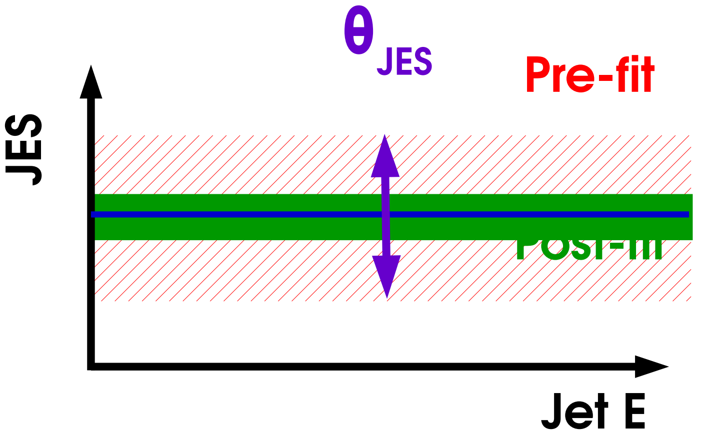


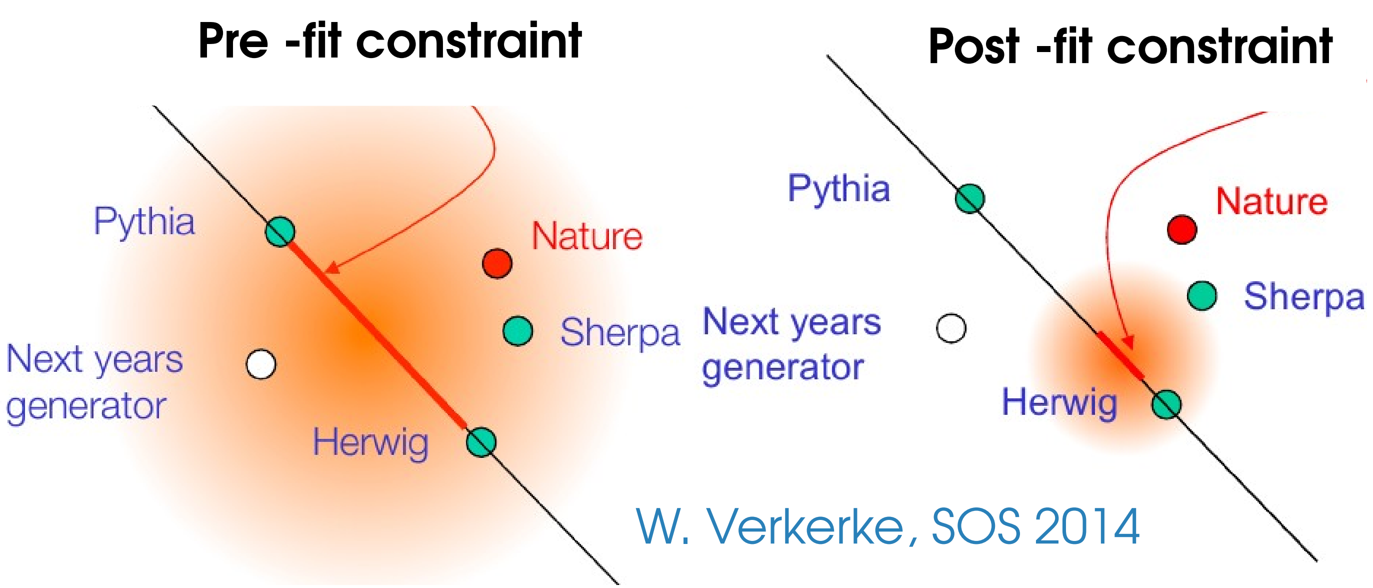

ATLAS-CONF-2016-08

# 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



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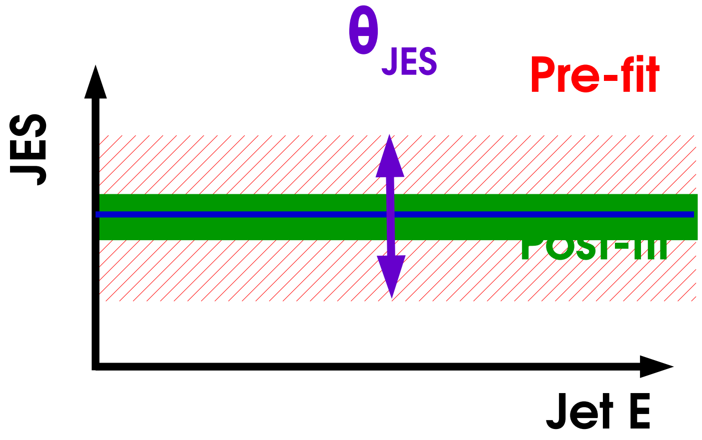


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