



SYSTEMATIC UNCERTAINTIES AND NUISANCE PARAMETERS

A. David (CERN and IST-Lisboa)

ABOUT THE SPEAKER

Detector builder, Nature scrutiniser, Engineer botherer, and Theory disprover.

PhD in NA60, until 2013 in CLOUD, and CMS since 2006:

- CMS ECAL, 1st LHC single isolated photon crosssection measurement, then two photons, then one Higgs, then COMBINE Higgs analyses, then Higgs co-convener.
- Presently building CMS HGCAL for Phase 2 #LifeWithHexagons.

Profiled as many nuisance parameters as there are millionaires in the world.



LIMITED ACCEPTANCE WARNING

I am not a statistician, just a physicist trying to be more accurate.

• Since 2000 that physicists and statisticians meet in PHYSTAT to figure out many of these issues.

This view is **incomplete** and **has biases**.

Both are my fault, not that of the sources I used.

My goal: share some of what I have found useful when building an analysis.

BEFORE DINNER AND ARE ALLA SPIAGGIA

What are systematic uncertainties.

- 2. \Rightarrow How we account for them using nuisance parameters.
- 3. We How frequentist inference is done in the present of such beasts.
- 4. 🧐 How to live with them and answer your reviewers' questions.
- 5. Malkthroughs of practices and caveats from experience in the wild.

Interrupt whenever you have a question.

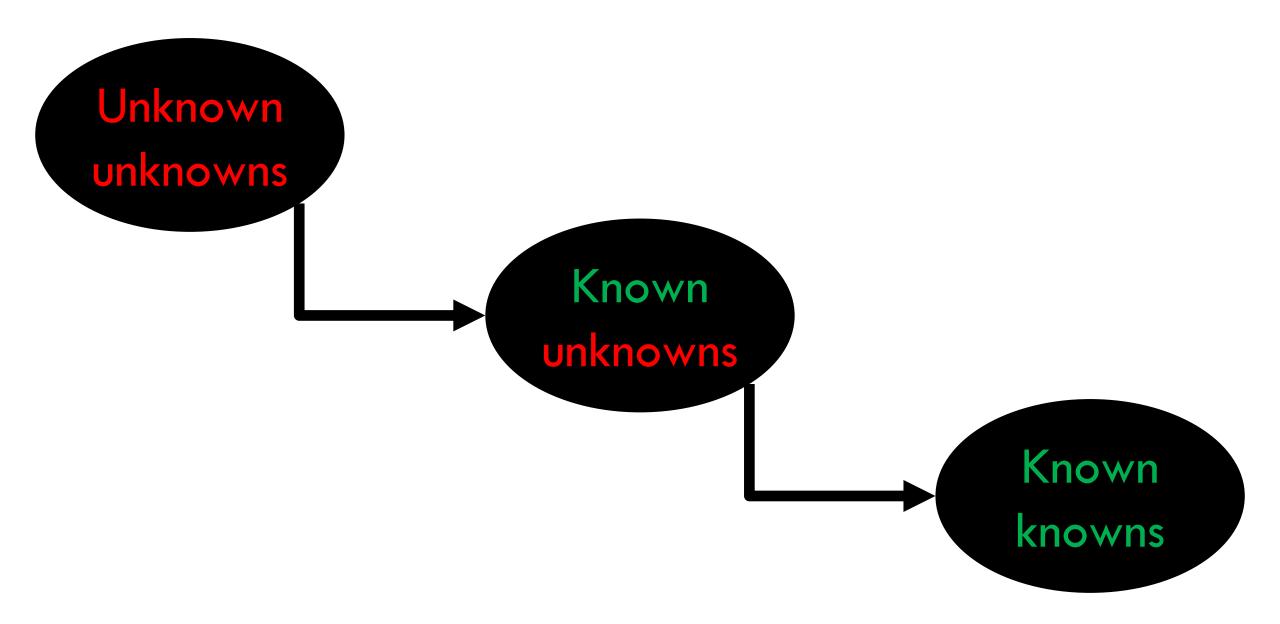
Worst that can happen is to discuss it alla spiaggia.

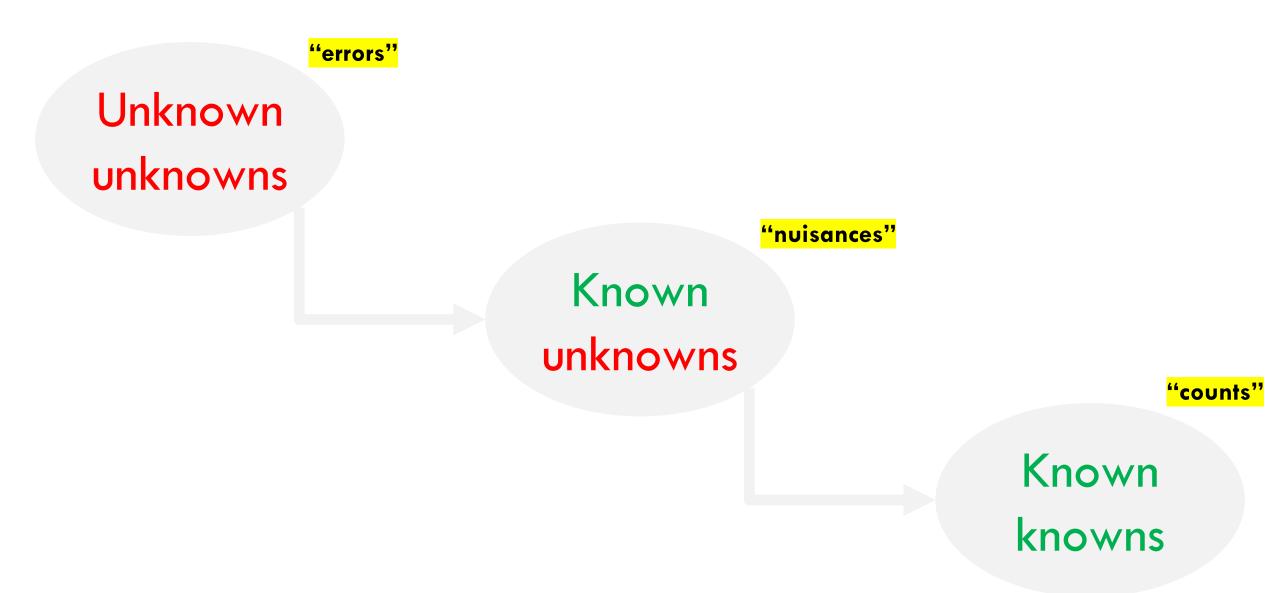
Dersonal disclaimer: publish frequentist results and take Bayesian decisions.

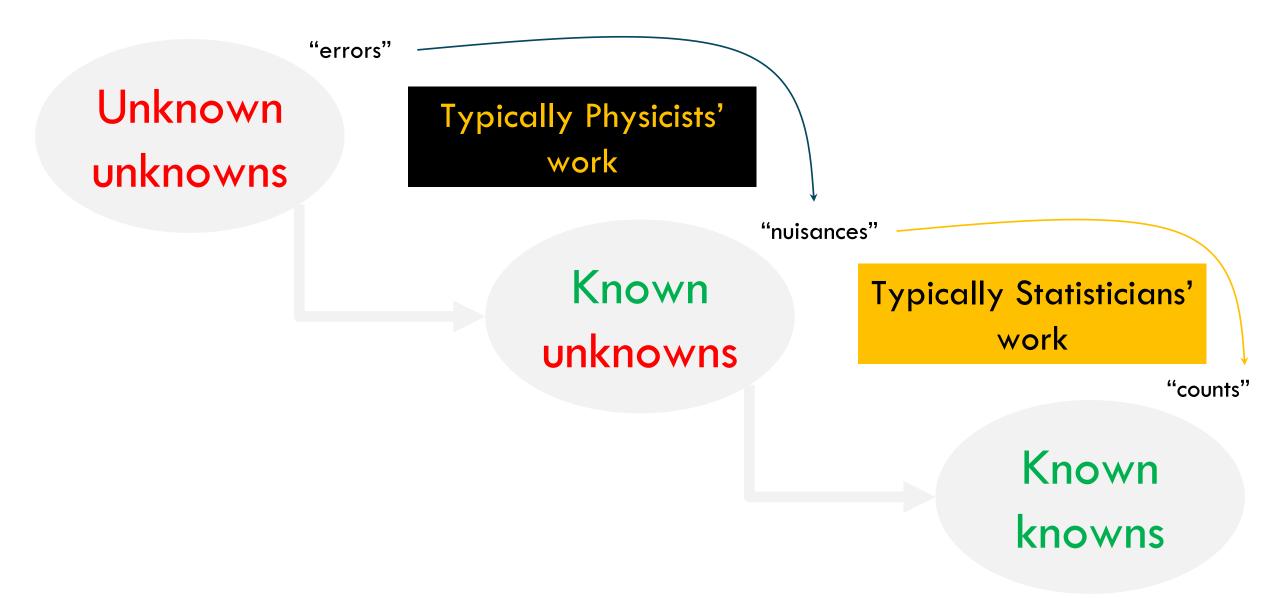


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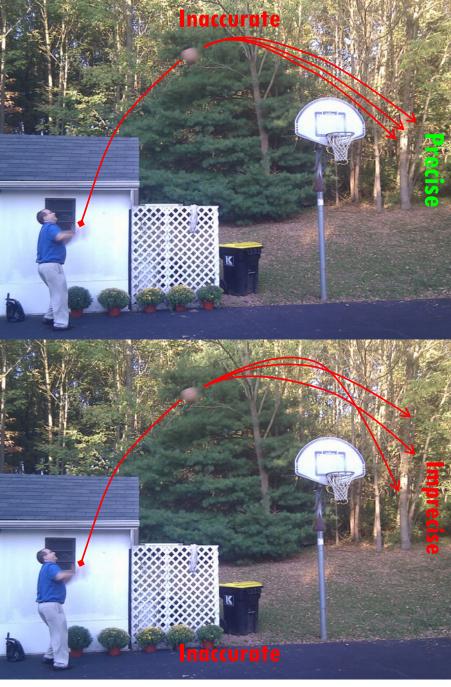




ACCURACY AND PRECISION

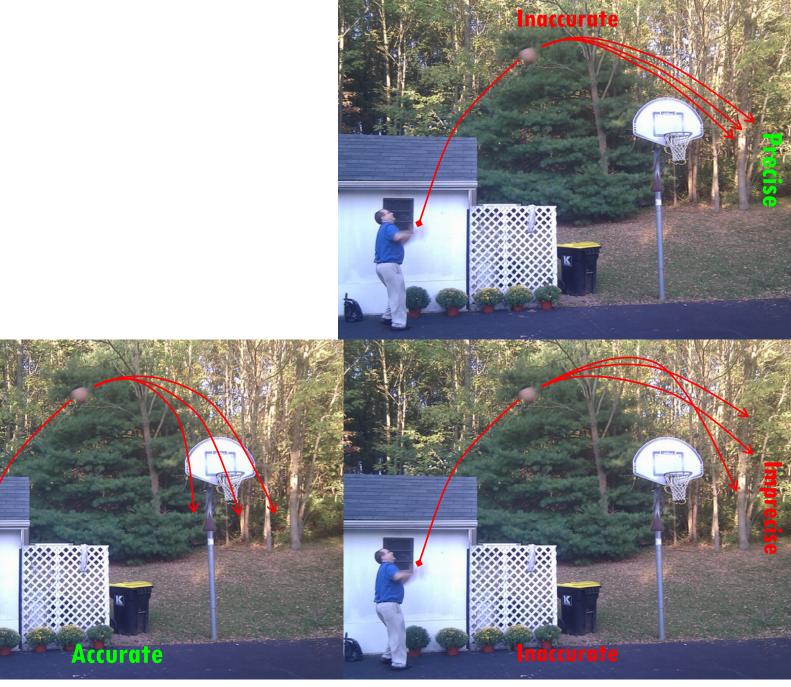


ACCURACY AND Precision



ACCURACY AND PRECISION

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ACCURACY AND PRECISION



TWO WORDS ON ERROR AND UNCERTAINTY

What I call error is the result of a bias or mistake.

What I call **uncertainty** is the degree to which something is (un)known.

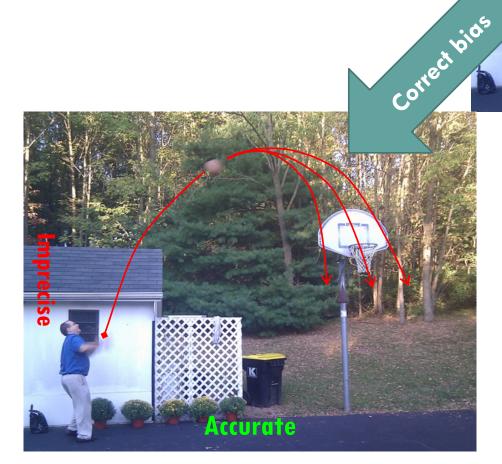
I think it's a mistake to call errors uncertainties.

E.g., experimentalists correct for systematic effects (biases).

Corrections come with added uncertainty.



BETTER ACCURACY AND DETERIORATED PRECISION



Inaccurate

BETTER ACCURACY AND DETERIORATED PRECISION

BIAS VS VARIANCE

Inaccurate

Correct bios

Accurate

EXAMPLE: METAL RULER ON A HOT DAY

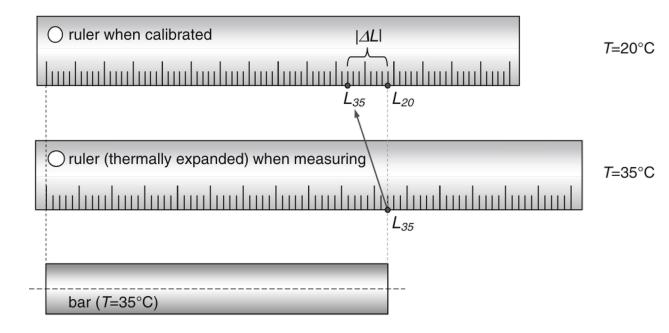
Givens:

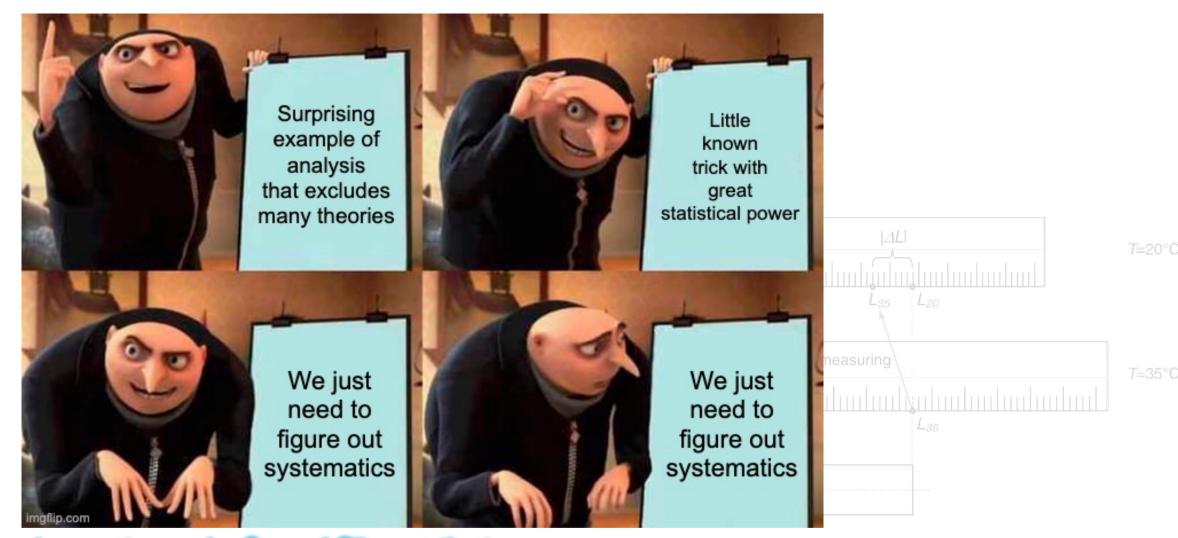
- Bar measured with ruler at $T_1 = 35$ °C.
- Metal ruler calibrated at $T_0 = 20$ °C.
- Ruler thermal expansion coefficient is α.
 - Measured in some way that will have uncertainty $\delta\alpha.$

Estimates:

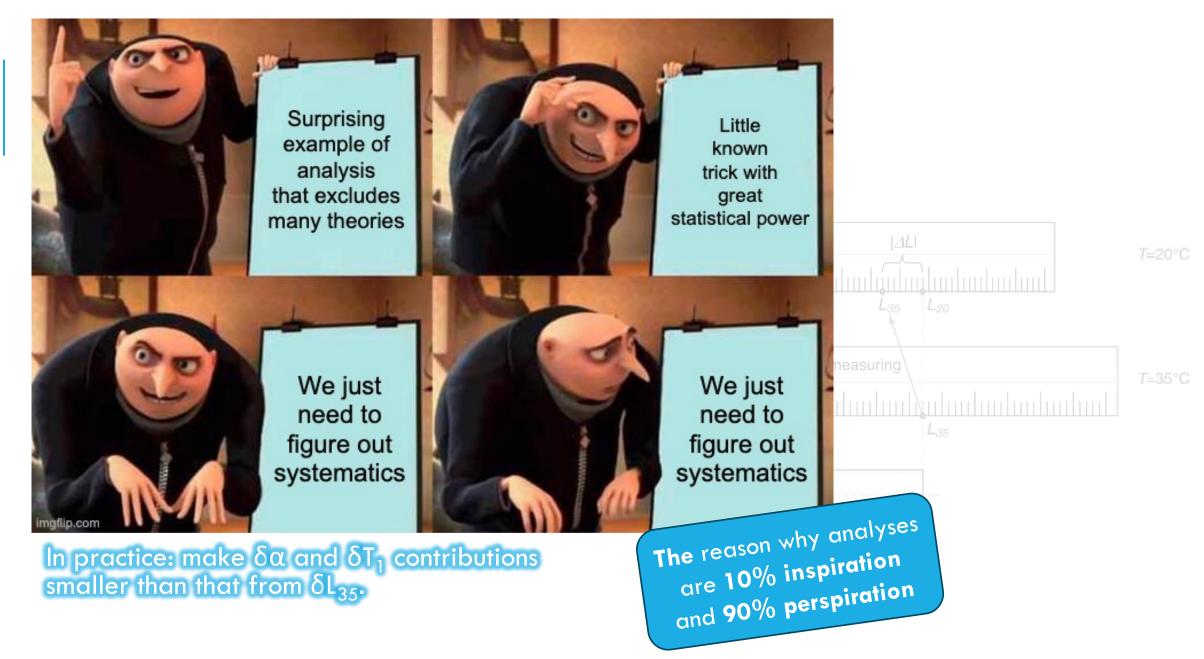
- Central value: L_{bar} = L₂₀ = L₃₅ [1+ α (T₀ T₁)]
 - Reduced bias !
- Unc. on L_{bar} includes uncertainties on L₃₅, α, T₁.
 - Additional uncertainty !

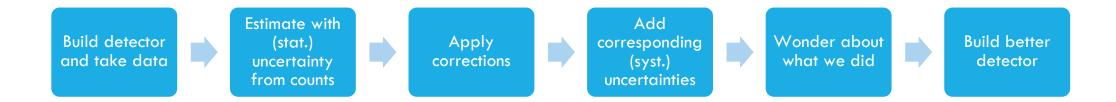
In practice: make $\delta \alpha$ and δT_1 contributions smaller than that from δL_{35} .

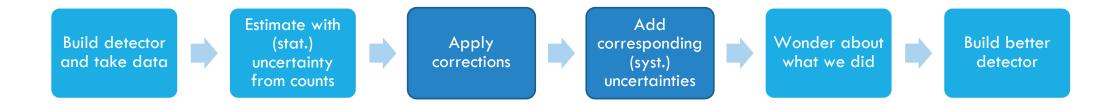


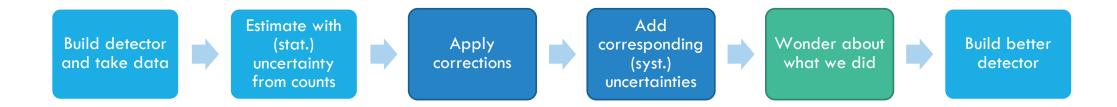


In practice: make $\delta \alpha$ and δT_1 contributions smaller than that from δL_{35} .



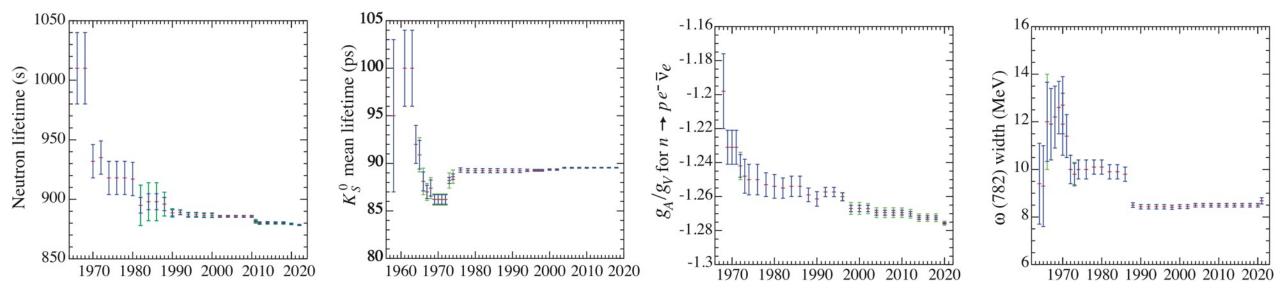




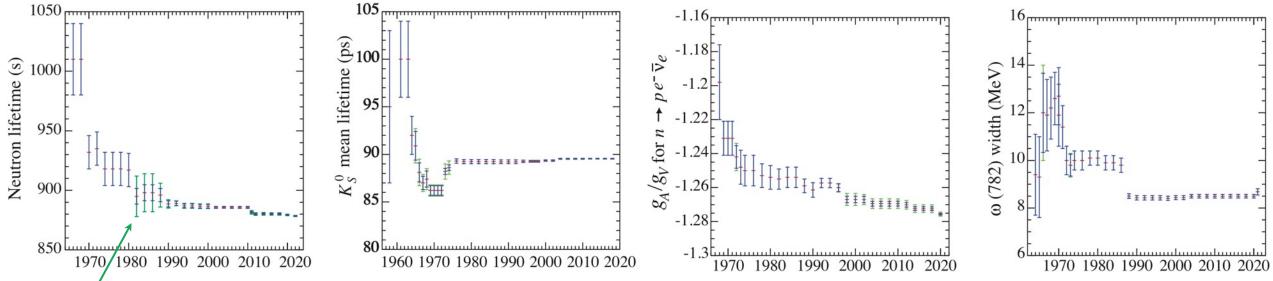




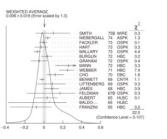
LOOKING BACK TO LOOK FORWARD



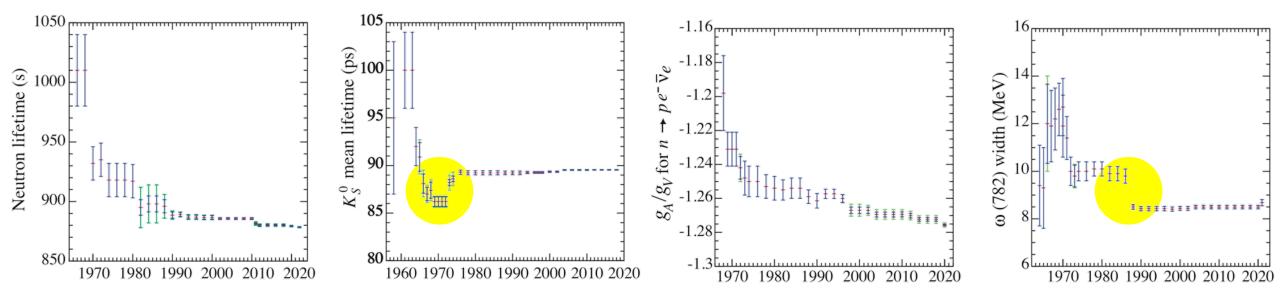
LOOKING BACK TO LOOK FORWARD



PDG scales uncertainties to deal with discrepant measurements.



LOOKING BACK TO LOOK FORWARD



A brief history of early Particle Data Group averages is given in Ref. [5]. Our History Plots show the time evolution of some of our values of a few particle properties. Sometimes large changes occur. These usually reflect the introduction of significant new data or the discarding of older data. Older data are discarded in favor of newer data when it is felt that the newer data have smaller systematic errors, or have more checks on systematic errors, or have made corrections unknown at the time of the older experiments, or simply have much smaller errors. Sometimes, the scale

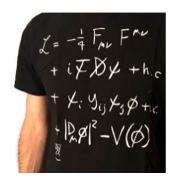
Yes, The PDG refers to uncertainties as "errors". 🗳



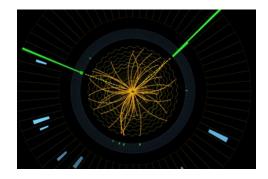
SYSTEMATIC UNCERTAINTIES AND NUISANCE PARAMETERS

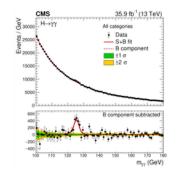
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ANATOMY OF A LHC MEASUREMENT







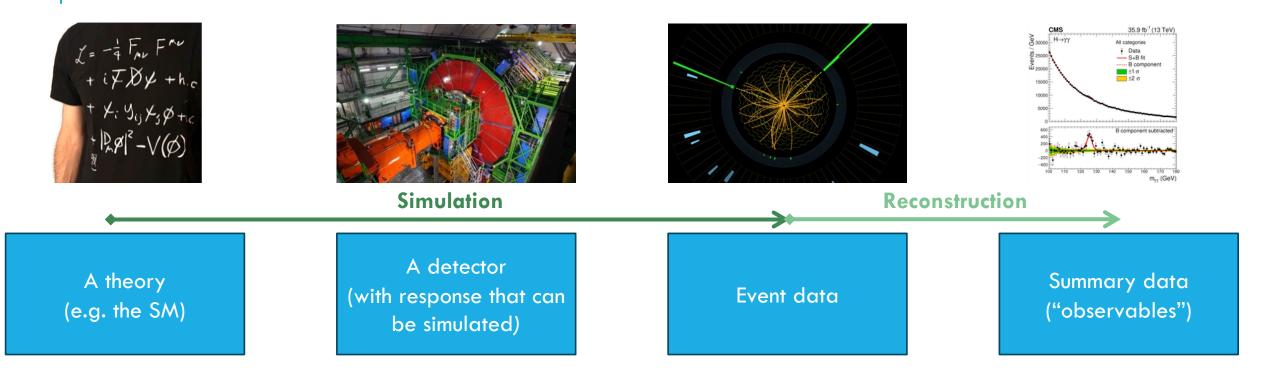


A theory (e.g. the SM) A detector (with response that can be simulated)

Event data

Summary data ("observables")

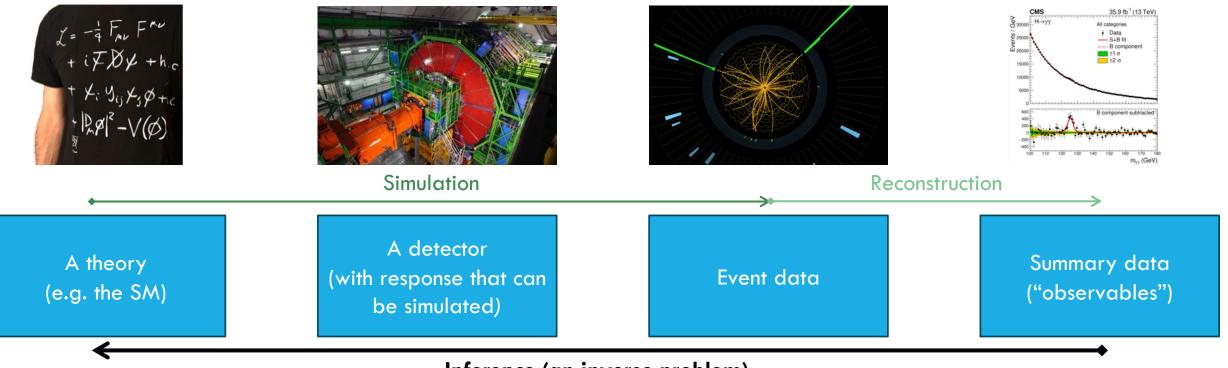
ANATOMY OF A LHC MEASUREMENT



Simulation encompasses both theory and experiment aspects.

Reconstruction also includes any aggregation (binning) or transformation (machine learning, calibration).

ANATOMY OF A LHC MEASUREMENT

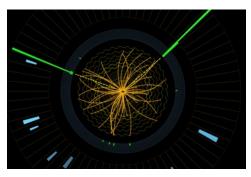


Inference (an inverse problem)

IN PRACTICE...



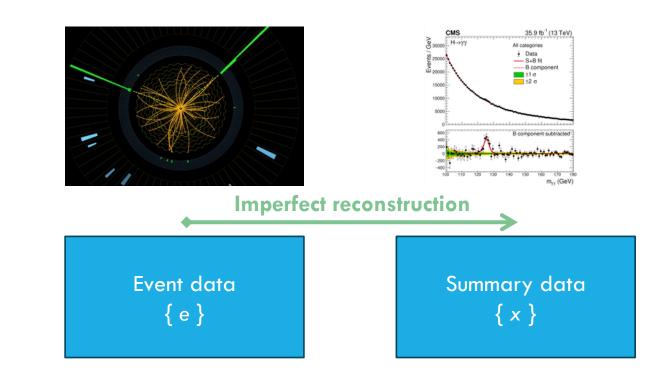




Simulation with imperfections (v) using Monte Carlo sampling

A theory (with parameters μ) A detector f(e ; μ, ν) Event data { e }

IN PRACTICE...



STEPS ALONG THE LHC WAY

Simulation of proton-proton collision at the LHC involves processes at many energy scales.

Different regimes require separate calculation approaches.

Implemented as chain of separate simulation packages.

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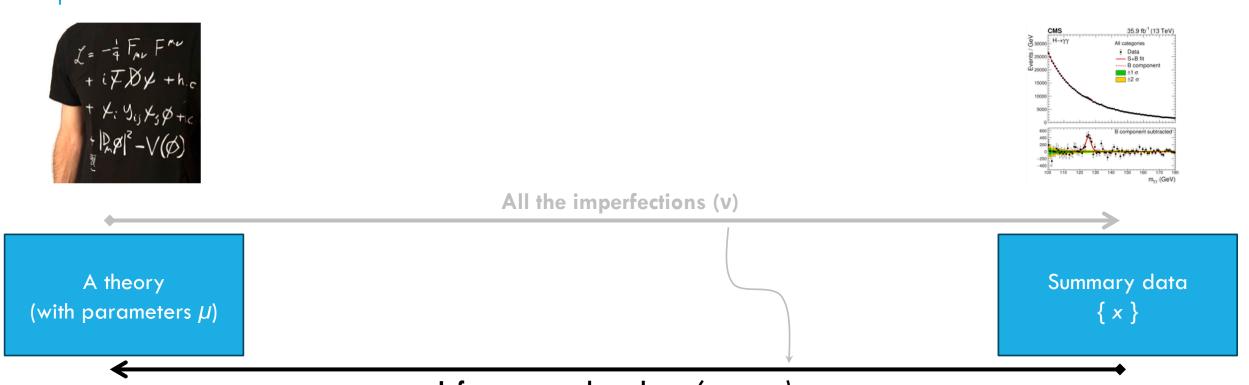
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inspired by W. Verkerke

IMPERFECTIONS ALONG THE LHC WAY

Ingredient	Estimate from	Uncertainty estimates include
Proton structure	Empirical; no first principles calculation.	Fit method and statistical uncertainties.
Matrix element calculation	Perturbative calculation from theory, resummed or fixed-order.	Missing higher orders.
Parton shower	Perturbative shower development.	Matching energy scale to Matrix element calculation.
{Hadroniz,Fragment}ation	MC simulation based on empirical models.	Tuneable parameters and different implementations.
Detector simulation	GEANT4 or Fast simulation.	GEANT tunes, parameterizations of digitisation.
Object reconstruction and identification	Custom-built algorithms (e, μ, τ, γ, b/c/q/g-jets,).	Data-driven calibration uncertainties.
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ANATOMY OF A MEASUREMENT

Inference on μ based on $p(x, y; \mu, v)$

What's **y** and where did that come from ?



THE STATISTICAL MODEL

The statistical model for inference is a function of the data given all parameters (Φ), $p({
m data};ec{\Phi})$

can be factorised into **primary data**, x, and **auxiliary observables**, y. For k systematic uncertainties, each y_k is paired with a nuisance parameter V_k :

$$p(\vec{x}, \vec{y}; \vec{\Phi}) = p(\vec{x}; \vec{\mu}, \vec{\nu}) \prod_{k} p_{k}(y_{k}; \nu_{k})$$

where p_k are the probability distribution functions of the auxiliary observables.

 $\cancel{1}$ \vec{x} is **one** data point (that can be multidimensional).



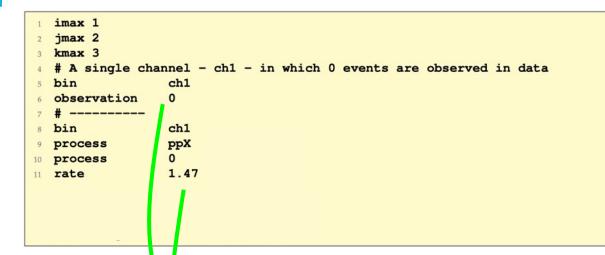
THE STATISTICAL MODEL

The "counts" and their estimates' dependency on all parameters.

$$p(\vec{x}, \vec{y}; \vec{\Phi}) = p(\vec{x}; \vec{\mu}, \vec{\nu}) \prod_{k} p_{k}(y_{k}; \nu_{k})$$

Information on how well any "nuisance" is known.



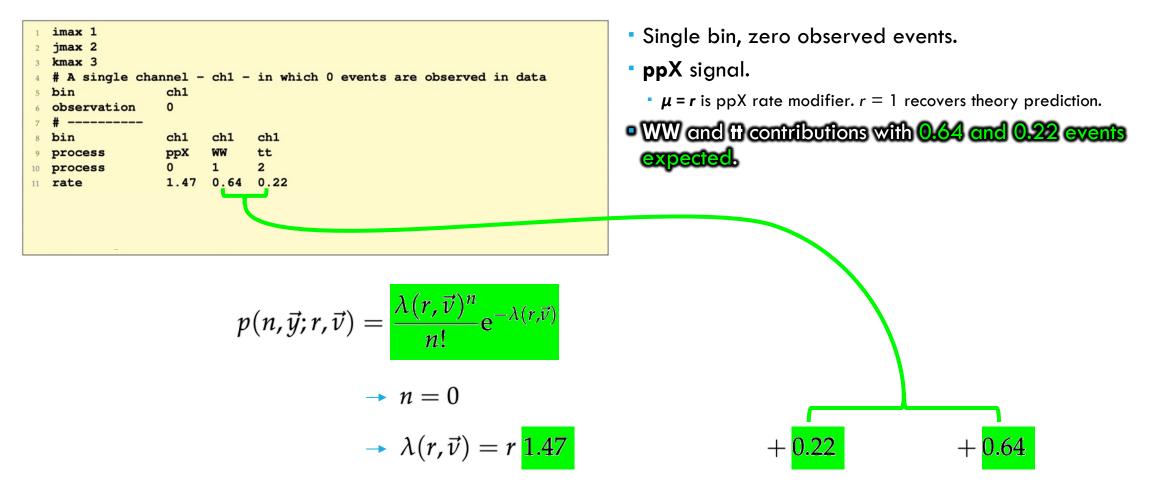


- Single bin, zero observed events.
- ppX signal, 1.47 events expected.

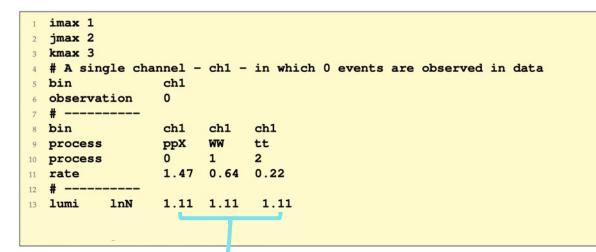
• $\mu \equiv r$ is ppX rate modifier. r = 1 recovers theory prediction.

$$p(n, \vec{y}; r, \vec{v}) = \frac{\lambda(r, \vec{v})^n}{n!} e^{-\lambda(r, \vec{v})}$$
$$\rightarrow n = 0$$
$$\rightarrow \lambda(r, \vec{v}) = r 1.47$$









- Single bin, zero observed events.
- **ppX** signal.
 - $\mu = r$ is ppX rate modifier. r = 1 recovers theory prediction.
- WW and **tt** backgrounds.
- **lumi:** all processes from simulation and since $N = \sigma \mathcal{L}$ all yields affected by luminosity measurement uncertainty.

$$p(n, \vec{y}; r, \vec{v}) = \frac{\lambda(r, \vec{v})^n}{n!} e^{-\lambda(r, \vec{v})} \frac{1}{2\pi} e^{-(v_{1umi} - y_{1umi})^2}$$

$$\rightarrow n = 0, y_{1umi} = 0$$

$$\rightarrow \lambda(r, \vec{v}) = r \frac{1.47}{1.47} (1.11)^{v_{1umi}} + \frac{0.22}{1.11} (1.11)^{v_{1umi}} + \frac{0.64}{1.11} (1.11)^{v_{1umi}}$$



1	imax 1						
2	jmax 2						
3	kmax 3						
4	# A single	channel -	ch1 -	in which	0 events	are observed	in data
5	bin	ch1					
6	observation	n 0					
7	#						
8	bin	ch1	ch1	ch1			
9	process	ppX	WW	tt			
10	process	0	1	2			
11	rate	1.47	0.64	0.22			
12	#						
13	lumi lnl	N 1.11	1.11	1.11			
14	xs lnl	N 1.20	-	-			

- Single bin, zero observed events.
- **ppX** signal.
 - $\mu = r$ is ppX rate modifier. r = 1 recovers theory prediction.
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- **lumi:** all processes affected by luminosity measurement uncertainty.
- **xs**: ppX has theoretical uncertainty on cross-section (σ).

$$p(n, \vec{y}; r, \vec{v}) = \frac{\lambda(r, \vec{v})^n}{n!} e^{-\lambda(r, \vec{v})} \frac{1}{2\pi} e^{-(v_{1umi} - y_{1umi})^2} e^{-(v_{xs} - y_{xs})^2}$$

$$\rightarrow n = 0, y_{1umi} = y_{xs} = 0$$

$$\rightarrow \lambda(r, \vec{v}) = r \frac{1.47}{1.47} (1.11)^{v_{1umi}} (1.2)^{v_{xs}} + \frac{0.22}{(1.11)^{v_{1umi}}} + \frac{0.64}{(1.11)^{v_{1umi}}}$$



<pre>1 imax 1 2 jmax 2 3 kmax 3 4 # A single channel - ch1 - in which 0 events are observed in data 5 bin ch1 6 observation 0 7 # 8 bin ch1 ch1 ch1 9 process ppX WW tt 10 process 0 1 2 11 rate 1.47 0.64 0.22 12 # 13 lumi lnN 1.11 1.11 1.11 14 xs lnN 1.20 15 nWW gmN 4 - 0.16 -</pre>	 Single bin, zero observed events. ppX signal. μ = r is ppX rate modifier. r = 1 recovers theory prediction. WW and the backgrounds. Iumi: all processes affected by luminosity measurement uncertainty. xs: ppX has theoretical uncertainty on cross-section (σ). nWW: WW yield estimated from 4 simulated events. 		
$p(n, \vec{y}; r, \vec{v}) = \frac{\lambda(r, \vec{v})^n}{n!} e^{-\lambda(r, \vec{v})} \frac{1}{2\pi} e^$	$-(v_{\text{lumi}}-y_{\text{lumi}})^2 e^{-(v_{xs}-y_{xs})^2} \frac{(v_{nWW})^{y_{nWW}}}{y_{nWW}!} e^{-v_{nWW}}$		
$ ightarrow$ $n=0, y_{ t lumi}=y_{ t xs}=$	$= 0, \text{ and } y_{\text{nWW}} = 4$		
■ 0.64 yield = 0.16 factor × 4 counts $ \rightarrow \lambda(r, \vec{\nu}) = r \frac{1.47}{1.47} (1.1)$	$11)^{\nu_{\text{lumi}}} (1.2)^{\nu_{\text{xs}}} + \frac{0.22}{0.22} (1.11)^{\nu_{\text{lumi}}} + \frac{0.64}{0.64} (1.11)^{\nu_{\text{lumi}}} \frac{\nu_{\text{nWW}}}{0.64}$		



-				
1	imax 1			
2	jmax 2			
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5	bin	ch1		
6	observation	n 0		
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12	#			
13	lumi ln	N 1.11	1.11	1.11
14	xs lnl	N 1.20	-	-
15	nWW gml	N4 –	0.16	-

1

- Single bin, zero observed events.
- **ppX** signal.
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- WW and **tt** backgrounds.
- **lumi:** all processes affected by luminosity measurement uncertainty.
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$$p(n, \vec{y}; r, \vec{\nu}) = \frac{\lambda(r, \vec{\nu})^n}{n!} e^{-\lambda(r, \vec{\nu})} \frac{1}{2\pi} e^{-(\nu_{\text{lumi}} - y_{\text{lumi}})^2} e^{-(\nu_{\text{xs}} - y_{\text{xs}})^2} \frac{(\nu_{\text{nWW}})^{y_{\text{nWW}}}}{y_{\text{nWW}}!} e^{-\nu_{\text{nWW}}}$$

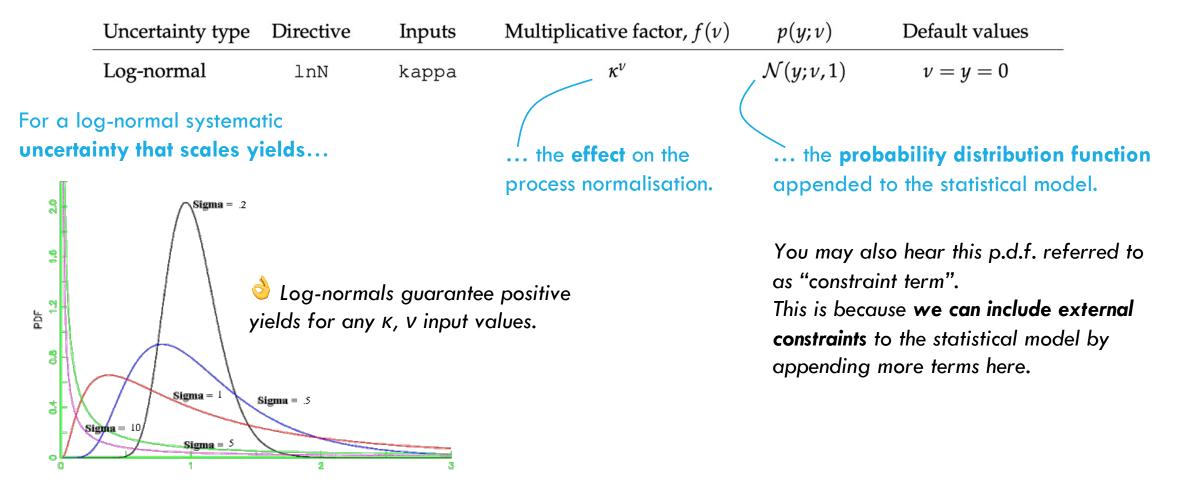
i Bin rate estimate λ does not depend on y_k, only v_k!

→
$$n = 0, y_{\text{lumi}} = y_{\text{xs}} = 0, \text{ and } y_{\text{nWW}} = 4$$

→ $\lambda(r, \vec{v}) = r \ 1.47 \ (1.11)^{\nu_{\text{lumi}}} (1.2)^{\nu_{\text{xs}}} + 0.22 \ (1.11)^{\nu_{\text{lumi}}} + 0.64 \ (1.11)^{\nu_{\text{lumi}}} \frac{\nu_{\text{nWW}}}{0.64}$



UNCERTAINTIES, EFFECTS, AND NUISANCES





UNCERTAINTIES, EFFECTS, AND NUISANCES

Uncertainty type	Directive	Inputs	Multiplicative factor, $f(v)$	p(y; v)	Default values
Log-normal	lnN	kappa	$\kappa^ u$	$\mathcal{N}(y;\nu,1)$	$\nu = y = 0$
Asymmetric log-normal	lnN	kappaDown, kappaUp	$(\kappa^{\text{Down}})^{-\nu}$ if $\nu < -0.5$, $(\kappa^{\text{Up}})^{\nu}$ if $\nu > 0.5$, $e^{\nu K (\kappa^{\text{Down}}, \kappa^{\text{Up}}, \nu)}$ otherwise.*	$\mathcal{N}(y;\nu,1)$	v = y = 0
Log-uniform	lnU	kappa	$\kappa^{ u}$	$\mathcal{U}\left(y,1/\kappa,\kappa ight)$	$ u = y = \frac{1}{2} \left(\kappa + 1/\kappa \right) $
Gamma	gmN	N,alpha [†]	ν/N	$\mathcal{P}(y; \nu)$	$\nu = N + 1, y = N^{\ddagger}$

* $K(\kappa^{\text{Down}}, \kappa^{\text{Up}}, \nu) = \frac{1}{8} \left[4\ln(\kappa^{\text{Up}}/\kappa^{\text{Down}}) + \ln(\kappa^{\text{Up}}\kappa^{\text{Down}})(48\nu^5 - 40\nu^3 + 15\nu) \right]$ ensures that the multiplicative factor and its first and second derivatives are continuous for all values of ν , and reduces to a log-normal for $\kappa^{\text{Down}} = 1/\kappa^{\text{Up}}$.

⁺The rate value for the affected process must be equal to $N\alpha$.

[‡]The default value for the nuisance parameter is set to the mean of a gamma distribution with parameters $\kappa = N + 1$, $\lambda = 1$, as defined in Ref. [20].



THE LIKELIHOOD FUNCTION

For *d* entries in the data set we tack on more "counts" terms to define the likelihood function:

$$\mathcal{L}(\vec{\Phi}) = \prod_{d} p(\vec{x}_{d}; \vec{\mu}, \vec{\nu}) \prod_{k} p_{k}(y_{k}; \nu_{k})$$



THE LIKELIHOOD FUNCTION

For *d* entries in the data set we tack on more "counts" terms to define the likelihood function:

$$\mathcal{L}(\vec{\Phi}) = \prod_{d} p(\vec{x}_{d}; \vec{\mu}, \vec{\nu}) \prod_{k} p_{k}(y_{k}; \nu_{k})$$

But what is this good for ?



THE LIKELIHOOD FUNCTION

For *d* entries in the data set we tack on more "counts" terms to define the likelihood function:

$$\mathcal{L}(\vec{\Phi}) = \prod_{d} p(\vec{x}_{d}; \vec{\mu}, \vec{\nu}) \prod_{k} p_{k}(y_{k}; \nu_{k})$$

1. Frequentist inference: \mathbf{V} profiled in a likelihood ratio: $q_{\text{LEP}}(\mu) = -2\ln\left(\frac{\mathcal{L}(\mu=0,\vec{v}_0)}{\mathcal{L}(\mu,\vec{v}_0)}\right) \qquad q_{\text{TEV}}(\mu) = -2\ln\left(\frac{\mathcal{L}(\mu=0,\hat{\vec{v}}(0))}{\mathcal{L}(\mu,\hat{\vec{v}}(\mu))}\right) \qquad \widetilde{q}_{\text{LHC}}(\mu) = \begin{cases} -2\ln\left(\frac{\mathcal{L}(\mu,\hat{\vec{v}}(\mu))}{\mathcal{L}(\mu,\hat{\vec{v}}(\mu))}\right) & \text{if } 0 \leq \hat{\mu} \leq \mu, \\ -2\ln\left(\frac{\mathcal{L}(\mu,\hat{\vec{v}}(\mu))}{\mathcal{L}(0,\hat{\vec{v}}(0))}\right) & \text{if } \hat{\mu} < 0, \\ 0 & \text{if } \hat{\mu} > \mu, \end{cases}$

2. Bayesian inference: v_k marginalised/averaged over their priors π_k :

$$\mathcal{L}_{\rm int}(\vec{\mu}) = \int \mathcal{L}(\vec{\Phi}) \prod_k \pi_k(\nu_k) d\vec{\nu}, \quad p_k(\nu_k | y_k) \propto p_k(y_k; \nu_k) \pi_k(\nu_k)$$

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FREQUENTIST INFERENCE WITHOUT NUISANCES

Statistical methodology in particle physics is (very) predominantly frequentist.

Notion of **coverage** is central to define uncertainties (68%, 95%).

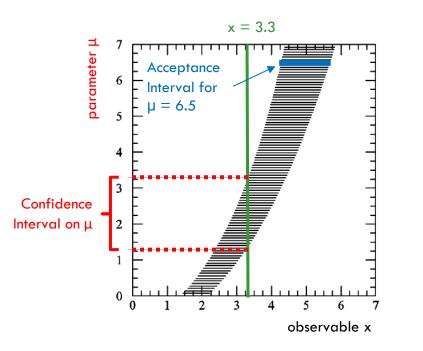
Computational procedures for frequentist methodology quite different from Bayesian: influences practical aspects of how systematics uncertainties are modelled.

30-second nutshell reminder of Frequentist approach:

- Observations { x } summarized by test statistic $q(\mu)$, typically a **likelihood ratio** testing for compatibility of the data with a certain hypothesis $\mu = \mu_0$.
- Knowing the distribution of q(μ) under given hypotheses μ = μ_i define a acceptance interval that contains 68% of the observed outcomes.
- A confidence belt maps the acceptance interval for each value of μ, and allows to construct a confidence interval in μ for a given observed value of q(μ).

FREQUENTIST UNCERTAINTIES IN HEPP

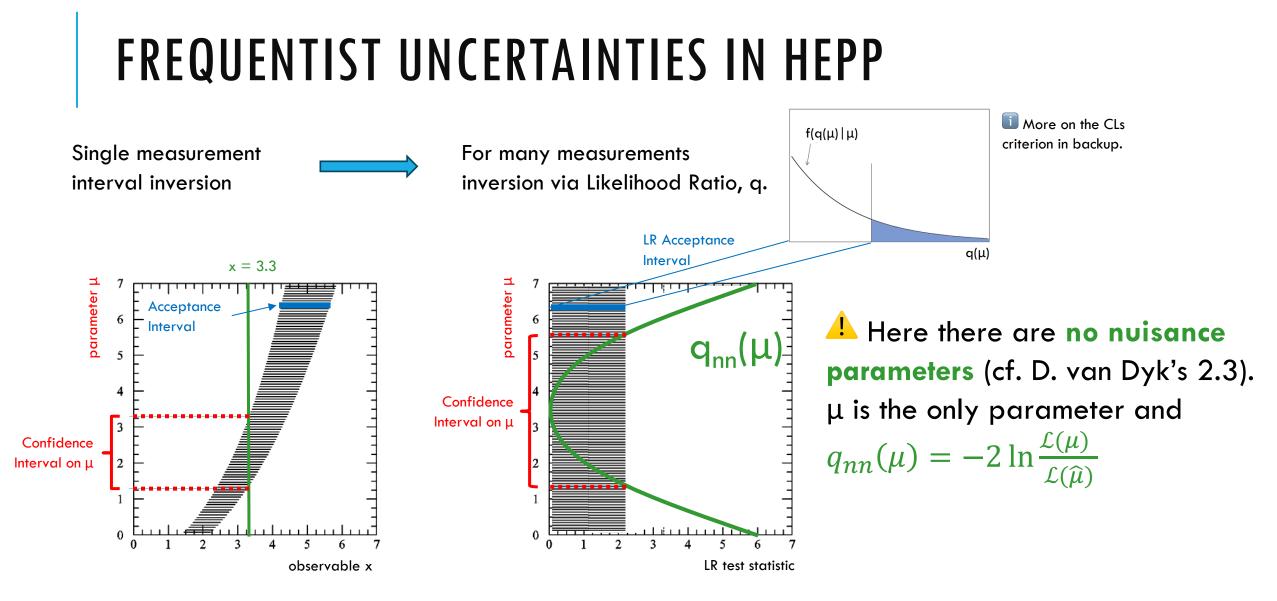
Single measurement interval inversion



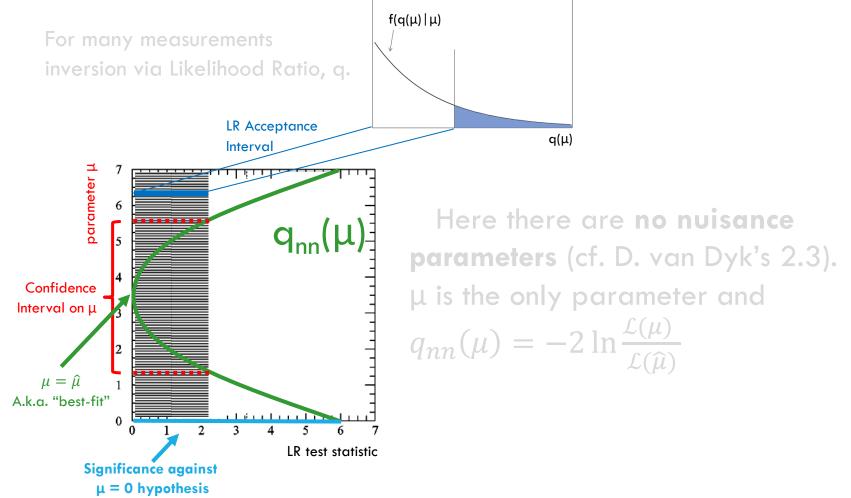
Neyman construction of the confidence belt Acceptance intervals defined by $P(x_{low} < x < x_{high}; \mu) = \int_{x_{low}}^{x_{high}} p(x; \mu) dx \ge 1 - \alpha$ where $1 - \alpha$ is the confidence level.

where $\mathbf{I} = \boldsymbol{\alpha}$ is the **confidence level.**

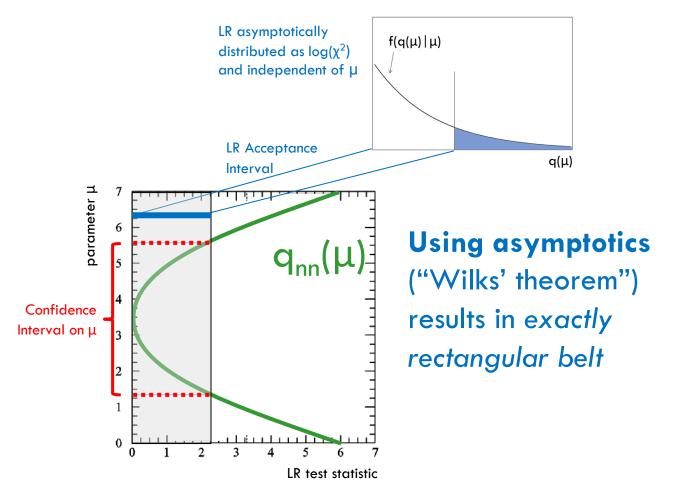
- Procedure in a nutshell:
- . For a given μ generate distribution of x, p(x; μ).
- 2. Use $p(x; \mu)$ to determine x_{low} and x_{high} and make horizontal line.
 - NB: acceptance interval depends on $1-\alpha$ choice and can be one-sided (for limits).
- 3. Repeat for many values of μ to construct the belt.
- 4. For a given x = 3.3 look up the confidence interval for μ from the belt. (Detailed step-by-step in backup.)



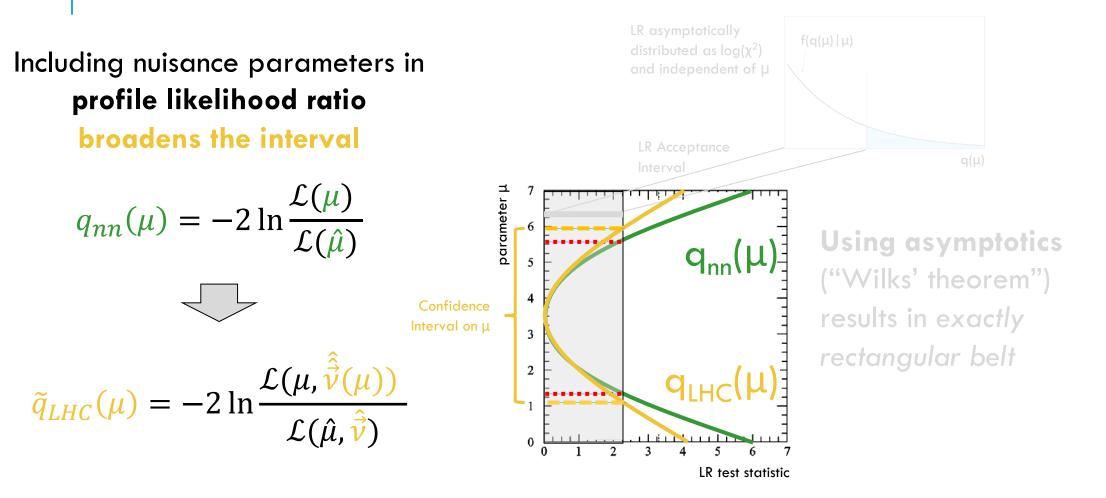
FREQUENTIST UNCERTAINTIES IN HEPP



ASYMPTOTIC APPROXIMATION



ADDING NUISANCES



ADDING NUISANCES

Including nuisance parameters in **profile likelihood ratio**

broadens the interval

 $\tilde{q}_{LHC}(\mu) = -2\ln\frac{\mathcal{L}(\mu, \hat{\vec{v}}(\mu))}{\mathcal{L}(\hat{\mu}, \hat{\vec{v}})}$

The workhorse of inference with nuisances at the LHC.

- Confidence regions, confidence intervals, and upper limits.
- Beware caveats concerning the asymptotic approximation.

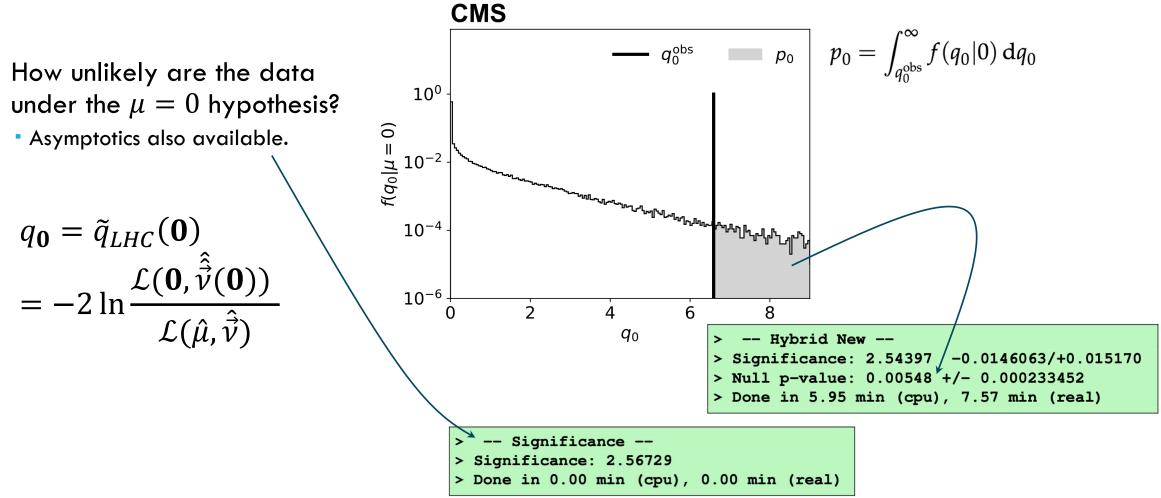
Computing $\tilde{q}_{LHC}(\mu)$ is **relatively cheap** even when dimension of \vec{v} is large.

- No practical penalty to introduce many nuisance parameters.
- Many LHC analyses have 10² to 10³.
- Combined CMS+ATLAS analyses can reach 10⁴.

 $\hat{\vec{v}}$ is the overall best-fit value of \vec{v} , i.e. when $\mu = \hat{\mu}$. $\hat{\vec{v}}(\mu)$ is the best-fit value of \vec{v} for a specific value of μ .



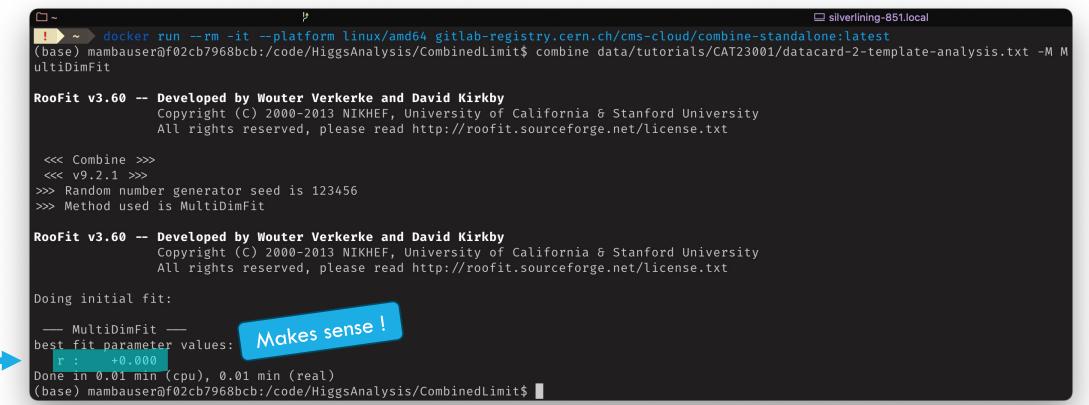
THE $\mu = 0$ case – "Significance"



SIMPLE COUNTING EXPERIMENT — SIGNIFICANCE

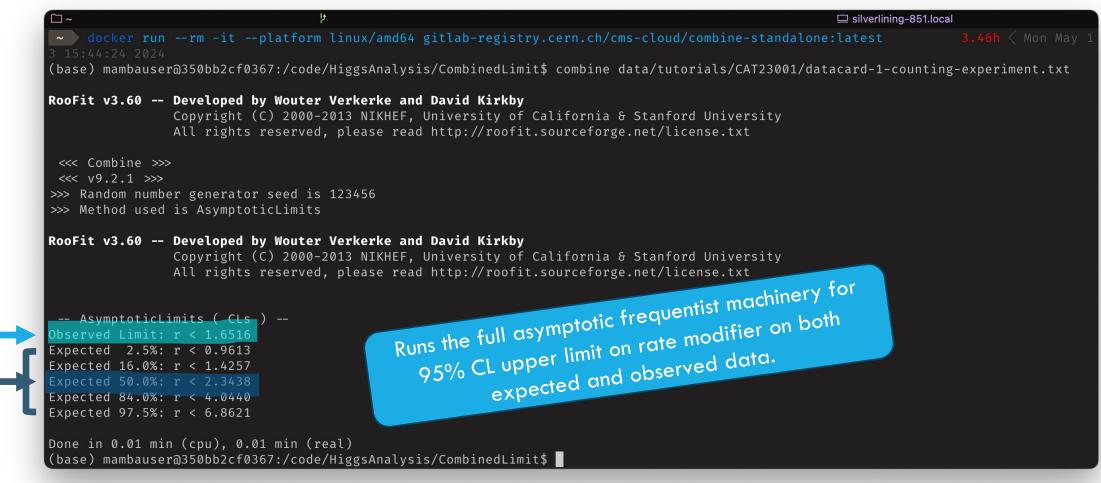
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Copyright (C) 2000-2013 NIKHEF, University of California & Stanford University All rights reserved, please read http://roofit.sourceforge.net/license.txt Significance Makes sense ! Significance: 0 Done in 0.01 min (cpu), 0.01 min (real) (base) mambauser@130e6b27ce0e:/code/HiggsAnalysis/CombinedLimit\$						

SIMPLE COUNTING EXPERIMENT — BEST-FIT



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SIMPLE COUNTING EXPERIMENT — LIMITS



HALF-TIME

All imperfections should give rise to an uncertainty.

- Some are more important than others.
- Some are important to one inference but not another.

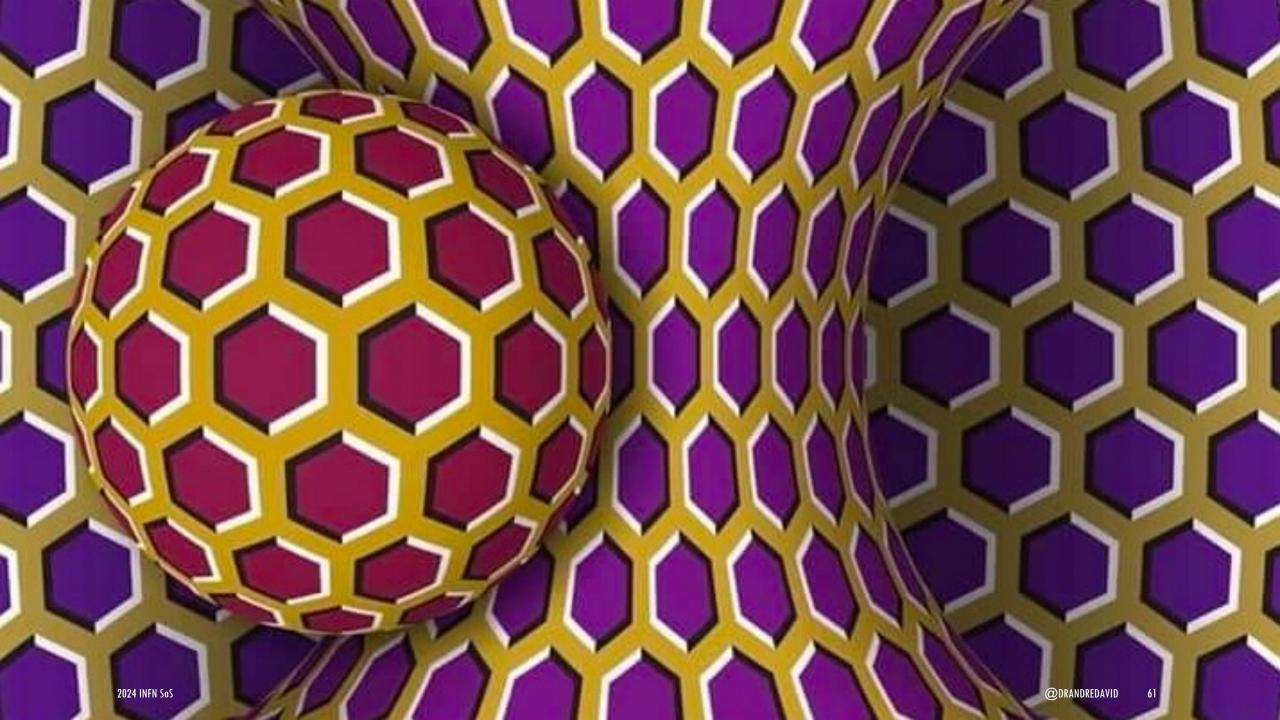
There are decades of practice on how to include them in the statistical model.

Make use of the tools that already exist.

Both Frequentist and Bayesian methods fail in some cases.

 Make sure to understand their limitations and strengths.





ONE LISTING OF NUISANCE PARAMETERS

Luminosity

Detector and per-particle type

- Acceptance
- Efficiency and misidentification
- Energy scales
- Energy resolutions

Templates of processes:

- Theory total cross section uncertainty
- Theory modelling uncertainties
- Limited MC statistics

Empirical process shape modelling

- Parameterisations
- Non-parametric smoothing
- Morphing of templates

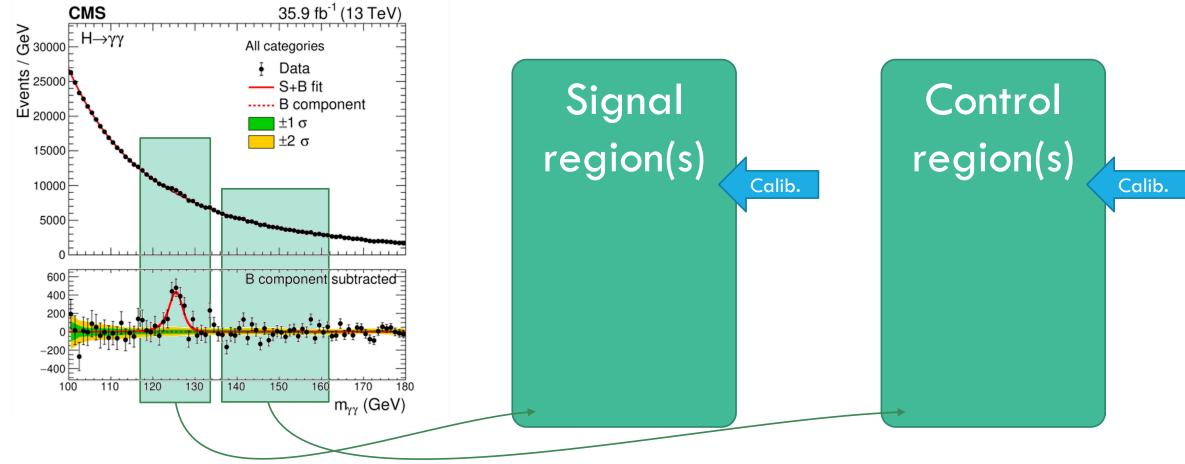
Nuisance parameters can be constrained by:

- Detector calibration data
- Control samples with different event selection
- The data distributions
- Measurements from other experiments
- Theory calculations

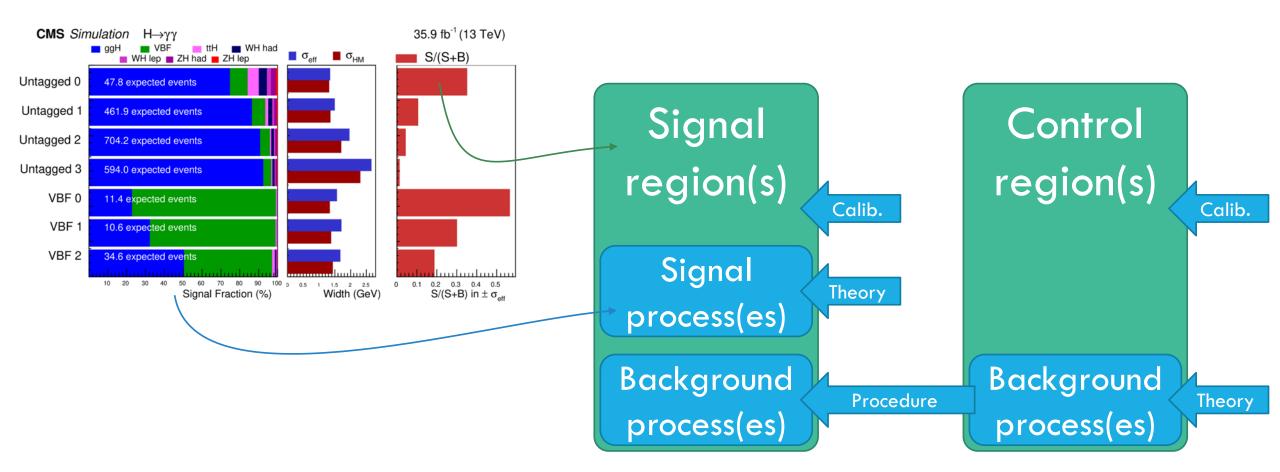




ERRORS – NUISANCES – COUNTS



ERRORS – NUISANCES – COUNTS



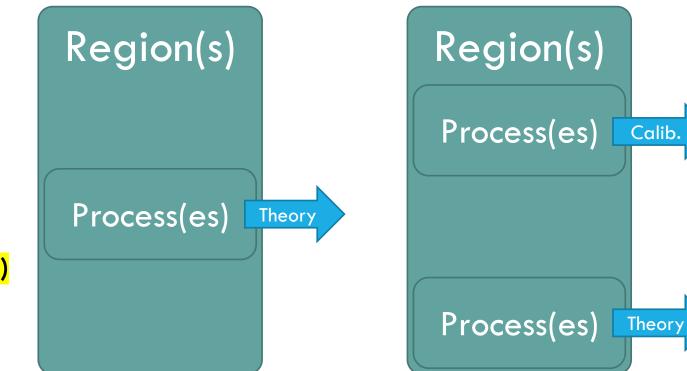
A REVERSIBLE PROCESS

Data also used to:

- Calibrate.
- Constrain theory parameters.
- Constrain non-perturbative inputs.
 - Perennial concern that parton distribution function fits may subsume BSM physics effects.

<mark>Same events ≠</mark> (Double-counting = Double-dipping)

 Avoiding circularity always in the back of our minds.



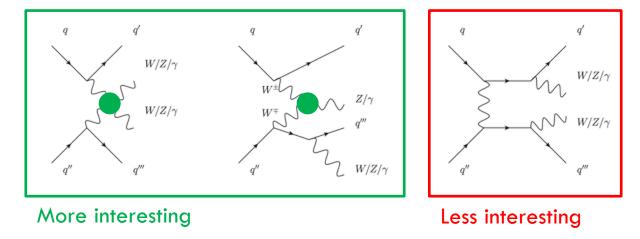
BEYOND S AND B — PROCESSES

Quantum-mechanically indistinguishable example.

- Use interference as systematic?
- Avoid interfering phase space?
- Estimate effects on the total?
- • •

Generally-speaking there are:

- Processes sensitive to the inference you want to make.
- Processes that are not.
 - Some you can estimate from MC.
 - Others may be better estimated from data.
 - Many have an impact on the power of your inference.
- Detector limitations (like noise).



or $\mu^+\mu^-$, a photon, and two jets are selected. The electroweak component is measured with observed and expected significances of 4.1 standard deviations. The fiducial cross-section for electroweak production is measured to be $\sigma_{Z\gamma jj-EW} = 7.8 \pm 2.0$ fb, in good agreement with the Standard Model prediction.

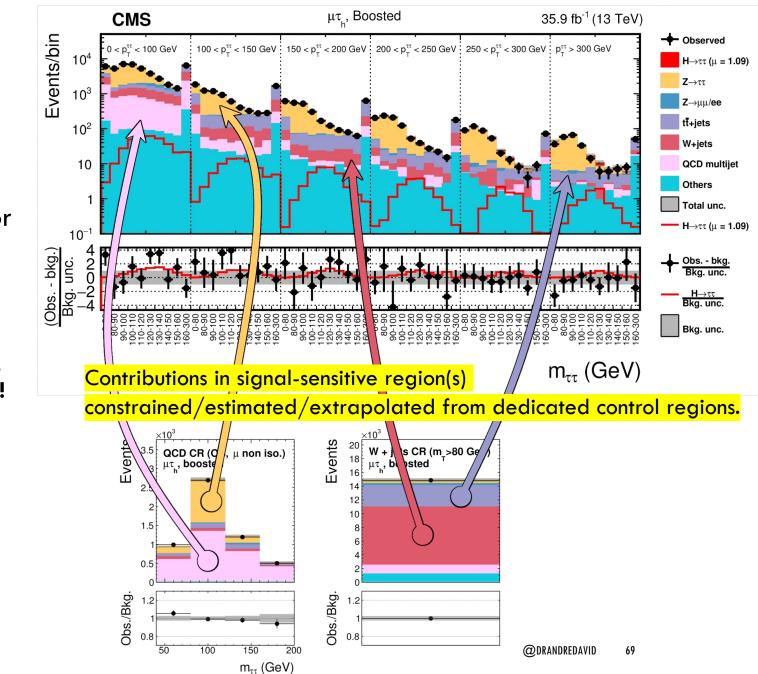
MADGRAPH5_AMC@NLO 2.3.3 MC cross-section prediction in the fiducial region ($\sigma_{Z\gamma jj-EW}^{\text{fid., MC}}$). Because the effect of interference between the $Z\gamma jj$ -QCD and the $Z\gamma jj$ -EW processes is not accounted for in the $Z\gamma jj$ -QCD contribution, the observed cross-section $\sigma_{Z\gamma jj-EW}^{\text{fid.}}$ formally corresponds to electroweak production plus the interference effects.

CONTRIBUTIONS, NOT CONTAMINATION

Simultaneous inference accounts for all processes in all regions.

Pure regions not as important as independent ones.

 Covering similar kinematics minimises extrapolation systematic uncertainties !



THE ASIMOV DATASET

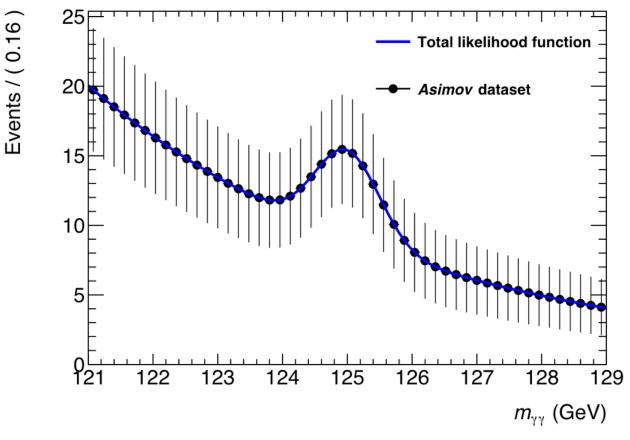
Procedure

- Fix all parameters of the model.
- Estimate corresponding expected counts.

Zero statistical fluctuations.

 Crucial property to explore the model's power without (Nature's) randomness added.

First used by <u>CCGV</u> for median significance and inspired by I. Asimov's <u>"Franchise"</u> short story.



70

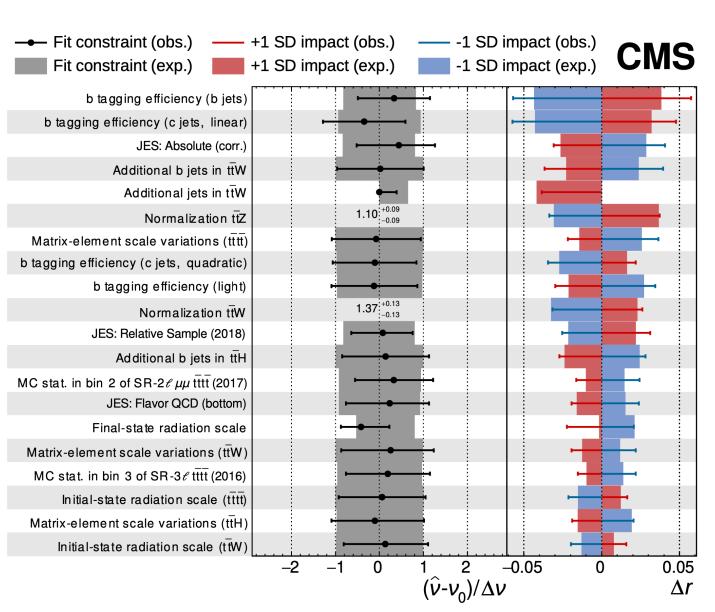
arXiv:2204.06614

PULLS, CONSTRAINTS, IMPACTS

Essential diagnostics that the tools can produce for you.

They cannot tell you whether you are missing something in your statistical model.

They provide insight on how the statistical model and the data interact and affect your inference.



arXiv:2204.06614

CMS

0.05

 Δr

PULLS, CONSTRAINTS, IMPACTS

How much does μ change when changing ν ?

- Fix v_i to $\hat{v_i} \pm \Delta v_i$ and refit all other parameters (μ , $\nu_{k\neq i}$).
- Δv typically chosen as 1 standard deviation value.
- Impact of $\hat{\nu} + \Delta \nu$ in red.
- Impact of $\hat{\nu} \Delta \nu$ in blue.

Two different cases shown:

- Full boxes are the impact after the fit to the Asimov dataset ("expected").
 - 4 "expected" does not imply "correct"; it's just a reflection of what to expect with this choice of statistical model and observables.
- Lines show the impact after the fit to collision data ("observed").

- +1 SD impact (exp.) b tagging efficiency (b jets) b tagging efficiency (c jets, linear) JES: Absolute (corr.) Additional b jets in ttW Additional jets in ttW Normalization ttZ Matrix-element scale variations $(t\bar{t}t\bar{t})$ b tagging efficiency (c jets, quadratic) b tagging efficiency (light) Normalization ttW JES: Relative Sample (2018) Additional b jets in ttH MC stat. in bin 2 of SR-2 $\ell \mu\mu$ tttt (2017) JES: Flavor QCD (bottom) Final-state radiation scale Matrix-element scale variations (ttW) MC stat. in bin 3 of SR-3 tttt (2016) Initial-state radiation scale (tttt) Matrix-element scale variations (ttH) Initial-state radiation scale (ttW)
- ---- Fit constraint (obs.) Fit constraint (exp.)

- +1 SD impact (obs.)

-2



0

-0.05

2

 $(\hat{v} - v_0) / \Delta v$

– -1 SD impact (obs.)

-1 SD impact (exp.)

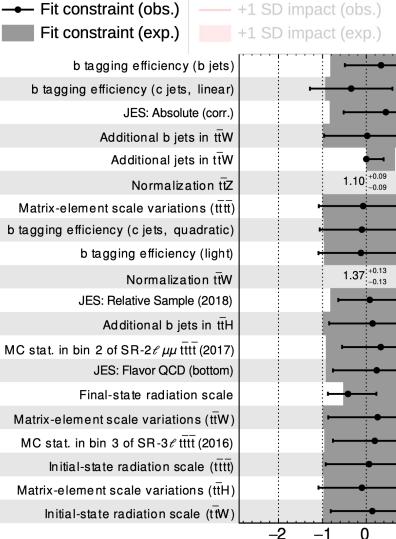


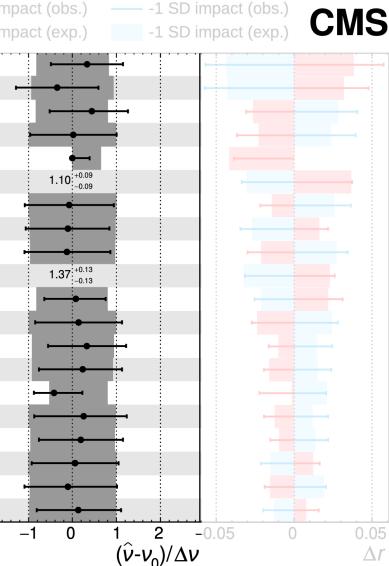
PULLS, CONSTRAINTS, IMPACTS

How much information is gained on each ν ?

Three things shown:

- ± 1 represents what you put in the model.
- Grey bars are the uncertainty after the fit to the Asimov dataset ("expected").
 - A "expected" does not imply "correct"; it's just a reflection of what to expect with this choice of statistical model and observables.
- Black uncertainties are the uncertainty after the fit to collision data ("observed").





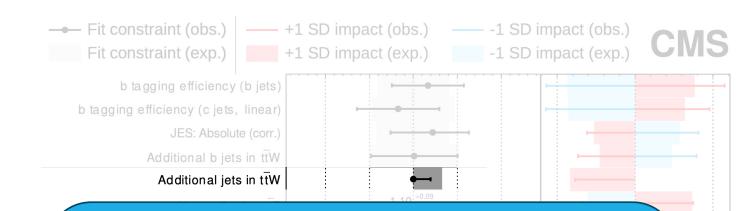
@DRANDREDAVID 73

PULLS, CONSTRAINTS, IMPACTS

How much information is gained on each ν ?

Three things shown:

- ± 1 represents what you put in the model.
- Grey bars are the uncertainty after the fit to the Asimov dataset ("expected").
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- Black uncertainties are the uncertainty after the fit to collision data ("observed").

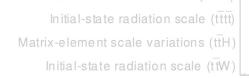


You can see here an expected uncertainty ~40% smaller than what was put in the model. So if someone says you should be "conservative" and put a

large(r) uncertainty in the model, that may have zero impact on the analysis if the data is able to constrain it.This is not necessarily a problem; e.g. here we have a theory uncertainty that was hard to gauge in the first place.

 \cap

-2



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 Λr

 $(\hat{v} - v_0)/\Delta v$

CMS



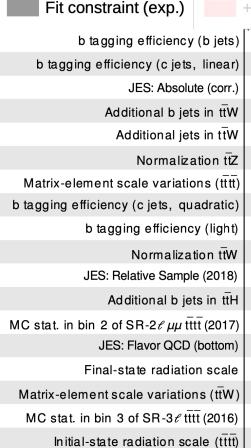
 Δr

PULLS, **CONSTRAINTS**, IMPACTS

How much information is gained on each ν ?

Different datasets tell us different things:

- Pre-fit expected (Asimov)
 - "What power is this model expected to have ?"
- Pre-fit toy data sets
 - "What do statistical fluctuations imply for that power ?"
- Post-fit expected (Asimov)
 - From partial data, e.g. only (some) CRs.
 - From whole data: CRs + SRs.
- Post-fit observed
 - Partial data or whole data.
 - Include statistical fluctuations.
- Post-fit toy data sets
 - "How unlucky was the observed ?"



---- Fit constraint (obs.) ---- +1 SD impact (obs.)

Matrix-element scale variations (ttH)

Initial-state radiation scale (ttW)

2

 $(\hat{\nu} - \nu_0) / \Delta \nu$

-1 SD impact (exp.)

1.10 +0.09 -0.09

1.37

+1 SD impact (exp.)

-2

_1

0

-0.05

75

– -1 SD impact (obs.)

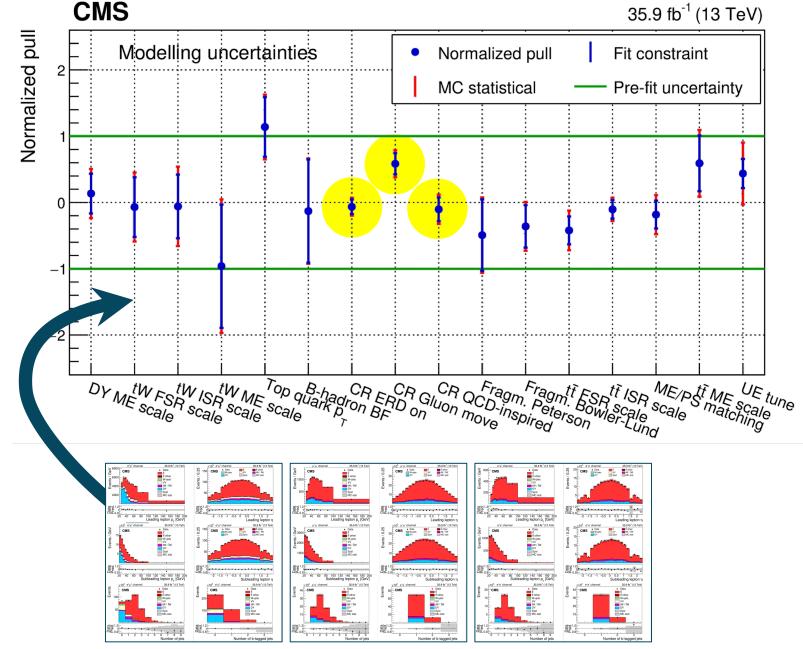
CMS-TOP-17-001

CONSTRAINING NUISANCES ?

From $t\bar{t}$ cross-section measurement: $e^{\pm}\mu^{\mp}$, $\mu^{+}\mu^{-}$, and $e^{+}e^{-}$.

"effects of **colour reconnection (CR)** processes on the top quark final state"

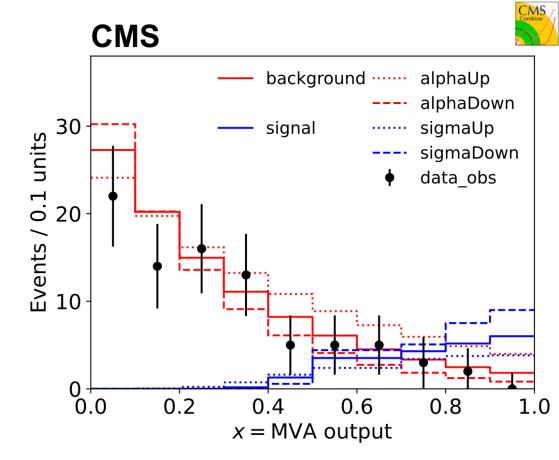
Is constraining these ok?



USE THE TOOLS TO SEE THE **INGREDIENTS**

Example analysis with two templates, each with a systematic shape variation:

- Observable x is a MVA output: more background at lower values and more signal at larger values.
 - One can see from the data that there is probably no signal in Nature.
- Signal syst. uncertainty controlled by nuisance parameter σ.
- Background syst. uncertainty controlled by nuisance parameter α.



USE THE TOOLS TO SEE THE **EFFECTS**

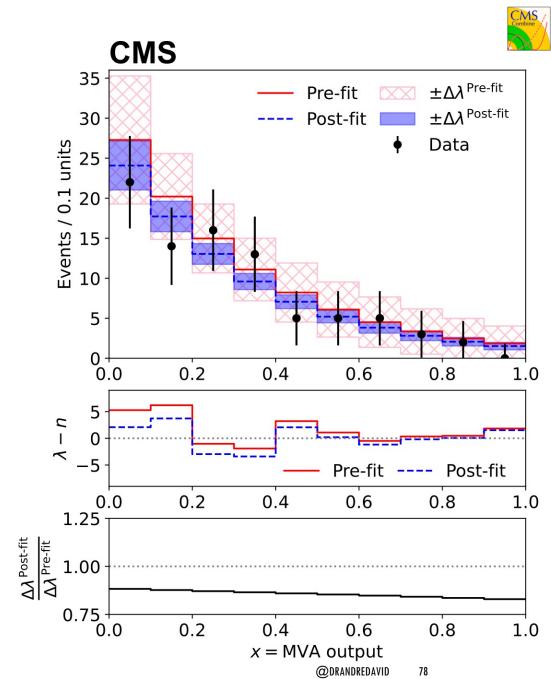
- Top panel bin contents:
- Black points: observed value.
- **Red**: pre-fit estimate and uncertainty.
- Blue: ditto post-fit.

Middle panel – bin contents differences:

- Difference between estimates (λ) and observations (n) both pre-fit and post-fit.
- Post-fit reduces discrepancies between model and data.

Lower panel – estimate uncertainties:

- Ratio between the estimated uncertainty post-fit and estimated uncertainty pre-fit.
- Post-fit reduces estimated uncertainties.



ASTRONOMERS AND CALIBRATORS

All-in-one in HEPP but not universal.

Also makes HEPP papers have very long, uninformative, author lists.

Cases in LHC where "interpreters" are "calibrators".

Cases where "interpretation" is blunted to not step beyond "calibration" stated ability.

My rule of thumb: if an analysis constrains a calibrationprovided nuisance parameter, stop and think.

And then possibly take action.



ALTERNATIVES AND MORPHING

Some alternatives are **physical deformations** with meaning.

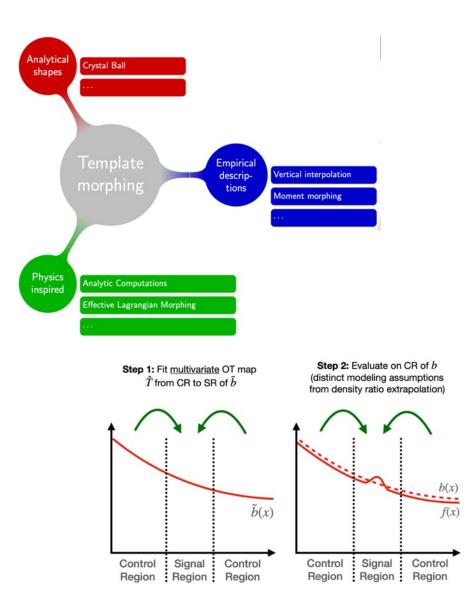
"Average"/morphing makes sense.

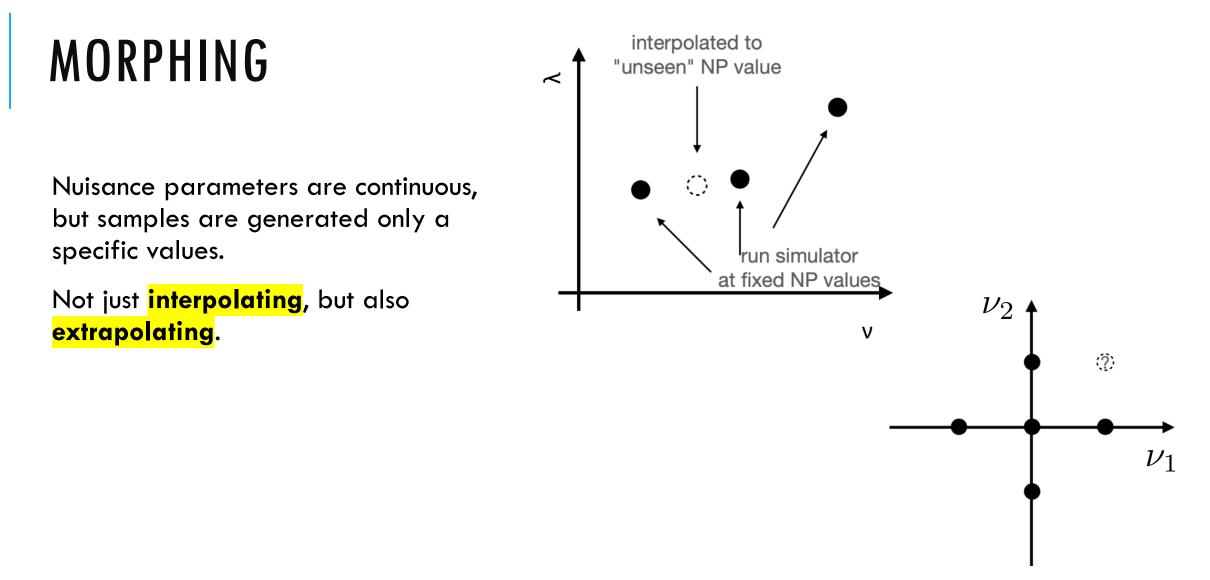
Some alternatives are really **just alternatives**.

 And if they end up mattering we'll likely throw one out as unphysical. (Cousins)

Perturbative theory uncertainties are a whole different beast altogether.

Limited but non-zero knowledge on the next term.



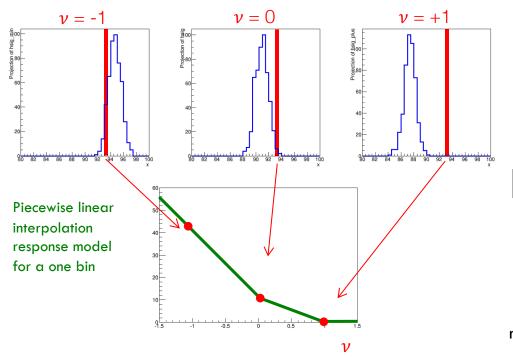


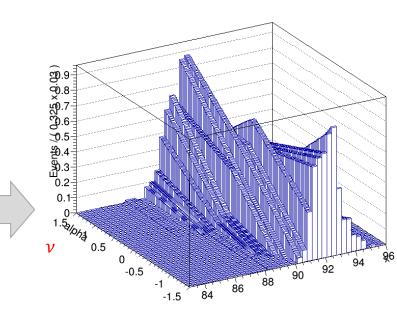
MORPHING

<mark>Main workhorse</mark> at LHC.

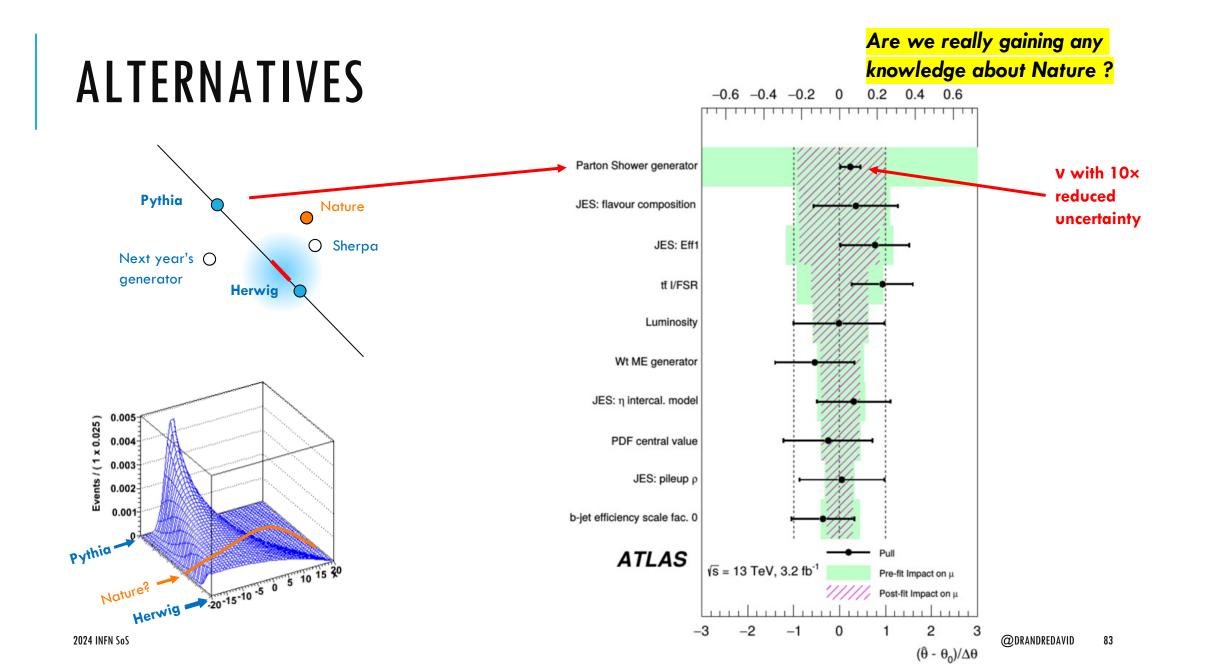
Several limitations known.

Now modern technology for multi-dimensional morphing now available.





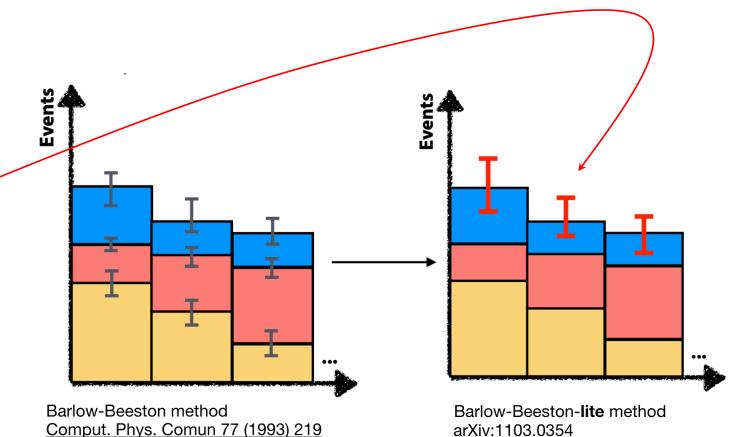
Bin-by-bin piece-wise interpolation robust enough for small-to-moderate distortions typically introduced by systematic variations



LIMITED SIMULATION STATISTICS

Account for uncertainties due to the limited sample size used when creating templates.

- Barlow-Beeston procedure widely available.
- "Lite" version reduces number of _ nuisance parameters.
 - No one prescription on how to merge nuisances.

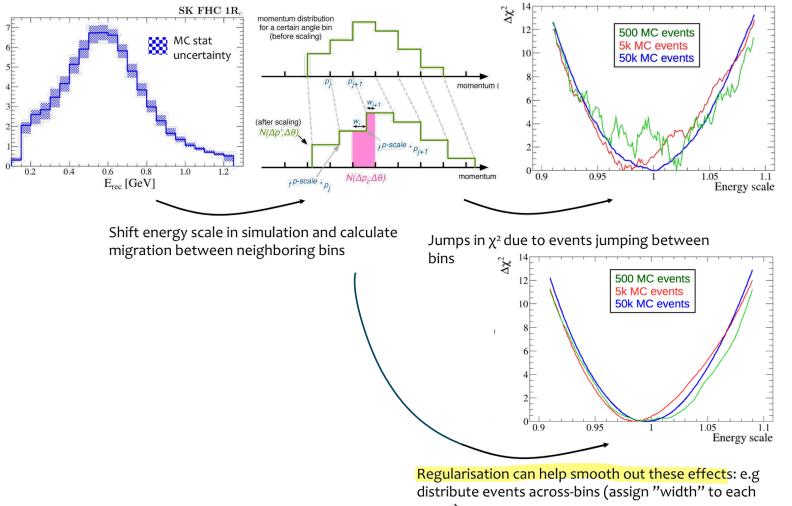


LIMITED SIMULATION STATISTICS

Events per Bin

Effects from "horizontal" migration of events.

- Induce "vertical" effects.
- Not related to bin-by-bin uncertainties (Barlow-Beeston).



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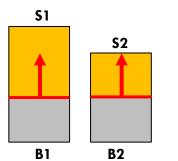
"BEING CONSERVATIVE"

Also: mass measurements and scale uncertainties.

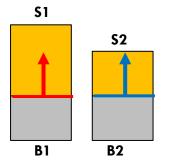
Should uncertainties be correlated or uncorrelated ? It depends.

Consider two bins, **Bi** with yields **Si**.

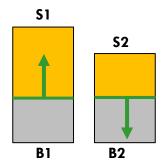
 $POI \propto S1 / S2$



Very Optimistic



Appropriate ?



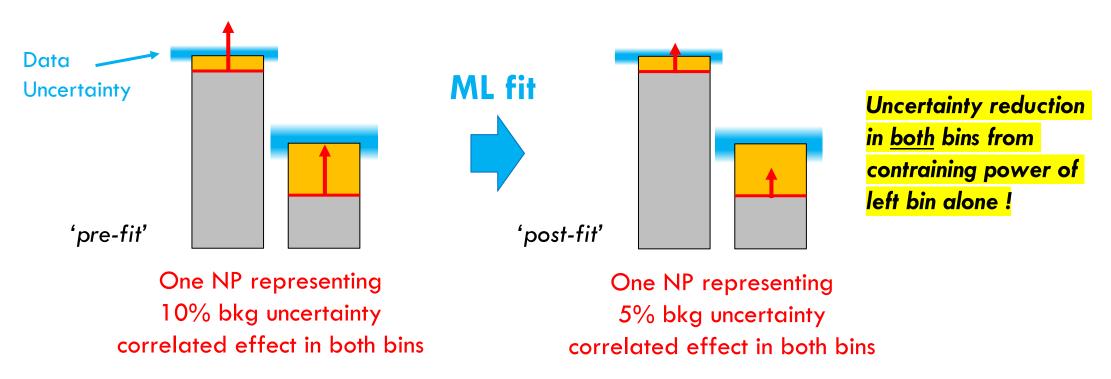
NP: 10% bkg uncertainty NP1: 10% bkg unc. - bin 1 NP: 10% bkg uncertainty correlated modeling NP2: 10% bkg unc. - bin 2 anti-correlated model
 POI ∝ S1 + S2 Conservative Appropriate ? Very Optimistic

Conservative

"BEING CONSERVATIVE"

Should uncertainties be correlated or uncorrelated ? It depends.

Consider bins with very different numbers of "counts".



ALTERNATIVES AND MORPHING

Some alternatives are physical deformations with meaning.

"Average"/morphing makes sense.

Some alternatives are really just alternatives.

 And if they end up mattering we'll likely throw one out as unphysical. (Cousins)

Perturbative theory uncertainties are a

whole different beast altogether.

• Limited but non-zero knowledge on the next term.

Parametrize and estimate the actual source of the uncertainty: f''(0)

$$f(x) = f(0) + f'(0) x + f''(0) \frac{x^2}{2} + \mathcal{O}(x^3)$$

source of the theory uncertainty

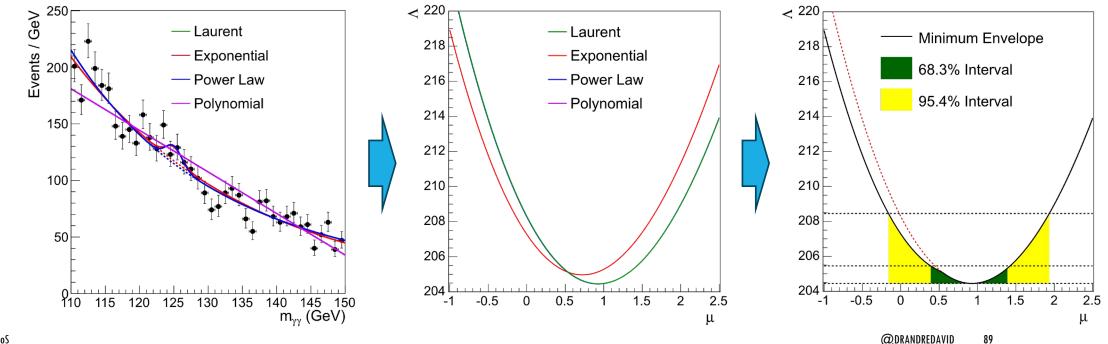
• We typically know a lot about the general structure of f''(0) even without explicitly calculating it

DISCRETE PROFILING

Invented in CMS $H \rightarrow \gamma \gamma$ to deal with **different parametric background choices**.

ATLAS uses "spurious signal" (different) method.

Extensively validated to not bias inference.



THE MOF DISCRETE PROFILING

Perhaps there is **hope to understand discrete profiling** in the model selection context.

 How do you feel about model averaging being the (weighted) average of estimates across different models?

Unavoidable comparison with spurious signal; both are prescriptions using statistical uncertainty under the signal as the gauge

- Discrete profiling functions are chosen to have bias smaller than O(10%) stat. unc.
- Spurious signal is chosen on similar basis and added to signal model.

Model	MLE of θ	Log likelihood at MLE	AIC	Akaike Weight
Linear	0.13	-174.79	355.58	≈ 0
Quadratic	0.84	-155.85	319.70	0.29
Cubic	1.14	-154.81	319.62	0.30
Quartic	1.21	-154.02	320.05	0.24
Quintic	1.18	-153.84	321.67	0.11
Sextic	1.24	-153.83	323.65	0.040
Septic	1.25	-153.34	324.69	0.024

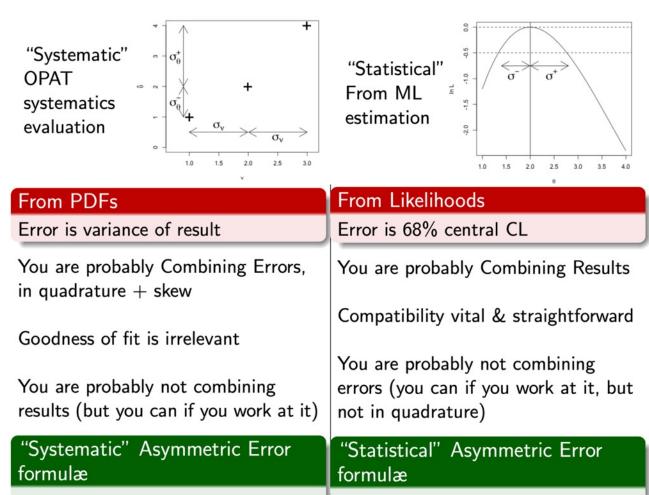
A WELCOME SYSTEMATISATION

OPAT vs APAST

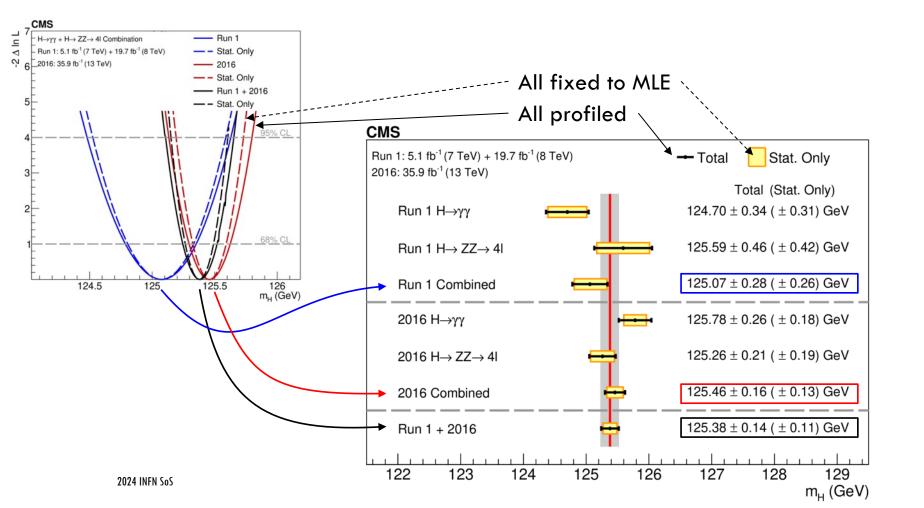
Combination of measurements vs combined measurement.

Discussion on **simplified likelihoods**:

- Taylor expansion seems to be founded.
- For PDFs a whole different story: cumulants, saddle point approximation, etc.

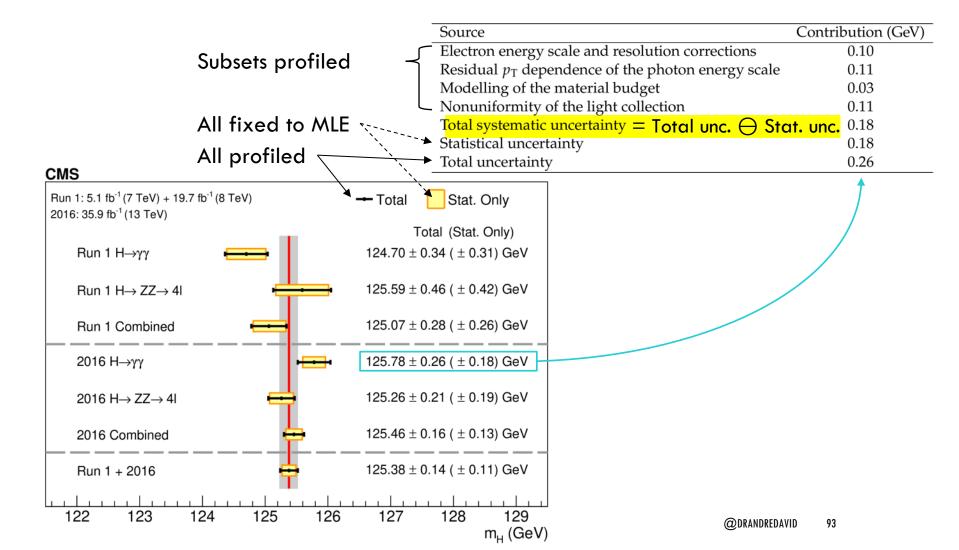


APAT — ALL PARAMETERS AT A TIME



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APAT — ALL PARAMETERS AT A TIME



BETTER ASYMPTOTICS

Sine qua non for "errors on errors" that can benefit all.

Correction can also be used as coverage diagnostic tool.

I wonder what happens in asymmetric cases...

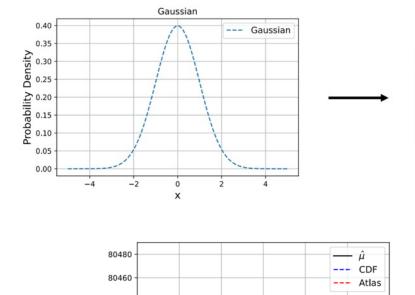
$$r_{\mu}^{*} = r_{\mu} + \frac{1}{r_{\mu}} \log \frac{q_{\mu}}{r_{\mu}} = \frac{r_{\mu} - E[r_{\mu}]}{V[r_{\mu}]^{1/2}} + \mathcal{O}(n^{-3/2})$$
$$r_{\mu}^{*} \sim \mathcal{N}(0,1) + \mathcal{O}(n^{-3/2})$$

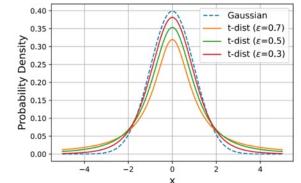
HOW CERTAIN IS THAT UNCERTAINTY?

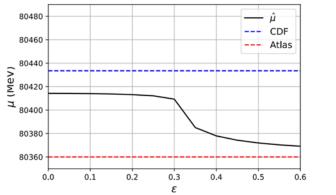
"Unleash the tails !"

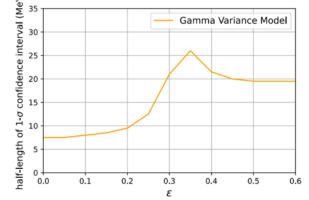
Discussion focused on applying these foremost to theory inputs.

- For exp. uncs. I wonder what the evaluation experiment_k by physicist_i would be.
 - Especially when k = i.
- Lots of interesting ideas to pursue to understand how it deals with outliers.
- I know at least one theorist seriously studying the method.









"LAST MILE" CORRECTIONS

Simulation imperfections can have substantial impact on inference.

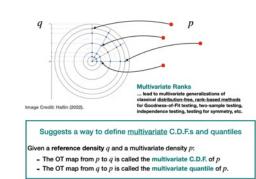
Example evolution with time:

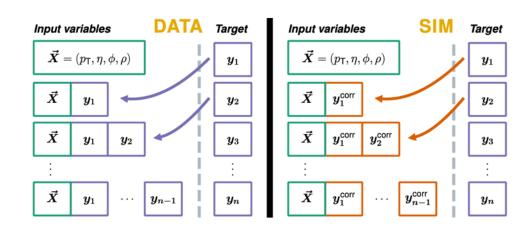
- "Multiply and smear".
- 1-D quantile regression.
- Chained quantile regression.

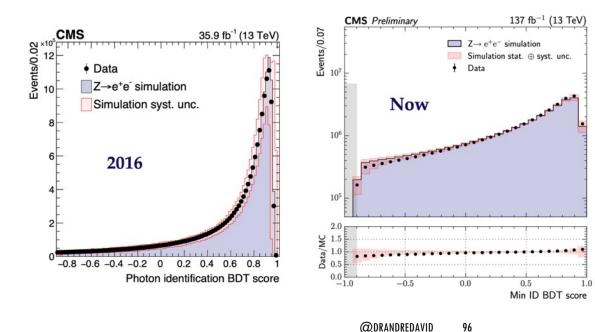
Is this the best that can be done?

Heard at PHYSTAT 2023:

- Multi-dim. quantile regression.
- Multi-dim. CDF.
- Optimal Transport maps.









\geq 1 PARAMETERS OF INTEREST

 $(1 - \alpha)$ (%)

68.27

90.

95.

99.

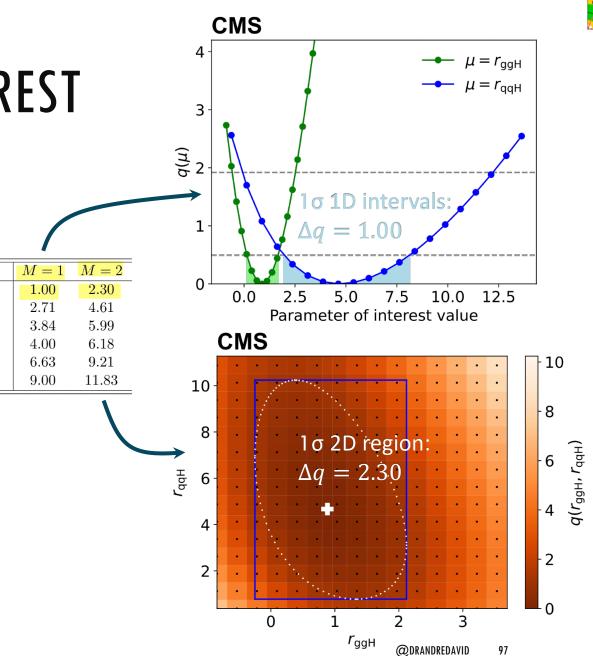
95.45

99.73

Thanks to Wald and Engle !

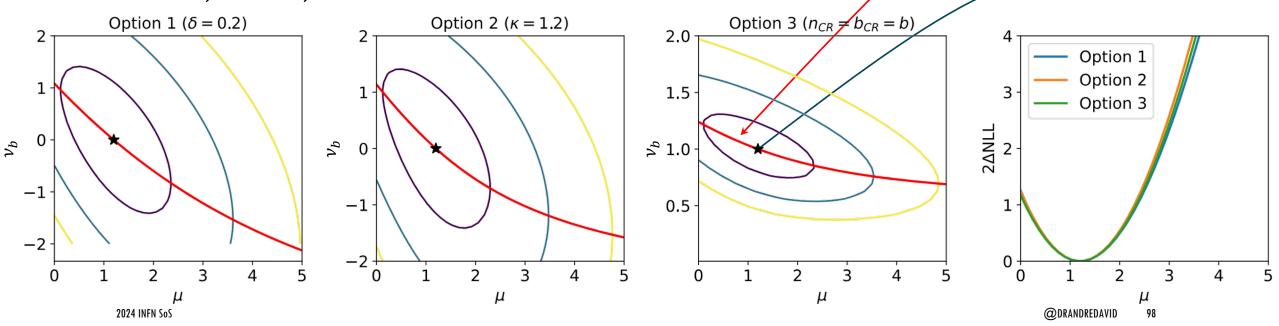
Joint inference can and should be done.

Same asymptotics but thresholds for regions depend on number of parameters.



KNOW YOUR APPROXIMATIONS

Background with 20% uncertainty modelled in three different ways. • Option 1 (Gaussian) $p(x; \mu, \nu_b) = P(x; \mu \cdot s + b(1 + \delta \cdot \nu_b)) \cdot N(y; \nu_b, 1).$ • Option 2 (Log-normal) $p(x; \mu, \nu_b) = P(x; \mu \cdot s + b \cdot \kappa^{\nu_b}) \cdot N(y; \nu_b, 1).$ • Option 3 (Gamma) $p(x; \mu, \nu_b) = P(x; \mu \cdot s + b \cdot \nu_b) \cdot P(n_{CR}; b_{CR} \cdot \nu_b).$ $q(\mu) = -2 \ln \frac{\mathcal{L}(\mu, \widehat{\nu_b}(\mu))}{\mathcal{L}(\hat{\mu}, \widehat{\nu_b})}$ s = 25, b = 25, x = 37



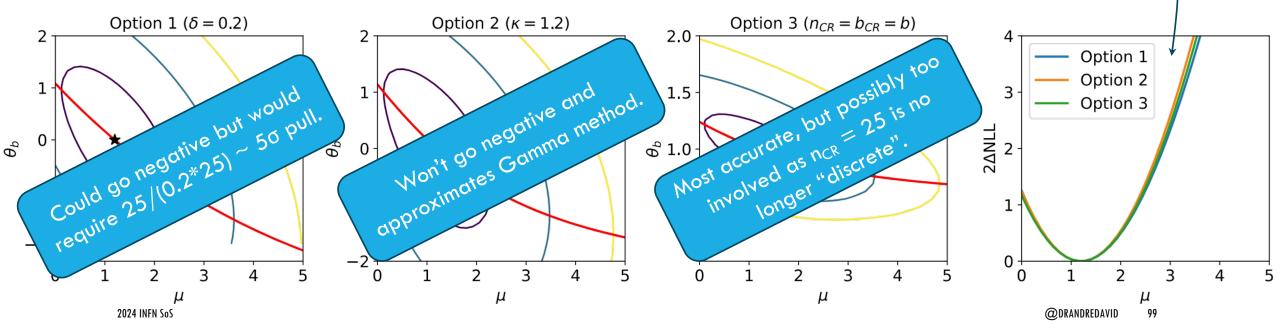
SAVED BY THE C.L.T.

Background with 20% uncertainty modelled in three different ways:

- $p(x;\mu,\nu_b) = P(x;\mu \cdot s + b(1 + \delta \cdot \nu_b)) \cdot N(y;\nu_b,1).$ Option 1 (Gaussian)

• Option 2 (Log-normal) $p(x; \mu, \nu_h) = P(x; \mu \cdot s + b \cdot \kappa^{\nu_b}) \cdot N(y; \nu_h, 1).$ • Option 3 (Gamma) $p(x; \mu, \nu_h) = P(x; \mu \cdot s + b \cdot \nu_h) \cdot P(n_{CR}; b_{CR} \cdot \nu_h).$

 $s = 10, b = 25, x = 37 \Rightarrow$ Small difference in the inference for this case.



PARTING THOUGHTS

You'll spend a lot of time correcting measurements.

 So make friends with the uncertainties that come with those corrections.

Whenever you have low counts, be very careful.

• If you have zero counts, welcome to the club.

Profiling nuisances has great power.

 Whether the power to constrain them is licit or not is another matter.



Vamos a la playa

>

Brano di Righeira



Righeira Vamos a la playa 1983 -YouTube

https://www.youtube.com > watch

Testo

Vamos a la playa, oh oh oh oh Vamos a la playa, oh oh oh oh Vamos a la playa, oh oh oh oh Vamos a la playa, oh oh... Testo completo

Fonte: LyricFind



FOR DISCUSSION

ACKNOWLEDGEMENTS

All who have contributed to more than two decades of PHYSTAT wisdom-building.

<u>https://phystat.github.io/Website/</u>

CMS's collective wisdom distilled into the COMBINE tool.

- <u>https://arxiv.org/abs/2404.06614</u>
- <u>https://github.com/cms-analysis/HiggsAnalysis-CombinedLimit</u>

Speakers at the 2021 and 2023 PHYSTAT workshops on systematic uncertainties.

- https://indico.cern.ch/event/1051224
- <u>https://www.birs.ca/events/2023/5-day-workshops/23w5096</u>

Wouter Verkerke's decades of material on the topic of modelling.

Dankjewel !

NOT ENOUGH TIME TO COVER DETAILS OF...

Multidimensional modern morphing.

"Marginalizing versus Profiling of Nuisance Parameters" <u>arXiv:2404.17180</u>

Diagonalization and externalisation of uncertainties.

Sampling nuisance parameters and constructing toy datasets.

The galaxy of asymptotics:

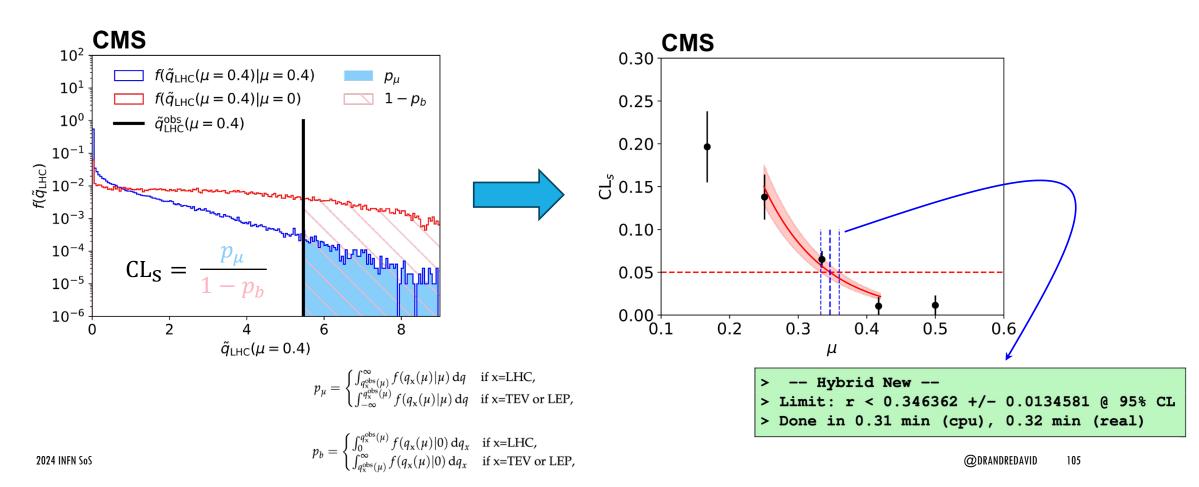
- Wilks (single parameter),
- Wald and Engle (multiple parameters), and
- Chernoff and Self-Liang (parameters at boundaries).

The Trials Factor or Look Elsewhere Effect and Machine Learning.



THE CL_S CRITERION — 95% CL LIMIT EXAMPLE

Motivation and description in <u>PDG RPP 40.4.2.4</u>.



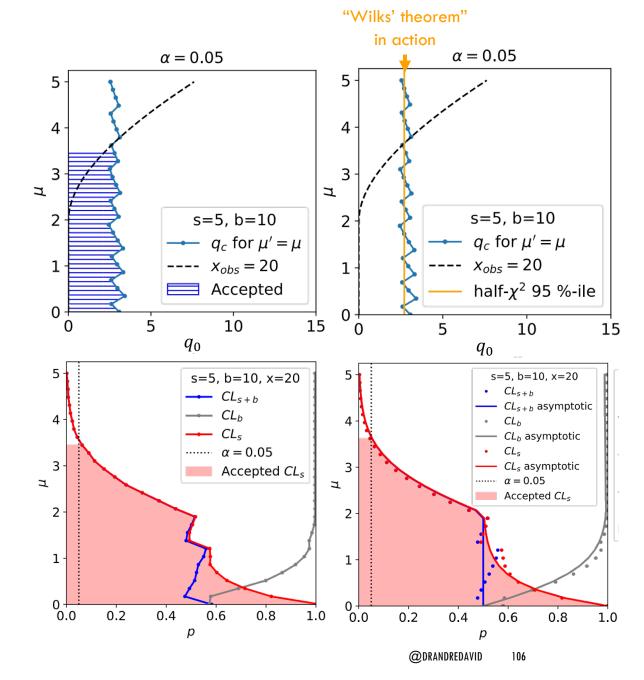
POISSON EXAMPLE WITHOUT NUISANCES

Model: $p(x; \mu s + b) = \frac{(\mu s + b)^x e^{-(\mu s + b)}}{x!}$

Known (fixed!) background.

Test statistic:
$$q_0(\mu) = -2 \ln \frac{\mathcal{L}(\mu)}{\mathcal{L}(\hat{\mu})}$$

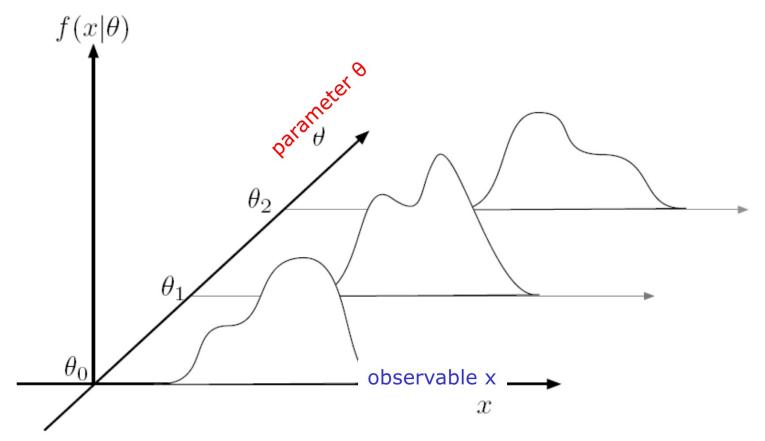
• Jagged behaviour of q_0 due to Poisson discrete nature, not by limited toy statistics (10⁴ in this case).





NEYMAN CONSTRUCTION

- Simplest experiment: one measurement (x), one theory parameter (θ)
- For each value of parameter θ , determine distribution in in observable x



 $\stackrel{!}{\frown}$ This $1 - \alpha$ region is:

two-sided for intervals, and

• one-sided for limits.

i $1 - \alpha = 68\%$ constructs $\pm 1\sigma$ intervals.

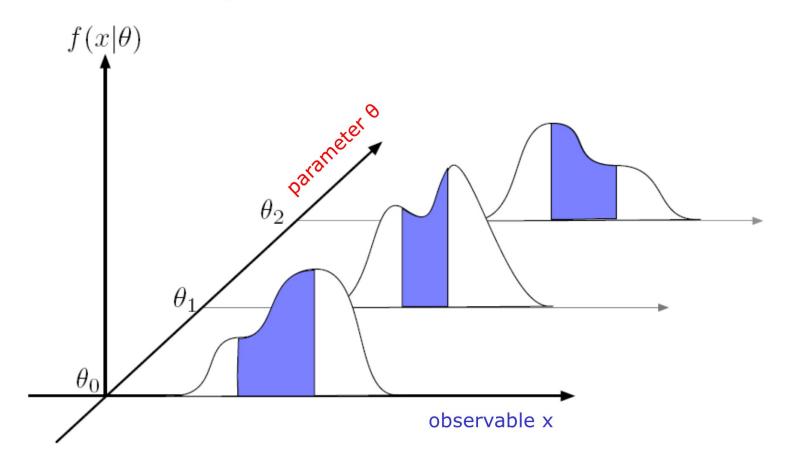
- Focus on a slice in θ
 - For a $1-\alpha$ confidence Interval, define *acceptance interval* that contains $100\%-\alpha^{\circ}$ of the distribution

pdf for observable x given a parameter value θ_0

 $f(x|\theta_0)$ $1-\alpha$

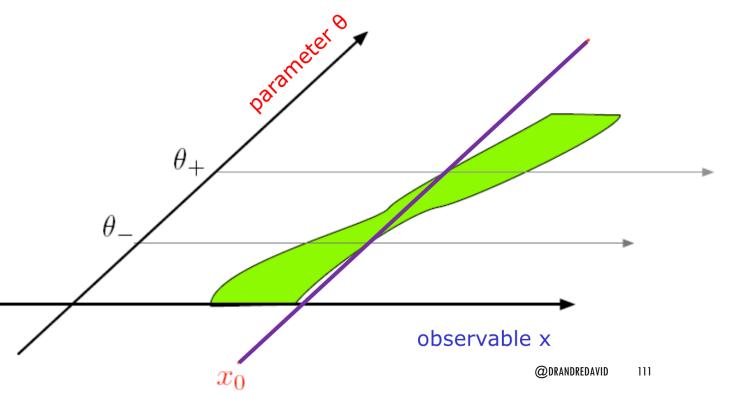
observable x

• Now make an acceptance interval in observable x for each value of parameter θ



Neyman invented this procedure as a "quality control" procedure. His goal was to guarantee that intervals from different people would be comparable.

- The confidence belt can constructed *in advance of any measurement*, it is a property of the model, not the data
- Given a measurement x₀, a confidence interval [θ₊,θ₋] can be constructed as follows
- The interval $[\theta_{-}, \theta_{+}]$ has a 68% probability to cover the true value





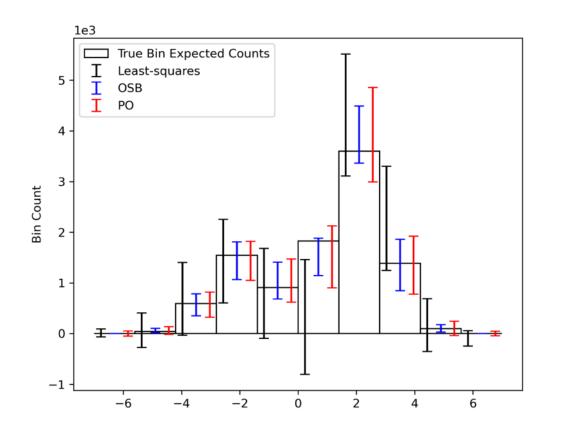
ADDITIONAL TOPICS

PROGRESS IN UNFOLDING

Important physics tool for theoryexperiment communication.

 Avoids theorists having to turn their calculations into full-fledged simulations.

Exciting progress with many open questions for future work.



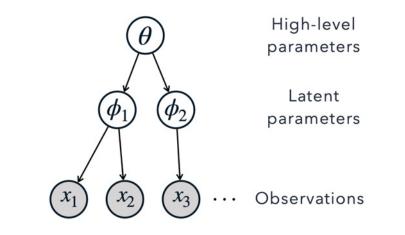
Inference

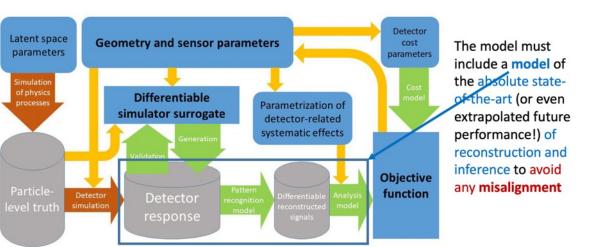
HIERARCHIES TO DIVIDE AND CONQUER

Specifying intermediate "quantities of interest" or "observables".

Not new: we calibrate energies of individual hits and reconstruct momenta of individual tracks.

Not a conclusion, just a feeling; a theme.





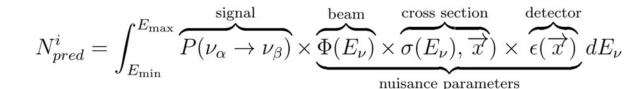
LHC'S BUT ONE CORNER OF PARTICLE PHYSICS

Specific issues that deserve just as much attention from statisticians.

 Fertile (safe?, welcoming?) ground for Bayesian methods.

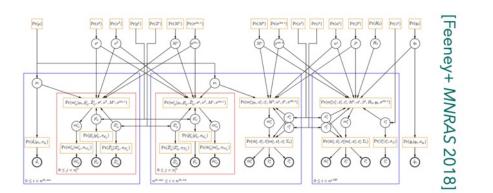
LHCb and Belle II: measurement style

For measuring \mathscr{B} of rare *B*-decays LHCb uses mostly relative and Belle II absolute approach: $\circ \ \mathscr{B}(B^+ \to \mu^+ \mu^- \mu^+ \nu) = \mathscr{B}(B^+ \to J/\psi(\to \mu^+ \mu^-)K^+) \times \frac{\varepsilon(B^+ \to J/\psi(\to \mu^+ \mu^-)K^+)}{\varepsilon(B^+ \to \mu^+ \mu^- \mu^+ \nu)} \times \frac{N(B^+ \to \mu^+ \mu^- \mu^+ \nu)}{N(B^+ \to J/\psi(\to \mu^+ \mu^-)K^+)}$ $\circ \ \mathscr{B}(B^+ \to K^+ \nu \bar{\nu}) = \frac{N(B^+ \to K^+ \nu \bar{\nu})}{\varepsilon(B^+ \to K^+ \nu \bar{\nu})}$



@DRANDREDAVID

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THE BULK AND THE TAILS

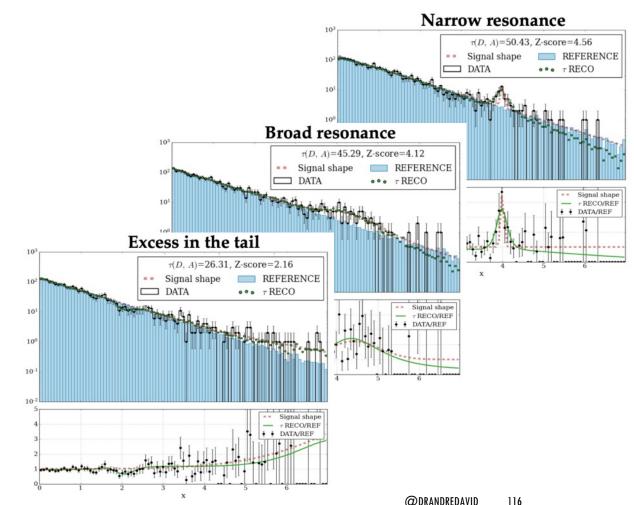
BSM physics unlikely to be the obvious stuff already looked for in the last 40 years.

- Must be within reach and be very subtle (bulk), or
- Out of reach and very energetic (tails).

Requiring same support as the SM simulation does not cover second case above.

- I.e. events beyond SM sim. support that could still be SM.
- Connected also to amount of SM sim. that can be afforded.

Can outlier estimation come to the rescue?



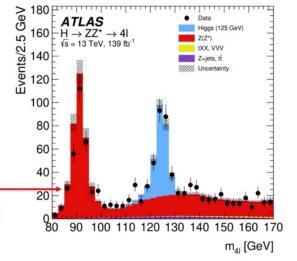
ML FOR AI — I.E. FOR ACTUAL INTELLIGENCE*

Progress: agreement that optimality and correctness are not the same.

- 90% of cases.
 - Can live with consequences.
- 10% of cases.
 - Can have dire consequences.

Question of optimality:

- Did ML get best reconstruction or event selection?
- Effects definition of discriminating variables, but doesn't affect compatibility with data



Things that affect $p(\cdot | \lambda(\theta))$

Questions of correctness:

- Did ML learn an accurate fast simulation?
- Did ML learn a good background estimate?
- Effects statistical model & compatibility with data!

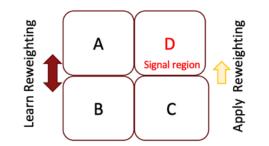
ML FOR AI — I.E. FOR ACTUAL INTELLIGENCE

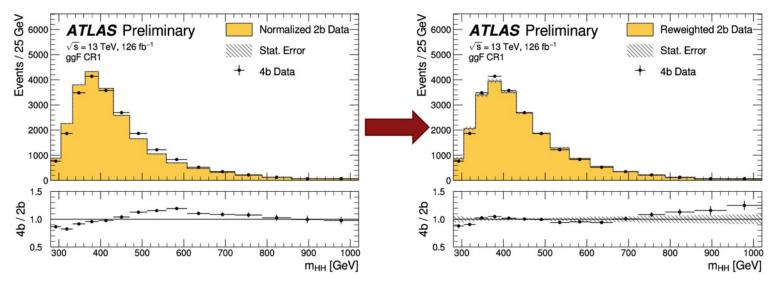
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ABCD excellent playground to test and learn.

 Also on density learning vs OT mapping.





ML FOR AI — I.E. FOR ACTUAL INTELLIGENCE

Large potential and broad applicability

- Detector operation.
- Construct observables.
- Detector designs.
- Model-independent methods vs SM sim. statistics.
- Skirt systematically-affected phase spaces.

• • • •

My take: algorithms can more easily explore outside the box **iff** we manage to write loss functions that can do that. Also, ML is not yet wise.

