



Science & Technology Facilities Council
Rutherford Appleton Laboratory

Hands-on Statistics

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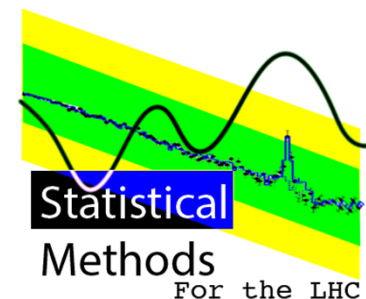
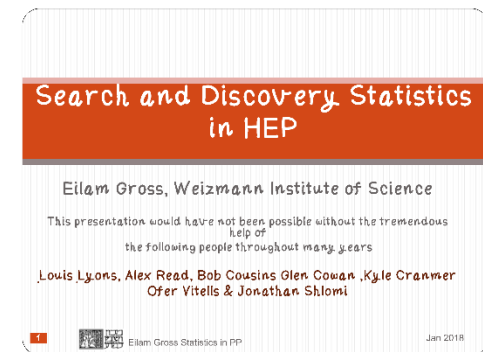
PPD Advanced Graduate Lectures
11th May 2020



ATLAS

Introduction

- This is not a statistics lecture!
 - Instead, I hope to give some hints on **how** to use some of the statistical methods you learned from the real expert lecturers.
 - I apologise in advance for sloppy language, unintroduced terms, and complete lack of proofs
- For a thorough introduction, I recommend:
 1. CERN Academic Training Lecture series, which has had 3–4 hour lectures by different HEP statistics experts every couple of years. I have found particularly helpful:
 1. Eilam Gross in 2018
 2. Glen Cowan in 2012
 3. Kyle Cranmer in 2011
 2. “Statistics Methods for the LHC” – online documentation from ATLAS, with RooFit / RooStats / RooUnfold code examples.



Introduction

- There are alternative concepts and methods that we could use, but I will only discuss techniques most common in Particle Physics today, notably:
 1. **Frequentist statistics**
 - Bayesian used in most other fields
 2. **profile likelihood ratio developed for the LHC**
 - You are probably already familiar with the other common method, least squares (χ^2) fit
 3. **CLs limits**
 - not widely accepted outside our field
- Due to lack of time or personal experience, I will **not** discuss
 1. **combination of results (BLUE etc)**
 - I will mention Likelihood combination
 2. **goodness-of-fit (χ^2 , KS tests, etc)**
 3. **... or any techniques used on event data, before the final statistical interpretation**
 - multivariate discrimination, machine learning, sPlots, etc.

Lecture plan

- Building a model
 1. PDF \otimes data \rightarrow Likelihood
 2. Asimov dataset
- Some typical types of statistical analysis
 - Testing a model, with an example from LHC Run1 Higgs measurements, demonstrates all three stages:
 3. Measurement
 4. Discovery
 5. Exclusion
 - ~~Presenting results without a model:~~
 6. ~~Unfolding~~ (but see [RooUnfold](#), very old [slides](#))
- Summary

Model building

PDF, dataset, and likelihood

- All the statistical tests we will be considering are based on the likelihood

$$L(\boldsymbol{\alpha}) = \prod_c \prod_i P_c(x_i|\boldsymbol{\alpha}) \cdot \prod_j C_j(\theta_j|\boldsymbol{\alpha}_j)$$

1. $L(\boldsymbol{\alpha})$ is a function of various parameters ($\boldsymbol{\alpha}$), some of which we wish to determine
 2. $P_c(x_i|\boldsymbol{\alpha})$ is the probability density function (PDF) for channel c , evaluated for each member of the dataset, x_i
 - The use (or not) of the parameters, $\boldsymbol{\alpha}$, in the different channels determines how they are constrained by the data
 - eg. for binned data in histogram h , with bins, i , $P_h(n_i|\boldsymbol{\alpha}) = \text{Poisson}(n_i|v_i(\boldsymbol{\alpha}))$
 3. $C_j(\theta_j|\boldsymbol{\alpha}_j)$ are additional PDFs that do not depend on the data
 - eg. constraint terms for systematic uncertainties, $C_j(\theta_j|\boldsymbol{\alpha}_j) = \text{Gaussian}(\mu_j|\boldsymbol{\alpha}_j, \sigma_j)$
- Bear in mind:
 - PDFs ($P_c(x)$ and $C_j(\theta)$) must be normalised to 1, or a constant independent of $\boldsymbol{\alpha}$
 - The likelihood, on the other hand, is not normalised
 - The absolute value of the likelihood ($L(\boldsymbol{\alpha})$) is irrelevant, only changes WRT $\boldsymbol{\alpha}$
 - It is usually used as $-\ln L$, or more commonly, $-2\ln L$
 - maximum likelihood is at minimum of $-2\ln L$
 - in the Asymptotic limit, $-2\ln L$ is distributed like a χ^2
- $$-2\ln L(\boldsymbol{\alpha}) = \sum_c \sum_i -2 \ln P_c(x_i|\boldsymbol{\alpha}) + \sum_j -2 \ln C_j(\theta_j|\boldsymbol{\alpha}_j)$$

- Roofit is a tool for creating models
 - RooAbsPdf: base class for PDFs. Will often be constructed from many PDF types.
 - eg. RooGaussian, RooProdPdf, RooSimultaneous
 - these are functions of each other, and of RooRealVar parameters that can be mapped to fit parameters
 - can be constructed directly from C++ or Python, or via a “factory” from a specification
 - eg. `SUM::model (f*RooGaussian::g(x,m[0],1), RooChebychev::c(x,{a0[0.1],a1[0.2],a2[-0.3]})`)
 - RooAbsData: abstract dataset type. Can hold binned and/or unbinned data
 - RooStats::ModelConfig: holds configuration information for a single model
 - PDF, POIs, NPs, observables, etc
 - RooWorkspace: container for PDFs, datasets, and ModelConfigs
 - This can be saved to a `workspace.root` file to allow separate statistical analysis
 - everything needed should be stored here, allowing sharing, combining, archiving
- Roofit also provides fitting and basic statistical analysis tools
 - RooNLLVar: $-\ln L$ constructed from PDF and dataset
 - RooMinimizer: uses Minuit to minimise RooNLLVar for specified parameters
- RooStats provides higher-level statistical analysis tools
 - eg. ProfileLikelihoodTestStat, AsymptoticCalculator, FrequentistCalculator, HypoTestInverter

HistFactory and pyhf

- HistFactory is a tool for creating models of binned data with systematics

$$L(\boldsymbol{\alpha}) = \prod_c \prod_i \text{Poisson}(n_i | \nu_i(\boldsymbol{\alpha})) \cdot \prod_j C_j(\theta_j | \alpha_j)$$

- Multiple disjoint channels, multiple samples contributing to each with additional (possibly shared) systematics
 - Many analyses can use HistFactory instead of calling RooFit directly.
 - Model specified with XML, which refers to histograms in hist.root files
-
- pyhf is a reimplementaion of HistFactory in pure-Python
 - no dependence on ROOT or RooFit
 - XML+histograms specification replaced by JSON
 - full conversion of models from HistFactory and back
 - reproduces HistFactory results, but much faster
 - tested on ATLAS Run-2 sbottom search, which ran >20 times faster

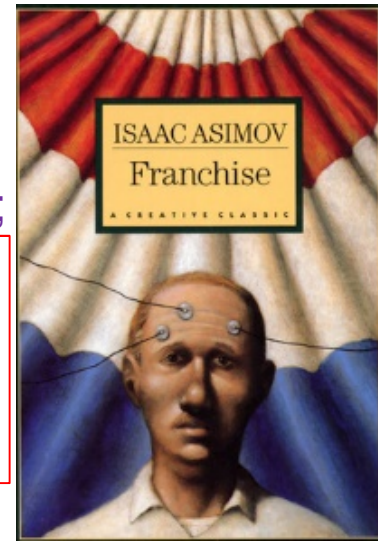
Asimov dataset

- An Asimov dataset [1] is generated for a particular set of model parameters such that the maximum likelihood best-fit value of all those parameters are equal to their generated values.
 - ie. maximising $L_A(\mu, \theta | \mu_0, \theta_0)$ will yield $\hat{\mu} = \mu_0, \hat{\theta} = \theta_0$
 - When used in a statistical test, it will return the result expected from that model configuration
 - eg. p_0 calculated using Asimov dataset generated with $\mu = 0$ will return the p-value expected from no signal
- Asimov datasets are built as binned datasets, in which the event count in each bin is set to the expected event yield for the chosen model parameters.
 - For unbinned models, a binned distribution is generated with chosen binning fine enough to reproduce all significant features of the model.
 - Note this means the Asimov dataset can look different from data or toy datasets: fractional bin contents or unbinned → binned
- For RooFit models:
dataset = RooStats::AsymptoticCalculator::GenerateAsimovData (pdf, observables);

[1] Named for SF author, Isaac Asimov, whose 1955 short story, *Franchise*, envisaged the 2008 US Presidential Election decided by one voter representative of the entire electorate.

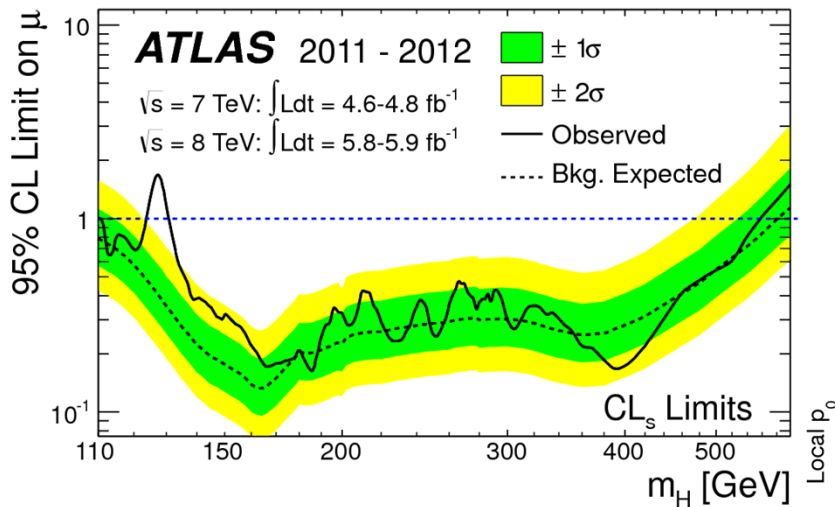
[arXiv:1007.1727]

As an Asimov fan of old, this name makes me very happy.

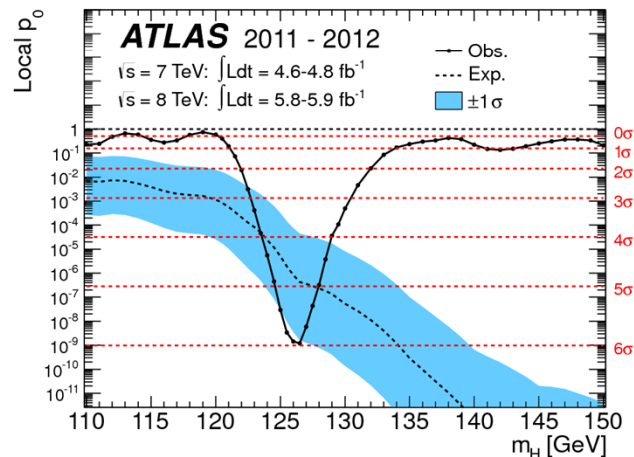


Statistical tests

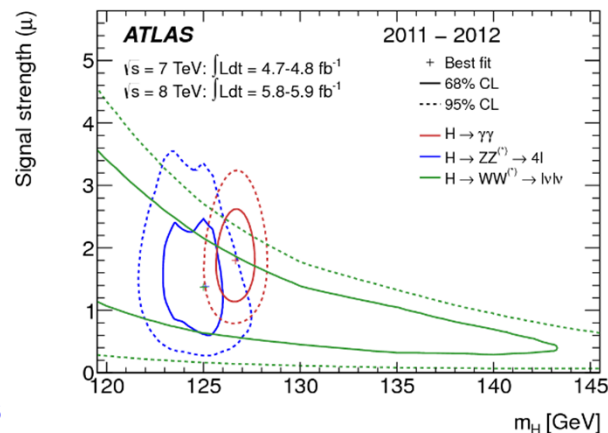
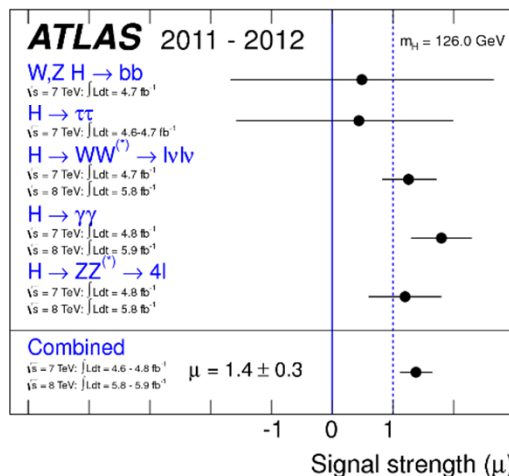
1. Exclusion: CLs



2. Discovery: p_0



3. Measurement: $\hat{\mu} \pm \sigma$ or more generally, confidence intervals



Measurement

- The likelihood is a function of our parameters of interest (POI), here μ , and various nuisance parameters (NP), θ : $L(\mu, \theta)$.

- Note that the θ are often dependent on μ .

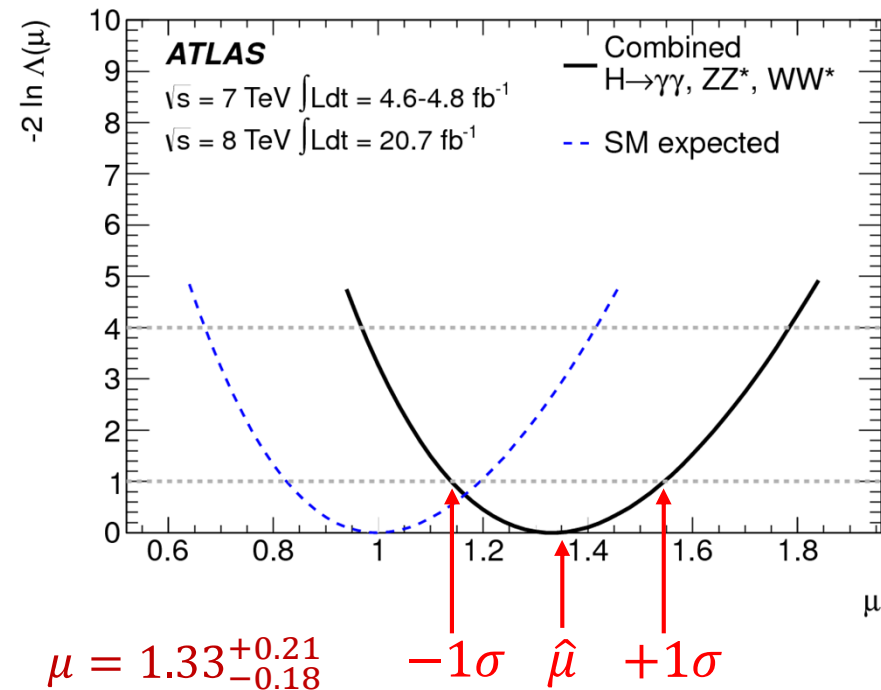
- We form the profile likelihood ratio as:
$$\Lambda(\mu) = \frac{L(\mu, \hat{\theta}(\mu))}{L(\hat{\mu}, \hat{\theta})}$$
 - maximise $L(\mu, \theta(\mu))$ for all $\theta(\mu)$ with specified μ
 - maximise $L(\mu, \theta)$ for all μ, θ

- $\Lambda(\mu)$ can be evaluated with two fits:

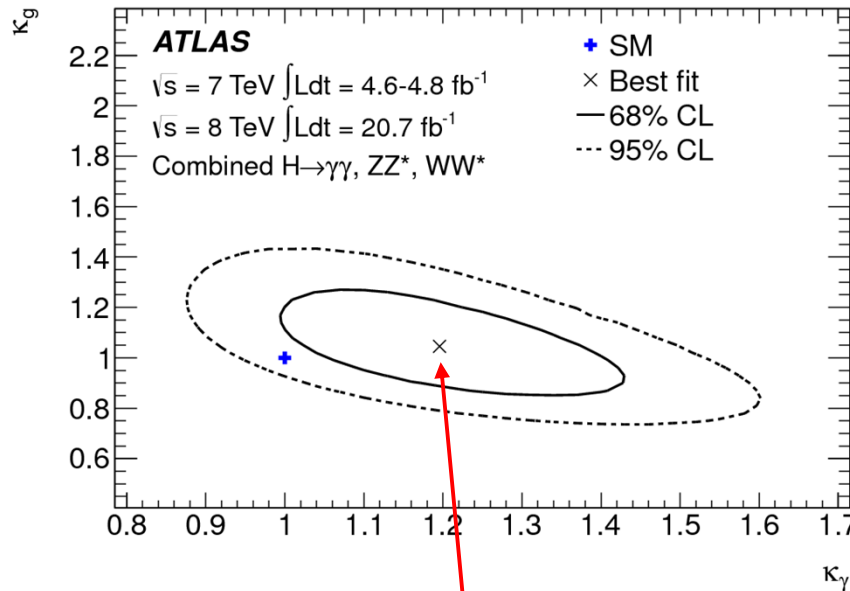
- $\hat{\mu}$ and $\hat{\theta}$ are the “best fit” (maximum likelihood estimate, MLE) values of μ and θ
- $\hat{\theta}(\mu)$ are the “conditional best fit” values for all the NPs at a given, specified, μ .

- Plot $-2 \ln \Lambda(\mu)$ against μ

- Minimum is at $-2 \ln \Lambda(\hat{\mu}) = 0$ (by definition)
- In the asymptotic limit (large N),
 - this will be distributed like a χ^2_1 distribution
 - or χ^2_n for n POIs
 - so 68% confidence interval is the range where $-2 \ln \Lambda(\mu) < 1$



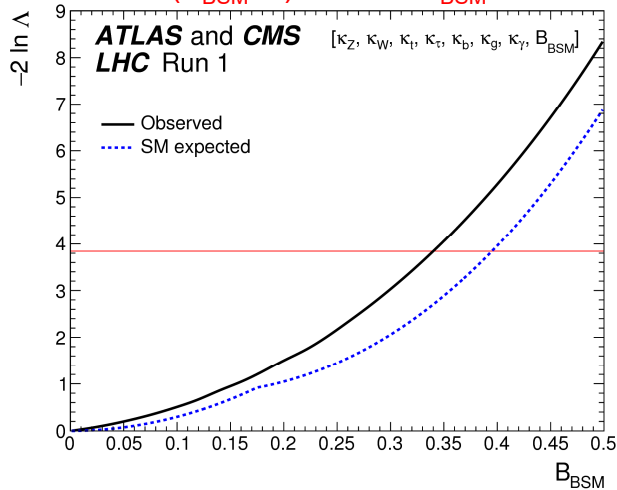
- For multiple POIs
 - calculate $-2 \ln \Lambda(\boldsymbol{\mu})$ for all points on a grid and
 - draw contours for regions $-2 \ln \Lambda(\boldsymbol{\mu}) < D^{-1}(\chi_n^2)$,
 - where $D^{-1}(\chi_n^2)$ is the inverse of the cumulative χ_n^2 distribution, for n POIs. [1]
 - 2D contours:
 - $D^{-1}(\chi_2^2(68\%)) = 2.30$
 - $D^{-1}(\chi_2^2(95\%)) = 6.18$



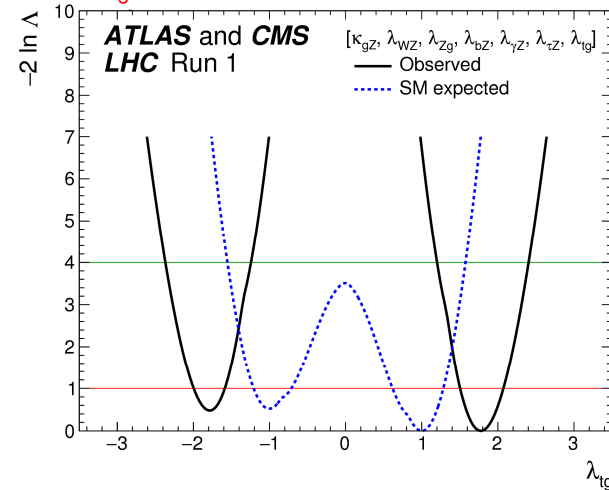
$-2 \ln \Lambda(\hat{\kappa}_\gamma, \hat{\kappa}_g) = 0$

[1] $D^{-1}(\chi_n^2(p)) = \text{ROOT::Math::chisquared_quantile}(p, n)$

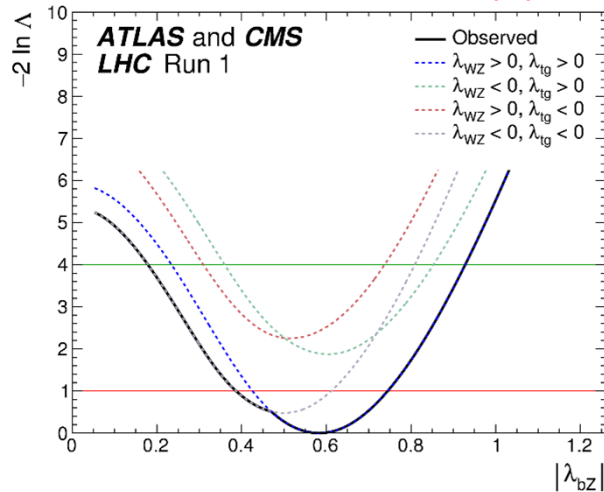
95% confidence interval
with $(B_{\text{BSM}} \geq 0)$ bound: $B_{\text{BSM}} < 0.34$



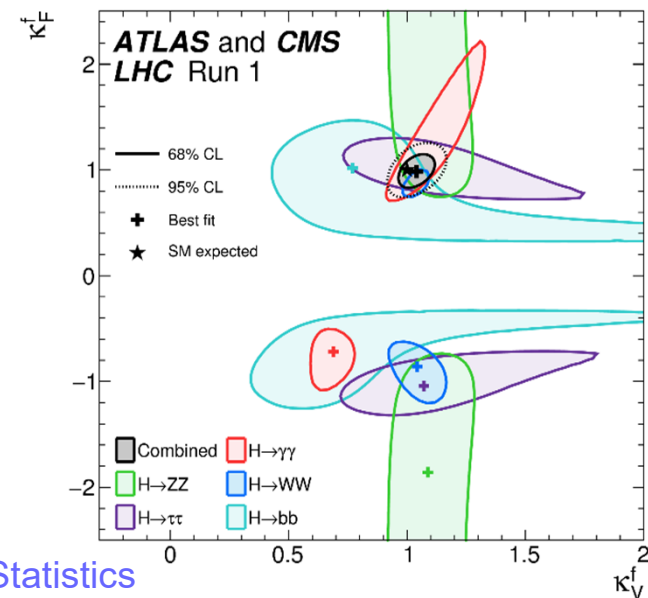
disjoint confidence interval:
 $\lambda_{t\bar{g}} = [-2.00, -1.59] \cup [1.50, 2.07]$



kink due to different sign combinations
of profiled NPs: $|\lambda_{bZ}| = 0.58^{+0.16}_{-0.20}$



multiple contours for different
channels and their combination

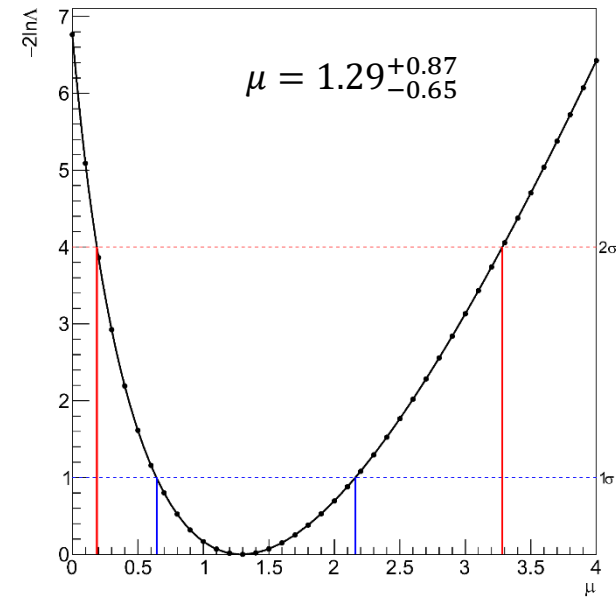


Measurement: scanning the likelihood curve

- To calculate a single PLR, require two fits:

$$\begin{aligned} \bullet \quad -2 \ln \Lambda(\mu) &= -2 \ln \frac{L(\mu, \widehat{\boldsymbol{\theta}}(\mu))}{L(\widehat{\mu}, \widehat{\boldsymbol{\theta}})} \\ &= -2 \ln L(\mu, \widehat{\boldsymbol{\theta}}(\mu)) - 2 \ln L(\widehat{\mu}, \widehat{\boldsymbol{\theta}}) \end{aligned}$$

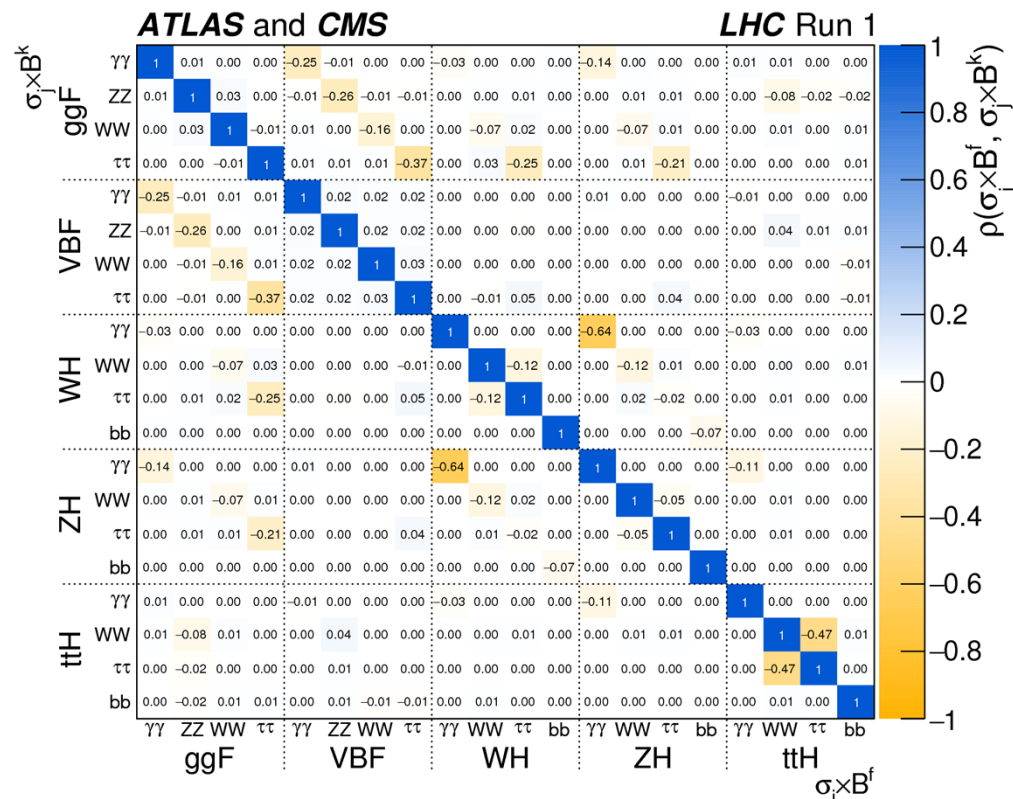
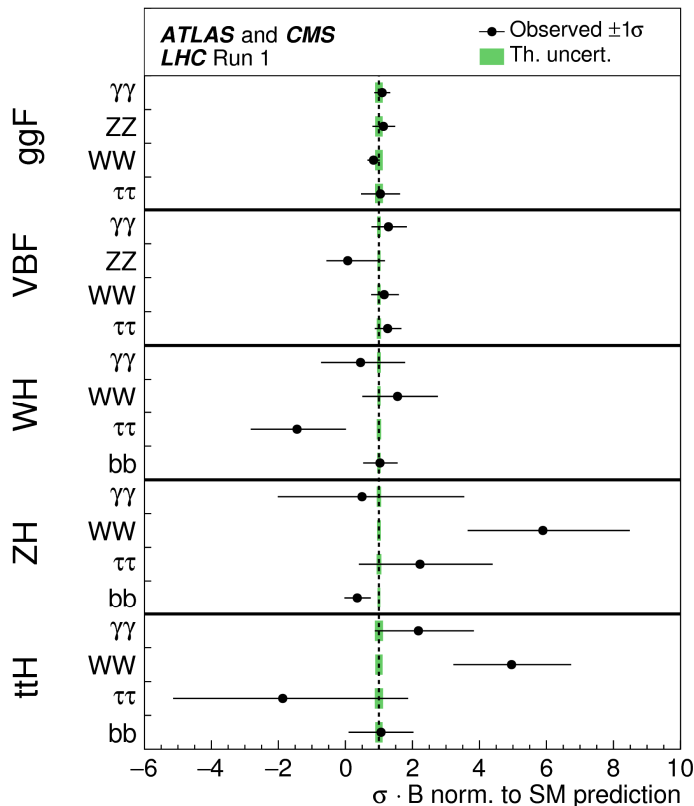
- The second term is independent of μ , so only needs to be evaluated once
- ... or not at all, if the minimum can be determined from the curve
 - removes ambiguity from the offset calculated in two ways (unconditional vs conditional fits)
 - should be \sim quadratic near minimum, so can use a quadratic interpolation of lowest 3 points
- Can (approximately) cross-check the result with the unconditional fit for $-2 \ln L(\widehat{\mu}, \widehat{\boldsymbol{\theta}})$:
 - $\widehat{\mu}$ should agree within the precision of the fit and of the interpolation
 - inverse Hessian at the minimum is the local covariance matrix, so $\sigma_0^2 = H^{-1}(\mu, \mu)$
 - Minuit will calculate (symmetric) errors from the Hessian
 - run with `strategy=2`, or call `Hesse()` explicitly.
 - Minuit's `Minos()` is similar to the curve scan, but without user control or diagnostic plot
 - Example comparison: $\mu = 1.29^{+0.87}_{-0.65}$ (curve) with $\mu = 1.29 \pm 0.73$ (Hessian)



Measurement: technical issues

- Sometimes significant CPU requirements
 - $\text{Time} = (\text{likelihood evaluation time}) * (\text{number of evaluations to fit}) * (\text{number of fits})$
 - Mitigations:
 - Simplify likelihood (faster likelihood evaluation)
 - Reduce or combine number of NPs (simplifies likelihood and fewer fit cycles)
 - Use fewer points in scan and interpolate (quadratic or spline)
 - 2D interpolation is more cumbersome
 - ROOT's `TGraph2D` can do linear interpolation of contours (use `GetContourList()` to extract)
 - Run different points in parallel, eg. in batch or on the Grid.
- Fit problems
 1. Fit failures reported by Minuit (or other minimiser)
 2. Bumpy curve, kinks, or bad points
- Possible causes:
 - Numerical precision in likelihood evaluation
 - Undefined component (eg. $-ve$ log for some parameter values) in likelihood evaluation
 - Minuit tolerance settings
 - NPs hitting their parameter limit
 - Some POIs or NPs don't budge from initial position
 - Minuit can't "tunnel" from secondary minimum

- For ≥ 3 POIs, it is not often practical to show contours
 - requires scanning a large number of points
 - results not easy to visualise
- Another option is to provide the correlation matrix at the best-fit point for all POIs
 - calculate using inverse Hessian $\rho(\mu_1, \mu_2) = H^{-1}(\mu_1, \mu_2) / (H^{-1}(\mu_1, \mu_1)H^{-1}(\mu_2, \mu_2))^{1/2}$
 - but beware that the correlations at the best-fit can be quite different elsewhere



- The NPs' effect on a model can be tested by determining by their post-fit pulls and impact on the POI

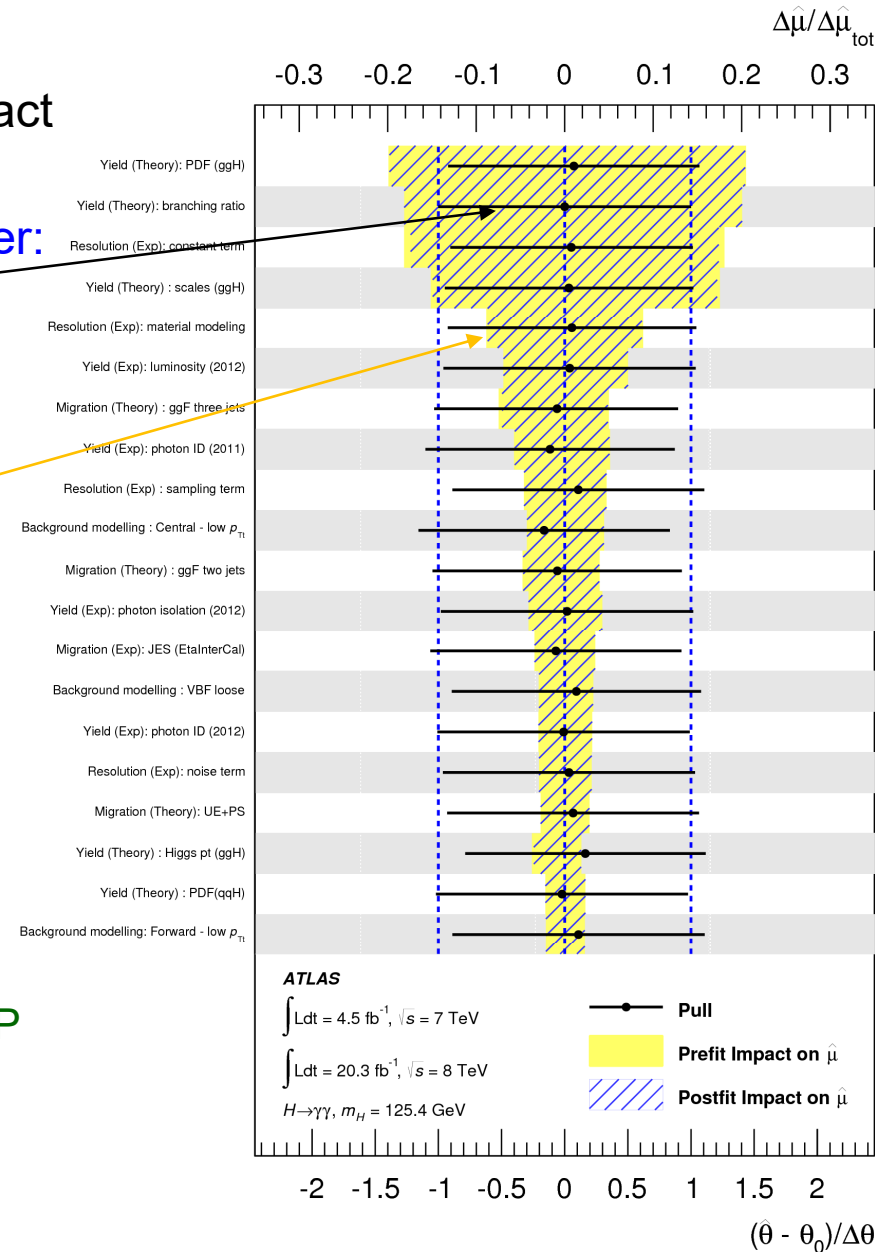
Often (perhaps confusingly) displayed together:

1. NP best-fit value and error

- relative to nominal, $(\hat{\theta} - \theta_0)/\Delta\theta$, here indicated by blue dotted lines at 0 ± 1 .
- refers to scale at the bottom

2. Impact of NP's error on POI

- $\pm\Delta\hat{\mu} = \hat{\mu}(\hat{\theta} \pm \sigma_{\theta}) - \hat{\mu}$
 - important to check relative sign of impact if correlating NPs in a combined workspace
- can use pre-fit (nominal) and/or post-fit NP errors
- refers to scale at the top, here relative to the total error, $\Delta\hat{\mu}/\Delta\hat{\mu}_{tot}$
- Size of impact indicates importance of each NP



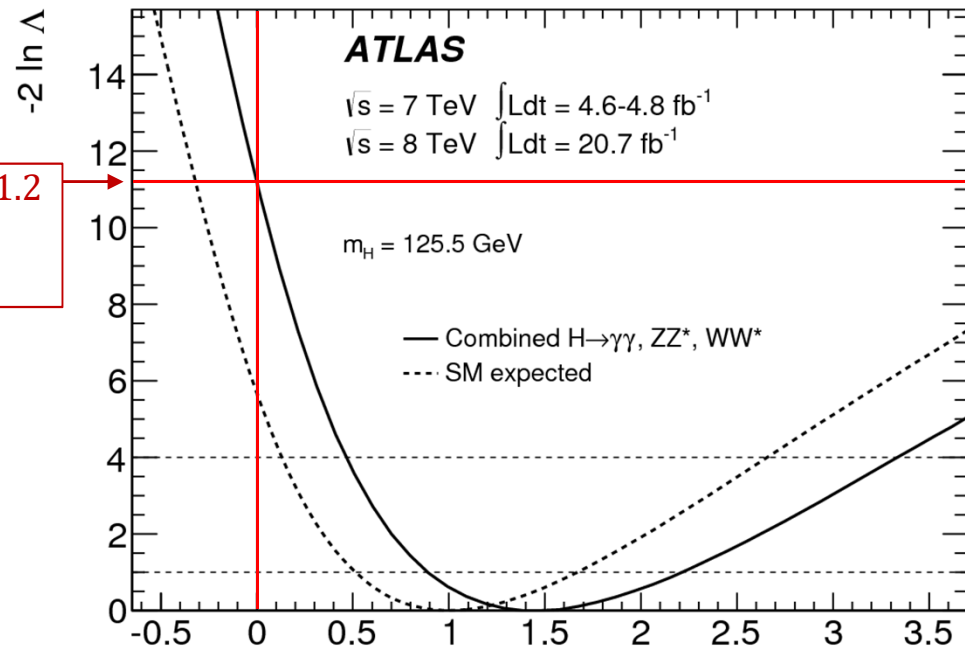
Discovery

- In the asymptotic limit (large N), the PLR, $\Lambda(\mu) = \frac{L(\mu, \hat{\theta}(\mu))}{L(\hat{\mu}, \hat{\theta})}$, gives the compatibility between μ and $\hat{\mu}$ hypotheses.
- Where μ is a ratio relative to the SM (eg. $\mu = \sigma/\sigma_{SM}$), we can test
 - Compatibility with background-only hypothesis: $Z_0 = \sqrt{-2 \ln \Lambda(\mu = 0)}$
 - Compatibility with SM (1 POI): $Z_{SM} = \sqrt{-2 \ln \Lambda(\mu = 1)}$
 - Compatibility with SM (n POIs): $Z_{SM} = D^{-1}(\chi_n^2(-2 \ln \Lambda(\mu)))$
- Z_μ is the significance ($N\sigma$), which (assuming χ_1^2 for 1 POI) has equivalent p-value, $p_\mu = s \Phi(-Z_\mu)$, where

- $s = 1$ for single-sided test like p_0 [1]
- $s = 2$ for double-sided test like p_{SM}
- $\Phi(Z)$ is the Gaussian CDF [2]

$-2 \ln \Lambda = 11.2$
 $Z_0 = 3.3\sigma$
 $p_0 = 0.04\%$

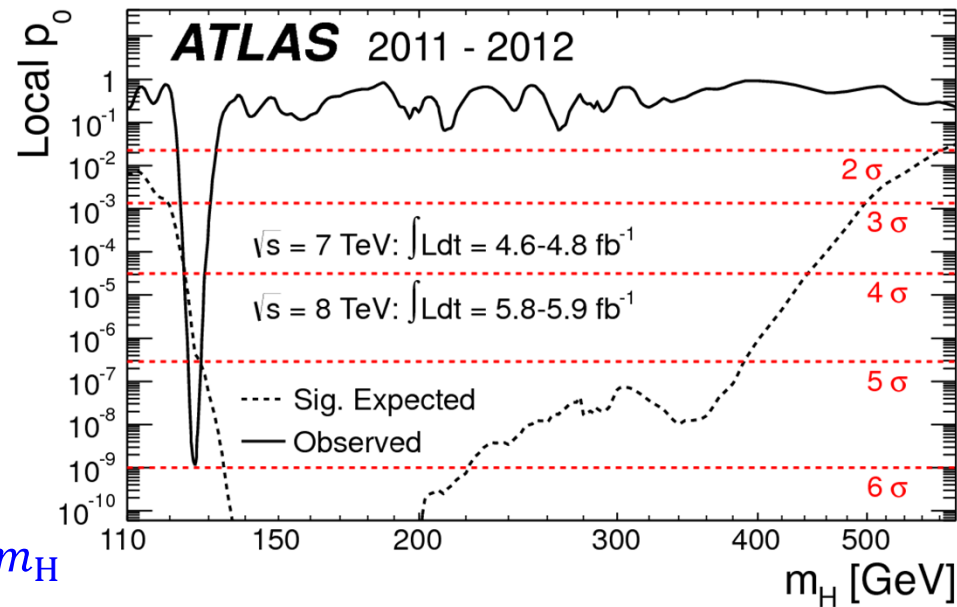
- p_0 interpreted as the significance of a signal, relative to a background-only hypothesis



[1] 1-sided p-value is capped at $p_0 < 0.5$. Can uncap by using $-Z_0$ for $\hat{\mu} < 0$

[2] $\Phi(Z) = \text{ROOT::Math::gaussian_cdf}(Z)$
 $\Phi^{-1}(p) = \text{ROOT::Math::gaussian_quantile}(p, 1.0)$

- Each mass hypothesis (m_H) has its own likelihood function, $L_{m_H}(\mu, \theta)$, eg.
 1. m_H hypothesis in kinematic fits
 2. $\mu = \sigma/\sigma_{SM}(m_H)$ so need m_H -specific SM production XS and decay BR
[LHC-H-XS-WG]
 3. each combined likelihood includes accessible decay modes at specified m_H



- p_0 vs m_H plot is the result of \sim independent fits to each L_{m_H} [1]
 - The largest local significance is 6.0σ ($p_0 \sim 10^{-9}$) at $m_H = 126.5$ GeV
 - the result of many (part-correlated) searches across the full $110 \leq m_H < 600$ GeV range
 - correct for the “look-elsewhere effect” using Gross-Vitells formula [arXiv:1005.1891]:
 - $p_{\text{global}} = p_{\text{local}} + \langle N(c_0) \rangle e^{-(c-c_0)/2} = 10^{-9} + 9 \cdot e^{-6.0^2/2} = 1.4 \cdot 10^{-7} \rightarrow 5.1\sigma$
- Still using asymptotic approximation, which we may not be confident in for new signal
 - test with toys

[1] except in m_H measurement, use single likelihood $L(m_H, \theta)$

- Toy MC (AKA “Monte Carlo pseudo-experiments”) can be generated directly from the components of the likelihood function

1. For each toy, generate

1. toy dataset (`pdf.generate(obs)`), with μ, θ determined from expectation or fit to data
2. set of global observables (`pdf.generate(globObs)`)
 - simulates variation of “NP truth”

2. Calculate a test statistic, $t_\mu = -2 \ln \Lambda(\mu)$, requiring:

1. conditional fit, under hypothesis being tested, eg. $\mu = 0$, background-only for p_0
2. unconditional fit for best-fit μ for this toy

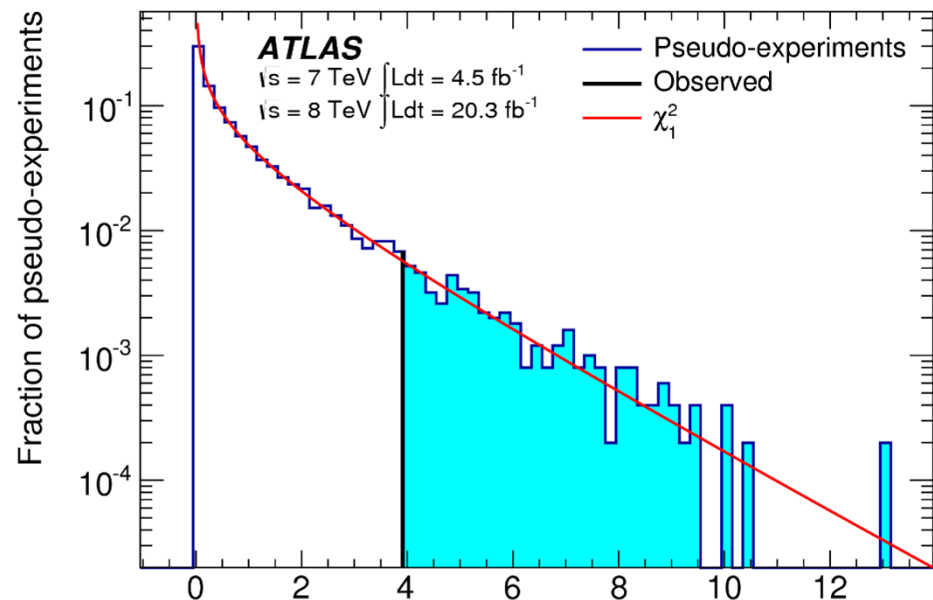
- `RooStats::FrequentistCalculator()` can be used to run this procedure for many toys

- The observed p-value is just the fraction of toys with test statistic larger than the observed:

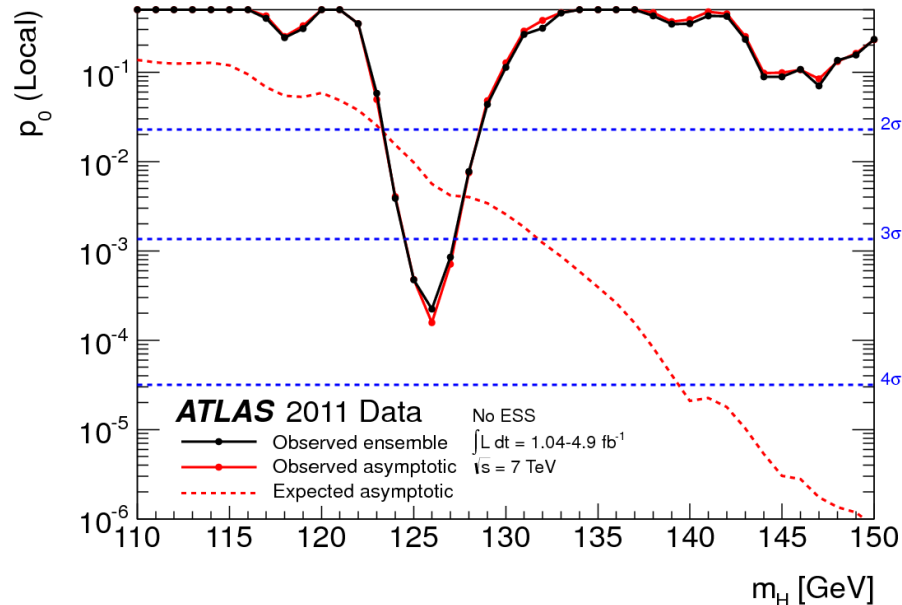
- $p_0 = N_{\text{toys}}(t_0 > t_{0,\text{obs}}) / N_{\text{toys}}$

Example distribution of t_0

(here for a 2-sided test of compatibility of two signals, not 1-sided signal significance)



- For the 2012 ATLAS Higgs discovery
 - the 6.0σ local significance was reduced to 5.9σ by including the effect of energy-scale systematics
 - ESS could only be measured using toys at $m_H = 126.5$ GeV
 - limited by CPU time available (used extrapolation from 300k toys)
- The cross-check with toys is more clearly seen with a previous sample
 - lower significance \rightarrow smaller number of toys required



Exclusion

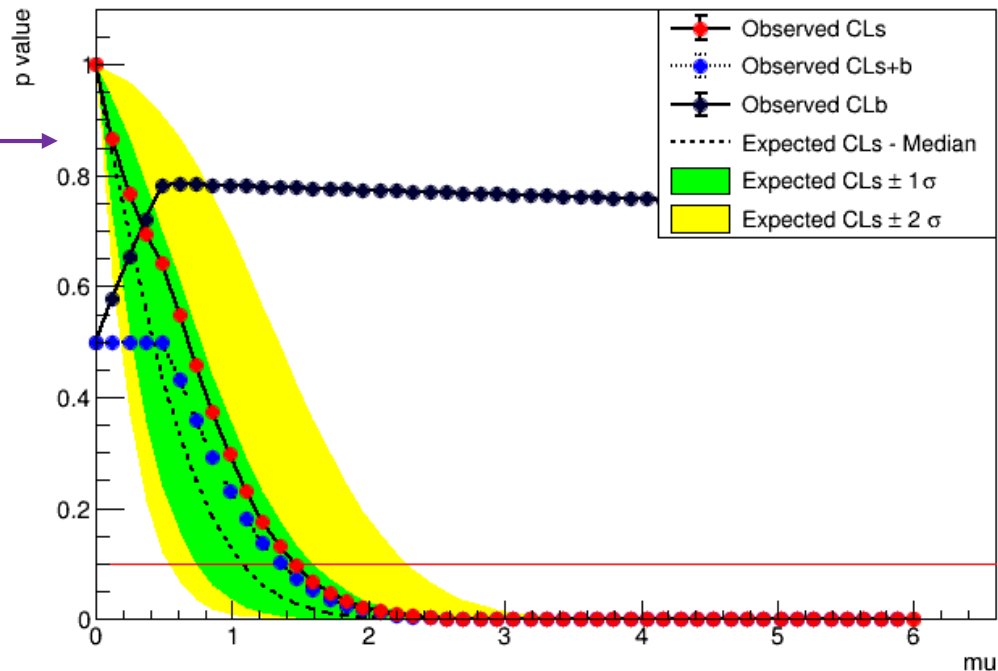
Exclusion: CLs

- CLs: $p'_\mu = p_\mu / (1 - p_0)$
 - CLs divides the tested p-value (CL_{s+b}) by the background-exclusion p-value (CL_b)
 - normally has little effect, but it is useful to inhibit a fluctuation spuriously excluding a hypothesis to which we have little sensitivity
 - p_μ and p_0 can be calculated as described previously for toys
- For a 95% CL limit, reject a particular μ (s+b) hypothesis if $p'_\mu \leq 0.05$.
 - to obtain a limit, find μ_{up} , the μ value for which $p'_\mu = 0.05$
- For toys, this means generating/fitting toys for various μ and interpolating μ_{up}
- Asymptotic limit obtained using the procedure from Asimov Paper [[arXiv:1007.1727](https://arxiv.org/abs/1007.1727)]
 - $q_\mu = -2 \ln \Lambda(\mu)$ PLR for observed data
 - $q_{\mu,A} = -2 \ln \Lambda_A(\mu|0)$ PLR for background-only Asimov dataset
 - $p'_\mu = (1 - \Phi(\sqrt{q_\mu})) / \Phi(\sqrt{q_{\mu,A}} - \sqrt{q_\mu})$
 - scan μ to find μ_{up} for which $p'_\mu = 0.05$.
 - For the median expected limit, $\mu_{up} = 1.96 \sigma(\mu_{up})$ [$\Phi^{-1}(1 - 0.05/2) = 1.96$]
 - where $\sigma(\mu_{up}) = \mu_{up} / \sqrt{q_{\mu_{up},A}}$, so again requires a numerical determination of μ_{up}
 - The expected bands, median $\pm N\sigma$, $\mu_{up+N} = (\Phi^{-1}(1 - 0.05\Phi(N)) + N) \cdot \sigma(\mu_{up+N})$

CLs procedure

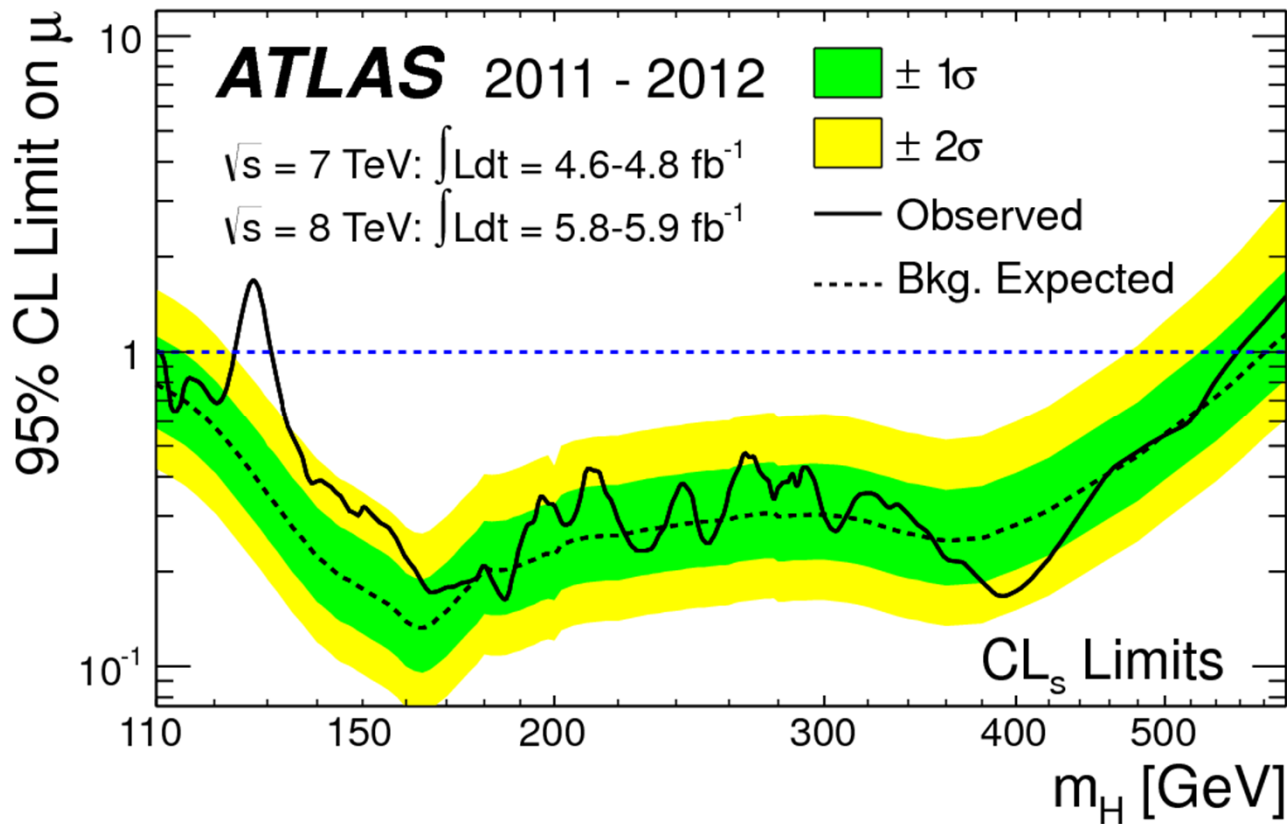
- For RooFit models, see:
 1. [RooStats StandardHypoTestInvDemo.C](#) tutorial, or
 2. [ATLAS CLs tutorial](#)
- In summary, create an asymptotic or toy calculator:
 1. `RooStats::AsymptoticCalculator calc (data, bModel, sbModel); // or`
 2. `RooStats::FrequentistCalculator calc (data, bModel, sbModel);`
- and pass that to the hypothesis test inverter:

```
RooStats::HypoTestInverter hypo (calc);  
result = hypo.GetInterval();  
RooStats::HypoTestInverterPlot (,result);
```

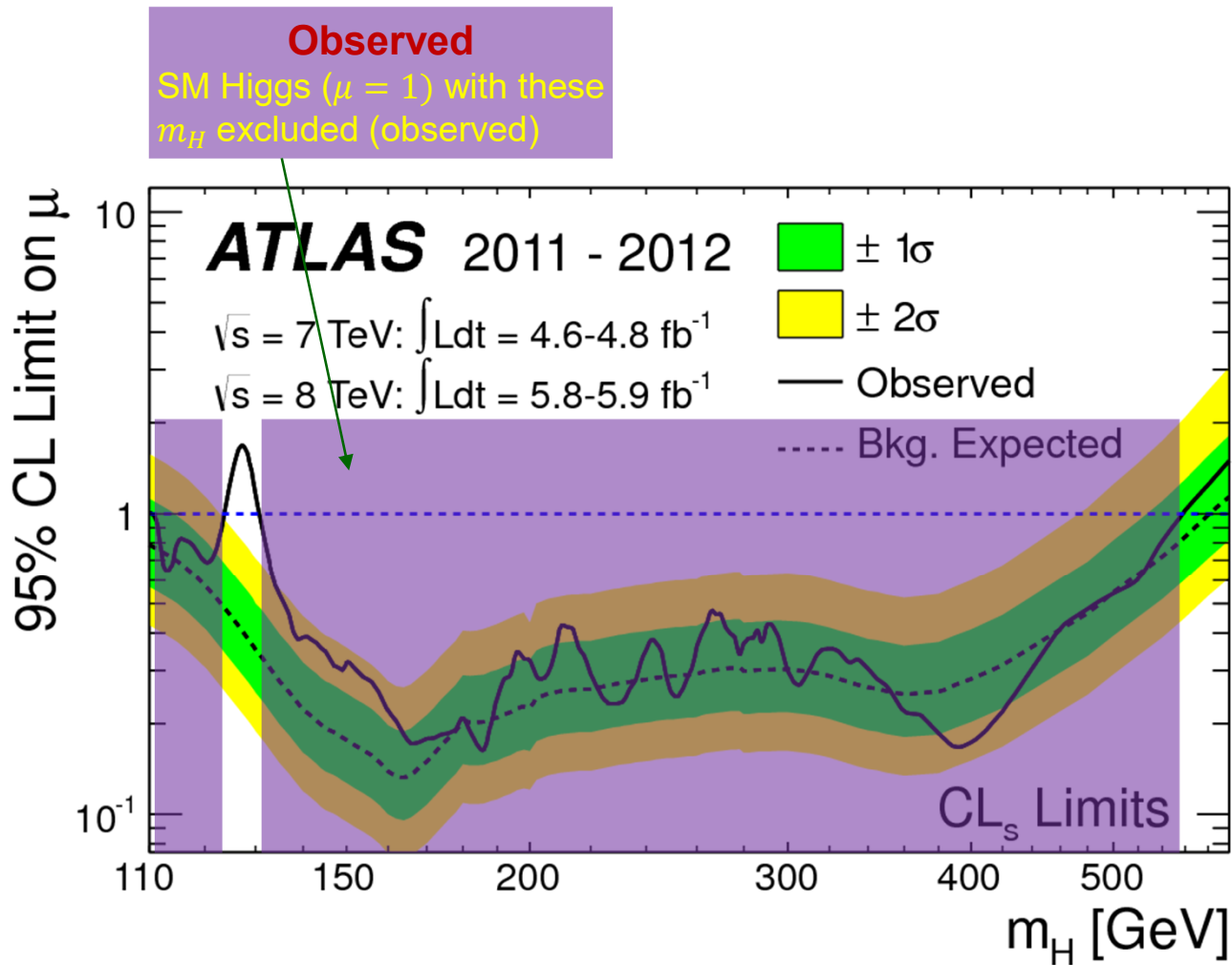


- For HistFactory-style models, [pyhf](#) has built-in tools to calculate CLs

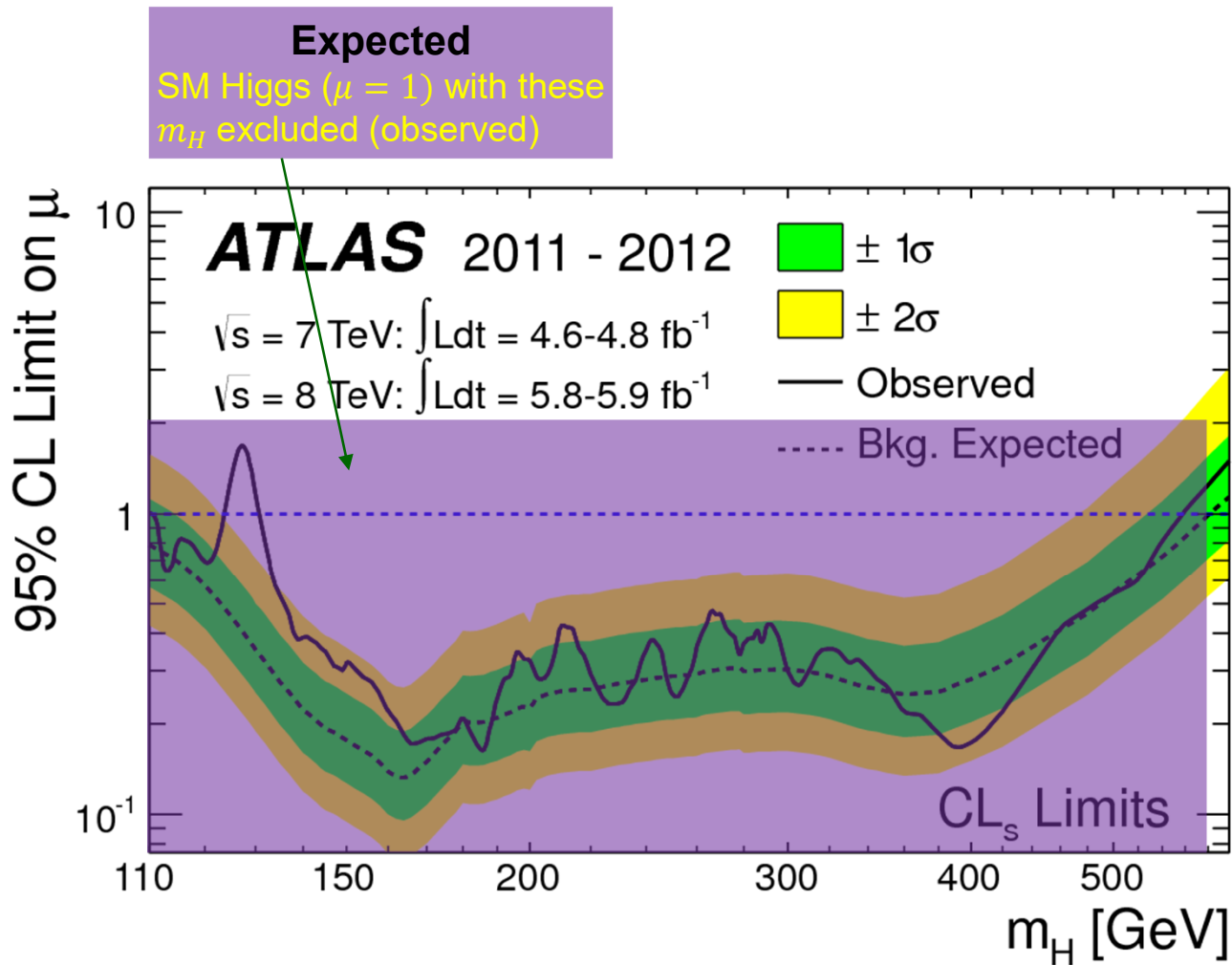
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 - different likelihood for each m_H , as before



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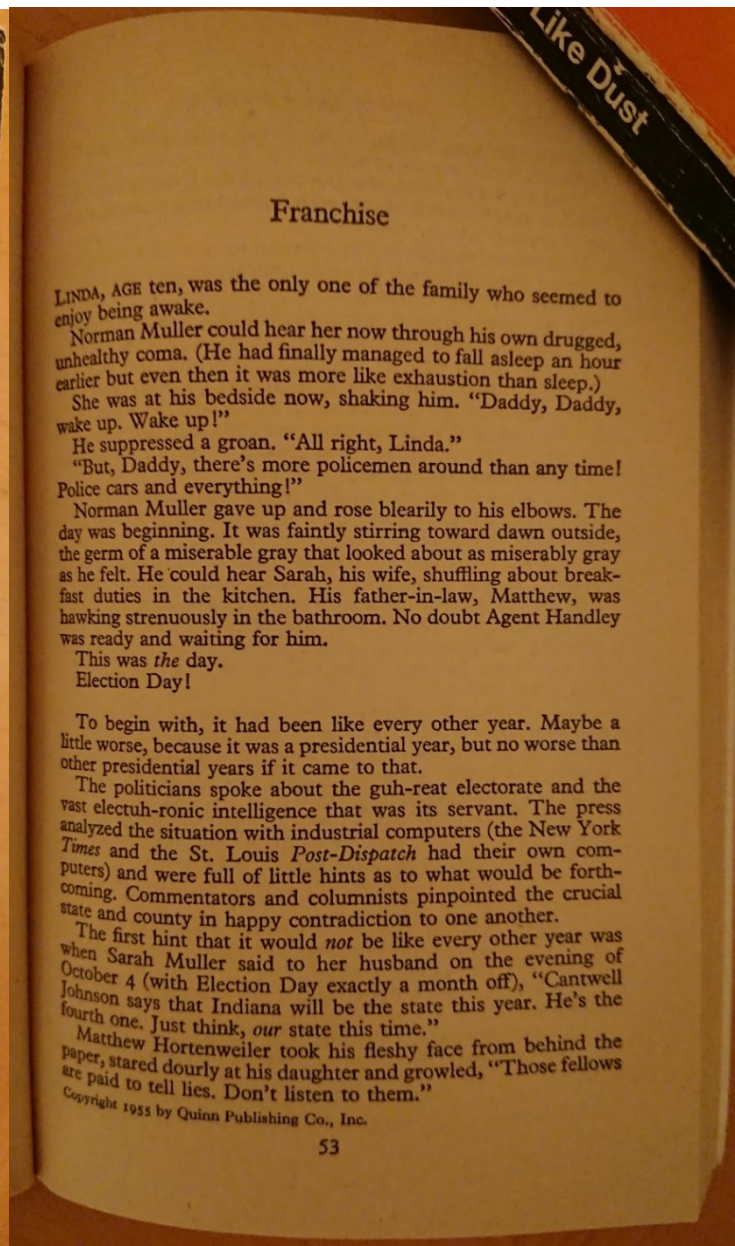
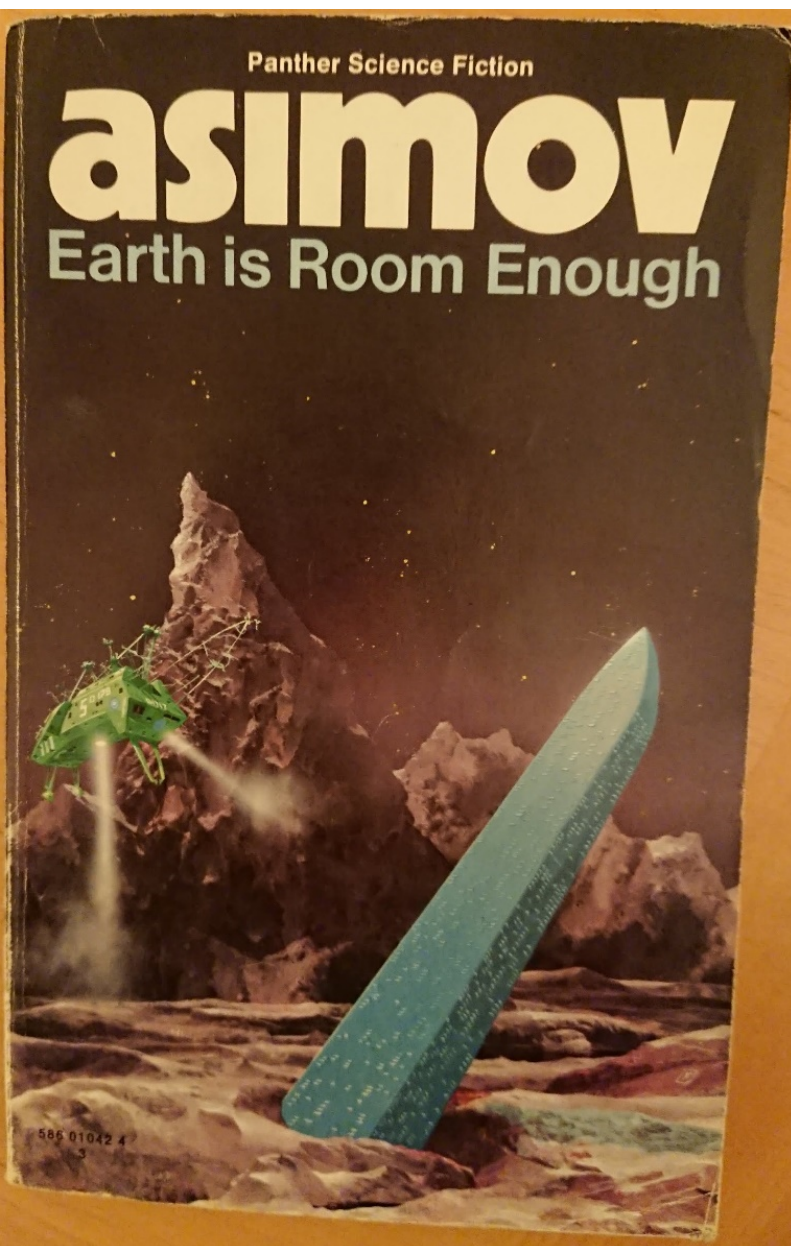
Summary

Summary

- Build models with
 - RooFit (C++, Python, or factory)
 - HistFactory (XML)
 - pyhf (JSON)
- Keep model and data in RooFit workspace files
 - Asimov dataset
- Statistical tests
 - Measurement, scanning profile likelihood ratio
 - RooFit
 - Discovery with profile likelihood ratio, asymptotic or toys
 - RooFit, RooStats
 - Exclusion with CLs, asymptotic or toys
 - RooFit, RooStats, or pyhf

Backup

Isaac Asimov – Franchise



The Asimov dataset [arXiv:1007.1727] is named for SF author, Isaac Asimov, whose 1955 short story, *Franchise*, envisaged the 2008 US Presidential Election decided by one voter representative of the entire electorate.

This is my copy of the story, in a collection.