

HIP SEMINAR

BACKGROUNI

PRECISION LIMIT?

IN-SITU Systematics

BINNING

CONSEQUENCE

Further Feature

RESULTS

SUMMARY

SOURCES



Profile Likelihood Methods in Top Quark Mass Measurements at the CMS $\,$

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 $25\mathrm{th}$ October, 2022



BACKGROUND

- PRECISION LIMIT?
- IN-SITU Systematics
- BINNING
- Consequence
- Further Features
- RESULTS
- Summary
- Sources

CMS

- **1** BACKGROUND
- **2** PRECISION LIMIT?
- **3** IN-SITU SYSTEMATICS
- **4** BINNING
- **6** CONSEQUENCES
- **6** FURTHER FEATURES
- **7** RESULTS
- **8** SUMMARY

9

Sources



TOP QUARK MEASUREMENTS AT THE LHC

BACKGROUND

- Precision Limit?
- IN-SITU Systematic
- BINNING
- Consequence
- Further Features
- RESULTS
- SUMMARY
- Sources



- At the LHC, direct measurements of the top quark mass (m_t) are the most precise
 - Direct \equiv reconstruction of decay products
 - Indirect \equiv anything else, e.g. based on cross-section
- In Run 2 conditions ($\sqrt{s} = 13 \,\mathrm{TeV}$):
 - Collision events producing a top quark pair are the most frequent $(832 \, \text{fb}^{-1})$
 - Events with a single top quark make a good number 2 $(264 \, \text{fb}^{-1})$



Visualized: the semileptonic top quark pair decay channel



TOP QUARK MEASUREMENTS AT THE LHC

BACKGROUND

- Precision Limit?
- IN-SITU Systematic
- BINNING
- Consequence
- Further Features
- RESULTS
- SUMMARY
- Sources



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DIRECT TOP QUARK MASS MEASUREMENTS

1.582/5

72.73 ± 0.346

 0.6733 ± 0.09427

 γ^2 / ndf

170





- Classical strategy:
 - Intricate parametrized fits on the observables are made against simulation truth values
 - The parameter dependence on e.g. m_t is fit against the **simulation** truth





Constructing A Likelihood

BACKGROUND

- Precision Limit?
- IN-SITU Systematics
- BINNING
- Consequences
- Further Features Results
- Sources



- Using the parametrized fits, a likelihood function for the observables can be constructed
 - This will depend on the chosen parameters
- CMS used to utilize m_t and Jet Scale Factor (JSF)
 - On the right is the CMS lepton+jets and all-jets likelihood combination on the 2016 data
 - The yielded result: $m_t = 172.26 \pm 0.07 (\text{stat}+\text{JSF}) \pm 0.61 (\text{syst}) GeV$
- ATLAS used in addition bJSF during Run1





Constructing A Likelihood

BACKGROUND

- Precision Limit?
- IN-SITU Systematic:
- BINNING
- Consequences
- Further Features Results
- SOURCES



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Constructing A Likelihood

BACKGROUND

- Precision Limit?
- IN-SITU Systematic:
- BINNING
- Consequences
- FURTHER FEATURES RESULTS
- Sources



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HAS THE PRECISION LIMIT BEEN REACHED?

- Background
- Precision Limit?
- IN-SITU Systematics
- BINNING
- Consequenci
- Further Feature
- RESULTS
- SUMMARY
- Sources



- The stat. (+ JSF) errors in the CMS 2016 measurement are vanishing vs. the systematics: 0.07 GeV vs. 0.61 GeV
 - In the classic treatment, the most important systematic error sources cannot typically be reduced by adding statistics
 - Such error sources include e.g. modelling uncertainties (in the simulations)
 - This indicates that adding limitless statistics to the measurement would at best yield an error of $\pm 0.00 (\text{stat+JSF}) \pm 0.61 (\text{syst}) \text{ GeV}$
- As modelling advances, an inverse trend is observed:
 - With better modelling, the number of potential systematic error sources tends to increase
 - With traditional methods, there is always a risk of double-counting and adding statistical noise to each additional error source



Precision Limit?

IN-SITU Systematics

BINNING

Consequenci

FURTHER FEATURE

RESULTS

SUMMARY

Sources



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BACKGROUND

Precision Limit?

IN-SITU Systematics

BINNING

Consequence

Further Feature

RESULTS

SUMMARY

Sources



CM	S Preliminary					36 f	b ⁻¹ (13 Te			
	I + jets 5D: m,	= 171.77 ±	0.38 GeV	pre-fit impacts						
			- pull	post-fit imp	acts∎ θ+ ∆θ	0 -∆θ	MC sta			
JEC flavor bottom		<u> </u>	0.89				0.3			
FSR PS scale X→Xg		→ •→	0.74				0.1			
FSR PS scale q→qg			0.46				0.1			
CR: gluon move			0.34				0.			
CR: QCD inspired			0.35				0.0			
BG W+jets		•	0.76				0.0			
Early resonance decay			0.33				0.0			
BG QCD multijet		<u>→</u> !	0.66				0.0			
JEC abs. MPF bias			0.95				0.0			
Underlying event			0.51				0.0			
ME/PS matching	-		0.48		and and a second second		0.0			
JEC rel. sample			0.90				0.0			
JES Bowler-Lund central			0.82				0.0			
e SFs			0.93				0.0			
bJES Peterson			0.50				0.0			
stat.							0.0			
JEC rel. FSR	_	_	0.97				0.0			
JER ŋ <1.93			0.33				0.0			
JEC abs. scale		_	0.98			1	0.0			
JEC flavor light guarks	-		0.97				0.0			
bJES Bowler-Lund		-	0.86				0.0			
FSR PS scale g→gg		-	1.02				0.0			
Calibration							0.0			
JEC pileup data/MC		_	0.96				0.0			
bJES semilep. B decays			0.96				0.0			
μ SFs		-	0.98				0.0			
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Apparently Not?



- Earlier this year preliminary results on a new measurement on the 2016 data was released:
 - $m_t = 171.77 \pm 0.04 \,(\text{stat}) \pm 0.38 \,(\text{syst}) \,\text{GeV}$
 - The analysis uses a split scheme of Final State Radiation (FSR) uncertainties: light quarks and heavy quarks handled separately
 - With the old FSR definitions one measures $m_t = 172.14 \pm 0.04 \text{ (stat)} \pm 0.31 \text{ (syst) GeV}$

BACKGROUND

Precision Limit?

IN-SITU Systematics

BINNING

Consequence

Further Feature

RESULTS

SUMMARY

Sources



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BACKGROUND

Precision Limit?

IN-SITU Systematics

BINNING

Consequence

Further Feature

RESULTS

SUMMARY

Sources



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					$(\theta - \theta_0)/\Delta \theta$						Δň	۱, [Ge۱

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WHAT HAS CHANGED?

BACKGROUND

Precision Limit?

- IN-SITU Systematics
- BINNING
- Consequences
- FURTHER FEATURES
- RESULTS
- SUMMARY
- Sources



- **1** The reconstructed m_t resonance
- 2 The reconstructed hadronic m_W resonance
- Three new observables were introduced in the new study
 - These include a ratio between b-jet and W jet p_T values, earlier utilized by ATLAS
 - Most importantly, the use of the partial resonance between a b-jet and the charged lepton was added in a phase-space region that was earlier unused
- These updates are still not sufficient for explaining the improvement
 - The missing piece is the introduction of a profile likelihood approach





WHAT HAS CHANGED?

BACKGROUND

Precision Limit?

- IN-SITU Systematic:
- BINNING
- Consequences
- Further Features
- RESULTS
- SUMMARY
- Sources



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WHAT HAS CHANGED?

BACKGROUND

Precision Limit?

- IN-SITU Systematics
- BINNING
- Consequences
- FURTHER FEATURES
- RESULTS
- SUMMARY
- Sources



- Earlier CMS measurements only used two observables, which excelled in a fit on m_t^{gen} and JSF
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BACKGROUND

Precisio Limit?

IN-SITU Systematics

BINNING

Consequence

FURTHER FEATURES RESULTS SUMMARY



A "Simple" In-Situ Measurement: JSF



- In the earlier iterations, the JSF **nuisance parameter** is measured in association to m_t in an *in-situ* manner
 - Measuring the additional dependence is possible, as the m_W distribution is present in the full likelihood
 - This allows reducing the jet calibration systematics

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More Nuisance Parameters



- LIMIT?
- IN-SITU Systematics
- BINNING
- CONSEQUENCE
- FURTHER FEATURES RESULTS SUMMARY SOURCES
- Could we do the same thing more comprehensively, making nuisance parameters from all systematic error sources?







A GENERALIZED IN-SITU MEASUREMENT

BACKGROUND

- PRECISION LIMIT?
- IN-SITU Systematics
- BINNING
- CONSEQUENC
- Further Features
- RESULTS
- SUMMARY
- Sources



- There is no fundamental obstacle for interpreting the systematic variations similarly as JSF variations
 - This is exactly what is done in the new CMS m_t analysis on the 2016 Data with a profile likelihood method
 - In practice this requires a higher level of automation
 - In a final analysis there can easily exist more than 100 systematic uncertainties
- In consequence, the auxiliary JSF parameter becomes unnecessary:
 - This task is already covered by the Jet Energy Uncertainties
- Systematic uncertainties are in general modelled with variations on the central simulated samples
 - This includes two-sided variations, interpreted as the corresponding $\pm \sigma$ uncertainties
 - ... and one-sided variations, which are interpreted as $+\sigma$ uncertainties



BACKGROUND

PRECISION LIMIT?

IN-SITU Systematics

BINNING

CONSEQUENCE

FURTHER FEATURES RESULTS SUMMARY

Sources



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BACKGROUND

PRECISION LIMIT?

IN-SITU Systematics

BINNING

Consequence

Further Features

RESULTS

Summary



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Systematics in the Likelihood

- In the old CMS analyses the best results were found with the **hybrid method**:
 - Here, a physically motivated Gaussian prior was imposed on the value of JSF
 - In the profile likelihood approach the systematics are interpreted as nuisance parameters θ_k
 - The $\pm \sigma$ variations are defined to correspond to the values $\theta_k = \pm 1$
 - The knowledge that the variations are the $\pm \sigma$ uncertainties is enforced by a Gaussian prior \mathcal{G} on all of the nuisance parameters θ_k
 - Similar Gaussian priors are also set on the normalization scales (η_j) of the simulated samples, according to the cross-section and luminosity uncertainties
 - In summary, starting from the likelihood without priors (\mathcal{L}_0) , the full likelihood stands as:

$$\mathcal{L} = \mathcal{L}_0 \times \prod_{k \in \text{nuisances}} \mathcal{G}(\theta_k) \times \prod_{j \in \text{samples}} \mathcal{G}(\eta_j).$$
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Background

Precision Limit?

IN-SITU Systematics

BINNING

Consequences

Further Feature

RESULTS

SUMMARY

Sources





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- Precisio Limit?
- IN-SITU Systematic
- BINNING
- Consequences
- FURTHER FEATURES
- RESULTS
- SUMMARY
- Sources



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PARAMETER AUTOMATIZATION?



- The automatization ends up being a major issue in the practical implementation
 - One method for tackling the issue is using a binned likelihood model
 - Here, the only parameters are the bin edges, and the only variables to fit the bin event counts
 - Each bin forms its own Poisson counting experiment

The 2016 CMS m_t analysis started with the 5 observables being handled by fit functions, but ended up handling 4/5 observables with binning (left)



PARAMETER AUTOMATIZATION?



- Precision Limit?
- IN-SITU Systematic:
- BINNING
- Consequence
- Further Features Results Summary
- Sources





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HIP Seminar



Considerations for a Binned Analysis

- BACKGROUND
- Precision Limit?
- IN-SITU Systematic
- BINNING
- Consequence
- Further Features Results
- GUMMARI
- Sources



- Maybe counter-intuitively, the binned approach is the most robust choice
 - Parametrized fit functions are notoriously volatile, even with a very good function
 - In contrast, a binned analysis derives its robustness from the simplicity of Poisson statistics
 - The CMS 2017–2018 m_t analysis uses the same 5 observables as the 2016 analysis, but all with a binned approach
 - This will be further handled in my thesis defence in Chemicum A129 on 22nd November, 1 pm



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- BACKGROUND
- PRECISION LIMIT?
- IN-SITU Systematic
- BINNING
- Consequences
- FURTHER FEATURES RESULTS SUMMARY
- Sources



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A BINNED LIKELIHOOD

- BACKGROUND
- PRECISION LIMIT?
- IN-SITU Systematics
- BINNING
- Consequence
- FURTHER
- RESULTS
- SUMMARY
- Sources



For a fully binned analysis the core likelihood in Eq. (1) can be expressed as:

$$\mathcal{L}_{0} = \prod_{i \in \text{bins}} \mathcal{P}\left(n_{i} \Big| \sum_{j \in \text{samples}} \left(1 + \kappa_{j}\right)^{\eta_{j}} \times \nu_{i}^{j}\left(\vec{\theta}, m_{t}\right)\right)$$
(2)

- $\mathcal{P}(n_i|\lambda)$ is the Poisson probability distribution for the (bin) event yield n_i
- ν_i^j the expected event yield for the simulated sample j in the bin i
- $\vec{\theta}$ collects the nuisance parameters
- κ_j is the fraction of normalization uncertainty for the sample j, controlled by the nuisance parameter η_j .
- As a reminder, Eq. (1) stands as

$$\mathcal{L} = \mathcal{L}_0 imes \prod_{k=1}^{n} \mathcal{G}\left(heta_k
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A BINNED LIKELIHOOD

- BACKGROUND
- Precision Limit?
- IN-SITU Systematics
- BINNING
- Consequence
- FURTHER
- RESULTS
- Summary
- Sources



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BACKGROUND

- Precision Limit?
- IN-SITU Systematics

BINNING

- Consequence
- FURTHER FEATURES RESULTS
- SUMMARY
- Sources



For a binned approach, interpolation between the central simulation sample and the variations is achieved through histogram morphing techniques

INTERPOLATION?



Visualization of bin-by-bin linear interpolation of distribution





Morphing Strategies

BACKGROUND

Precision Limit?

IN-SITU Systematics

Binning

- Consequence
- FURTHER FEATURES RESULTS SUMMARY
- Sources



- The two main classes of histogram morphing are vertical morphing (see previous slide) and horizontal morphing
 - Vertical morphing (seen on the previous slide) is relatively simple: each bin is considered separately
 - Horizontal morphing can be implemented with various algorithms, and it usually considers both bin migration and vertical effects
- Vertical morphing is preferred by its simplicity:
 - No migration between bins, so each bin receives its own parameters
 - The morphing parameters are easy to determine automatically
 - Typically a smooth interpolation function is utilized
 - The parametrization of each nuisance for each bin can be parametrized either
 - as a multiplicative factor (more common) or ...
 - as a direct offset



Morphing Strategies

BACKGROUND

Precision Limit?

IN-SITU Systematics

BINNING

Consequence

FURTHER FEATURES RESULTS SUMMARY



- The two main classes of histogram morphing are vertical morphing (see previous slide) and horizontal morphing
 - Vertical morphing (seen on the previous slide) is relatively simple: each bin is considered separately
 - Horizontal morphing can be implemented with various algorithms, and it usually considers both bin migration and vertical effects
- Vertical morphing is preferred by its simplicity:
 - No migration between bins, so each bin receives its own parameters
 - The morphing parameters are easy to determine automatically
 - Typically a smooth interpolation function is utilized
 - The parametrization of each nuisance for each bin can be parametrized either ...
 - as a multiplicative factor (more common) or ...
 - as a direct offset



Morphing Strategies

BACKGROUND

Precision Limit?

IN-SITU Systematics

BINNING

Consequence

FURTHER FEATURES RESULTS SUMMARY



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BACKGROUND

PRECISION LIMIT?

IN-SITU Systematics

BINNING

Consequenci

Further Features Results Summary

Sources



Even if vertical morphing is preferable, horizontal morphing becomes necessary when the variations are too big

VERTICAL VS. HORIZONTAL MORPHING

Limitations of piece-wise linear interpolation

- Bin-by-bin interpolation looks spectacularly easy and simple, but be aware of its limitations
 - Same example, but with larger 'mean shift' between templates







Wouter Verkerke, NIKHEF



HIP Seminar



Determination of a Good Binning

BACKGROUND

Precision Limit?

In-situ Systematic

BINNING

Consequence

Further Features

RESULTS

SUMMARY

Sources



• Strict rules follow from the preference of vertical morphing:

- **Bins must be wide enough**, so that the variations impose relatively small changes in bin contents
- Simultaneously the bins should be **narrow enough** to provide resolution to measure the problem at hand

Different problems may prefer different solutions:

- A "bump hunt" is best done on an evenly spaced binning on the mass axis
- A precision measurement (such as that of m_t) is best performed with bins with even statistics
HIP Seminar



Determination of a Good Binning

BACKGROUND

Precision Limit?

IN-SITU Systematic

BINNING

Consequences

Further Features Results Summary

Sources



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WHAT IS THIS ALL GOOD FOR?

BACKGROUND

Precision Limit?

IN-SITU Systematic

BINNING

Consequences

Further Features Results Summary Sources



Nomenclature:

- There can be one or more **unconstrained Parameters of Interest**
- For us, there is only one: $\mathbf{m_t}$
- This is in contrast to the nuisance parameters $\vec{\theta}$ with Gaussian constraints

We can define the following **profile likelihood ratio**:

$$\lambda(m_t) = \frac{\mathcal{L}\left(m_t, \hat{\vec{\theta}}_{m_t}\right)}{\mathcal{L}\left(\hat{m}_t, \hat{\vec{\theta}}\right)} \tag{3}$$

- Here, \$\vec{\theta}\$ is the global maximum likelihood solution for the nuisance parameters
 And \$\vec{\theta}\$ m_t the solution at \$m_t\$
- According to Wilks' theorem $-2 \ln \lambda(m_t)$ asymptotically approaches the χ^2 distribution at good statistics (error $\mathcal{O}\left(\frac{1}{\sqrt{n}}\right)$ for the 1D profile)



WHAT IS THIS ALL GOOD FOR?

BACKGROUND

Nomenclature:

Precision Limit?

IN-SITU Systematic

BINNING

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WHAT IS THIS ALL GOOD FOR?

BACKGROUND

- Precision Limit?
- IN-SITU Systematic
- BINNING

Consequences

FURTHER FEATURES RESULTS SUMMARY SOURCES



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NUISANCE PARAMETER CONSTRAINTS

- Precision Limit?
- IN-SITU Systematics
- BINNING
- Consequences
- FURTHER FEATURES RESULTS SUMMARY

- The *a priori* $\pm \sigma$ uncertainties correspond to the index *k* nuisance parameter values $\theta_k = \pm 1$
- Considering the full likelihood function, the nuisance parameter can be constrained *a posteriori* to a smaller uncertainty
 - This can be understood through applying Wilks' theorem to the nuisance
 - The nuisance parameter $\pm \sigma$ (*a posteriori*) limits are found at $-2 \ln \lambda(\theta_k) = 1$
 - Here, $\lambda(\theta_k)$ is understood in analogy to $\lambda(m_t)$ i.e. all parameters but θ_k being fixed at the maximum likelihood values
- On the next two slides an example borrowed from Ref. 4 is presented





NUISANCE PARAMETER CONSTRAINTS

- Precision Limit?
- IN-SITU Systematics
- BINNING
- Consequences
- Further Features Results Summary
- Sources



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- Precision Limit?
- IN-SITU Systematic:
- BINNING
- Consequences
- FURTHER FEATURES RESULTS SUMMARY
- Sources



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NUISANCE PARAMETER CONSTRAINTS

BACKGROUND

- Precision Limit?
- IN-SITU Systematic
- BINNING
- Consequences
- FURTHER FEATURES RESULTS SUMMARY
- Sources



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- Precision Limit?
- IN-SITU Systematic:
- BINNING
- Consequences
- FURTHER FEATURES RESULTS
- Sources



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Example: Loose Constraint





• The Parameter of Interest μ is measured aside the Jet Energy Scale (JES) nuisance α , yielding a slight constraint on α from the *a priori* values $\alpha = \pm 1$



EXAMPLE: TIGHT CONSTRAINT





• Here, statistics start to take over, constraining α to ± 0.31 , bringing down also the uncertainty on μ



WHICH NUISANCES CAN BE CONSTRAINED

BACKGROUND

Precision Limit?

IN-SITU Systematic:

BINNING

Consequences

FURTHER FEATURES

RESULTS

SUMMARY

Sources



It is important to emphasize that the systematics that can be constrained usually have an experimental connection

- This includes e.g. the energy scales of jets and charged leptons
- ... and jet flavor tagging (mainly b-jets)

But also the choices in the simulation are uncertain and (maybe less obviously) connected to the experiment:

- Parton Showers (Initial and Final State Radiation)
- Parton Density Functions
- Hadronization
- Underlying event



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BACKGROUND

Precision Limit?

IN-SITU Systematics

BINNING

Consequences

Further Features

RESULTS

SUMMARY

Sources



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NUISANCE PARAMETER IMPACTS

BACKGROUND

- Precision Limit?
- IN-SITU Systematics
- Binning
- Consequences
- FURTHER FEATURES RESULTS

- The uncertainty δm_t imposed by the index k nuisance θ_k on the parameter of interest (m_t) is called the **impact** of θ_k on m_t
- The impacts are found in a few steps
 - First fitting all the nuisance parameters and the parameter of interest
 - Then, fixing θ_k to +1 and -1, are then fitting on all the other parameters
 - The difference in the value of the parameter of interest is the impact





The same approach works both on the *a priori* nuisance limits $\theta_k = \pm 1$ and the possibly constrained *a posteriori* limits $\theta_k = \pm \sigma_{\text{posteriori}}$, where $|\sigma_{\text{posteriori}}| < 1$



NUISANCE PARAMETER IMPACTS

BACKGROUND

- Precision Limit?
- IN-SITU Systematics
- BINNING
- Consequences
- FURTHER FEATURES
- Councilla

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NUISANCE PARAMETER IMPACTS

- Precision Limit?
- IN-SITU Systematics
- BINNING
- Consequences
- Further Features
- RESULTS
- SUMMARY
- Sources



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NUISANCE PARAMETER IMPACTS

- Precision Limit?
- IN-SITU Systematic:
- BINNING
- Consequences
- Further Features
- RESULTS
- SUMMARY
- Sources



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NUISANCE PARAMETER IMPACTS

BACKGROUND

- Precision Limit?
- IN-SITU Systematics
- BINNING
- Consequences
- Further Features
- RESULTS
- SUMMARY
- Sources



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NUISANCE PARAMETER IMPACTS

- Precision Limit?
- IN-SITU Systematic:
- BINNING
- Consequences
- Further Features
- RESULTS
- SUMMARY
- Sources



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NUISANCE PARAMETER PULLS



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- Impacts an pulls can be **blinded or** .

CM	S Prelimir	nary								36 ft	o ⁻¹ (13	TeV)
[I + jets	5D: m,	= 171.7	77 ± 0	.38 GeV	pre-fit	impa	cts 🔲	}+∆ 0	∂- ∆θ		
					+ pull	post-fi	t imp	acts	}+ ∆θ	θ- Δθ	МС	stat.
JEC flavor bottom					0.89							0.20
FSR PS scale X→Xg					0.74							0.14
FSR PS scale q→qg	-	•			0.46							0.14
CR: gluon move			-	•	0.34							0.11
CR: QCD inspired					0.35							0.09
BG W+jets		-	•		0.76							0.09
Early resonance decay					0.33							0.09
BG QCD multijet					0.66							0.08
JEC abs. MPF bias		—			0.95							0.08
Underlying event				-	0.51							0.07
ME/PS matching			•		0.48							0.06
JEC rel. sample			•	-	0.90							0.05
JES Bowler-Lund central		-	•		0.82							0.05
e SFs			•		0.93							0.05
bJES Peterson			- • - •		0.50							0.05
stat.												0.04
JEC rel. FSR		-	-	-	0.97							0.04
JER n_ <1.93		-			0.33							0.04
JEC abs. scale		<u> </u>	+	-	0.98							0.04
JEC flavor light quarks		-			0.97							0.04
bJES Bowler-Lund		-	•	•	0.86							0.04
FSR PS scale g→gg		-		-	1.02							0.04
Calibration												0.03
JEC pileup data/MC		-	+	-	0.96							0.03
bJES semilep. B decays			•		0.96							0.03
μ SFs					0.98							0.03
	-2	-1	0	1	2 (θ̂-θ ₀)/Δθ	-0.3	-0.2	-0.1	0	0.1	0.2 ∆m _t).3 [GeV]

26/34

NUISANCE PARAMETER PULLS



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26/34

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NUISANCE PARAMETER PULLS

- Background
- Precision Limit?
- In-situ Systematic
- BINNING
- Consequences
- FURTHER FEATURES
- RESULTS
- SUMMARY
- Source



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• In the unblinded case notable pulls can appear but they are expected to be less than a unity (one sigma) 26/34



STATISTICAL UNCERTAINTIES

- BACKGROUND
- Precision Limit?
- IN-SITU Systematics
- BINNING
- Consequences
- FURTHER FEATURES
- SUMMARY
- Sources



- When estimating the expected number of events in a bin, the **statistical uncertainties are also a kind of modelling uncertainty:**
 - This means that every simulated sample in each bin should receive their statistical nuisance parameter
 - At low statistics they follow the Poisson distribution, which converges to a Gaussian at large statistics
 - If around 10 simulated samples are combined, the number of parameters quickly explodes
- Visualized from Ref. 4: Atlas Higgs combination model (23.000 functions, 1600 parameters)
- Partial cure: the **Barlow-Beeston** approach allows the combination of statistical errors from separate samples





STATISTICAL UNCERTAINTIES

- BACKGROUND
- PRECISION LIMIT?
- IN-SITU Systematics
- BINNING
- Consequences
- Further Features
- RESULTS
- SUMMARY
- Sources



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- BACKGROUND
- Precision Limit?
- IN-SITU Systematics
- BINNING
- Consequences
- FURTHER FEATURES
- RESULTS
- Summary
- Sources



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COMBINATION OF SIMULATIONS

- Integrated luminosity $\mathcal L$ is the general measure for the amount of events in a sample
- When simulation and data are compared, each sample should be weighted by:

 $w^{\mathrm{Sim}} = rac{\mathcal{L}^{\mathrm{Data}}}{\mathcal{L}_{\mathrm{Eff}}^{\mathrm{Sim}}} = rac{\sigma^{\mathrm{Sim}}\mathcal{L}^{\mathrm{Dat}}}{N_{\mathrm{Eff}}^{\mathrm{Sim}}}$

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- $N_{\rm Eff}^{\rm Sim}$ is the effective number of events in each simulated sample, considering event weights



28/34





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28/34



STATISTICAL VARIATION UNCERTAINTIES

- There are three common methods for quantifying systematics
 - Reweighting the simulated sample 1 (almost 100% statistical correlation)





STATISTICAL VARIATION UNCERTAINTIES

There are three common methods for

(almost 100% statistical

Reweighting the simulated sample

Rescaling object (e.g. jet) energies

(quite close to 100% statistical

quantifying systematics

correlation)

correlation)

Background

1

0

- Precision Limit?
- In-situ Systematic
- BINNING
- Consequences
- Further Features Results
- Summary
- Sources



- In the third case one should provide separate bin-wise nuisance parameters fo the systematic variation sample
 - This is often a weak point and poorly implemented in the common tools





STATISTICAL VARIATION UNCERTAINTIES

There are three common methods for

(almost 100% statistical

statistical correlation)

Reweighting the simulated sample

Rescaling object (e.g. jet) energies

(quite close to 100% statistical

Separate simulated samples (no

quantifying systematics

correlation)

correlation)

Background

1

0

3

- Precision Limit?
- IN-SITU Systematic:
- BINNING
- Consequences
- FURTHER FEATURES
- RESULTS
- SUMMARY
- Sources



- In the third case one should provide separate bin-wise nuisance parameters for the systematic variation sample
 - This is often a weak point and poorly implemented in the common tools





STATISTICAL VARIATION UNCERTAINTIES

- Background
- Precision Limit?
- IN-SITU Systematic:
- BINNING
- Consequences
- FURTHER FEATURES
- RESULTS
- Summary
- Sources



- There are three common methods for quantifying systematics
 - Reweighting the simulated sample (almost 100% statistical correlation)
 - 2 Rescaling object (e.g. jet) energies (quite close to 100% statistical correlation)
 - Separate simulated samples (no statistical correlation)



- In the third case one should provide separate bin-wise nuisance parameters for the systematic variation sample
 - This is often a weak point and poorly implemented in the common tools



A FINAL LOOK AT THE NEW CMS RESULTS

BACKGROUND

Precision Limit?

- IN-SITU Systematics
- BINNING
- CONSEQUENCE
- FURTHER
- RESULTS
- Summary
- Sources



CM	SPrelim	inary								36	ib⁻¹ (1 3	TeV)
	I + jets	5D: r	n, = 171	.77 ±	0.38 GeV	pre-fit	impa	cts 🔲 🕯	+ ∆θ	0 -∆€	,	
	-		•		+ pull	post-fi	it imp	acts <mark> </mark> 🖗	+ ∆θ	<mark>0</mark> -∆€	МС	stat.
JEC flavor bottom			•		0.89							0.20
FSR PS scale X→Xg					0.74							0.14
FSR PS scale q→qg	ļ	•			0.46							0.14
CR: gluon move			-	•	0.34							0.11
CR: QCD inspired					0.35							0.09
BG W+jets		+			0.76							0.09
Early resonance decay				•	0.33							0.09
BG QCD multijet			•		0.66							0.08
JEC abs. MPF bias		1			0.95							0.08
Underlying event					0.51							0.07
ME/PS matching					0.48							0.06
JEC rel. sample		-			0.90							0.05
bJES Bowler-Lund central		+		-	0.82							0.05
e SFs					0.93							0.05
bJES Peterson					0.50							0.05
stat.												0.04
JEC rel. FSR		-	-		0.97							0.04
JER ŋ <1.93		÷	- 1		0.33							0.04
JEC abs. scale		-		-	0.98							0.04
JEC flavor light quarks				-	0.97							0.04
bJES Bowler-Lund		-	-	- 1	0.86							0.04
FSR PS scale g→gg		-	-		1.02							0.04
Calibration												0.03
JEC pileup data/MC		-	-	_	0.96							0.03
bJES semilep. B decays			-	-	0.96							0.03
μ SFs		-	-	_	0.98							0.03
·	-2	-1	0	1	2	-0.3	-0.2	-0.1	0	0.1	0.2	0.3
					(θ-θ ₀)/Δθ						Δm _t	[GeV]

- In the new 2016 analysis especial quark Final State Radiation (FSR) and Jet Energy Resolution (JER) are constrained to less than ± 0.5
- This is explained by the hadronic W boson resonance
- The constraints are OK, but the notable **pulls** are a point of concern
- Without the constraints, the total error would be around $\pm 0.5 \,\mathrm{GeV}$

WERSTY OF HELSING

A FINAL LOOK AT THE NEW CMS RESULTS

BACKGROUND

Precision Limit?

IN-SITU Systematics

BINNING

CONSEQUENCE

Further Feature

RESULTS

SUMMARY

Sources



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]	I + je	ts 5D	: m, =	: 171.	77 ± ().38 GeV	pre	fit impa	acts 📔	}+ ∆θ	<mark> θ-∆</mark> €	Ð	
						- pull	pos	t-fit imj	oacts	}+ ∆0	 	е 🛛 м	C stat.
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A FINAL LOOK AT THE NEW CMS RESULTS

BACKGROUND

Precision Limit?

- IN-SITU Systematics
- BINNING
- Consequence
- FURTHER
- RESULTS
- SUMMARY
- Sources



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What to expect for 2017-2018



- Precision Limit?
- IN-SITU Systematic:
- BINNING
- Consequences
- FURTHER FEATURES
- RESULTS
- SUMMARY
- Sources



- The number of recorded events is around 3 times larger in 2017–2018 w.r.t. 2016
 - Statistical error for N events is according to Poisson statistics proportional to $1/\sqrt{N}$
 - For systematics that are well constrained by the measured data, one can optimistically expect similar scaling as for statistical errors
 - In consequence, the error scaling factor in 2017–2018 w.r.t. 2016 can go to $1/\sqrt{3}\approx 0.58$
- Other improvements:
 - The method is more stable with a binned with also for m_{t}
 - The 2016 analysis scales away the even yield both in the central simulation and systematic variations
 - With Poisson statistics the (absolute) event yields are an important part of the whole picture, so we see including these as an important improvement

What to expect for 2017-2018



- Precision Limit?
- IN-SITU Systematics
- BINNING
- Consequences
- Further Features
- RESULTS
- SUMMARY
- Sources



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- IN-SITU Systematics
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- Consequences
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- RESULTS
- SUMMARY
- Sources



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- Precision Limit?
- IN-SITU Systematic:
- BINNING
- Consequences
- Further Features
- RESULTS
- SUMMARY
- Sources



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UNVERSITY OF HELSHOE

BACKGROUND

- Precision Limit?
- IN-SITU Systematics
- BINNING
- Consequences
- Further Features
- RESULTS
- Summary
- SOURCES



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HISTORICAL REVIEW

- Precision Limit?
- IN-SITU Systematics
- BINNING
- Consequences
- Further Features
- RESULTS
- SUMMARY
- Sources



- Tools have evolved and gotten more wide-spread
- Slow diffusion from one field of study to another:
 - The early adopters at the LHC were the Higgs hunters, as can be reviewed from this profile likelihood article and this article on CMS/ATLAS methods on Higgs boson searches
 - In the top quark community, the methods first spread to inclusive cross-section measurements, and then to differential cross-section measurements
 - At the final step, also precision measurements (such as the m_t measurement) are taking up the tools





HISTORICAL REVIEW

Background

- Precision Limit?
- IN-SITU Systematics
- BINNING
- Consequences
- Further Features
- RESULTS
- SUMMARY
- Sources

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HISTORICAL REVIEW

- Precision Limit?
- IN-SITU Systematics
- BINNING
- CONSEQUENCES
- FURTHER FEATURES
- RESULTS
- SUMMARY
- Sources



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HISTORICAL REVIEW

- Precision Limit?
- IN-SITU Systematics
- BINNING
- Consequences
- Further Features
- RESULTS
- SUMMARY
- Sources



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- Precision Limit?
- IN-SITU Systematics
- BINNING
- Consequence
- FURTHER FEATURES
- RESULTS
- SUMMARY
- Sources



- In early Run 2 it seemed that the precision limit for such m_t measurements had been reached
 - This is ruled by irreducible (systematic) error sources
- Profile likelihood methods ruled this as a false assumption
 - The systematic errors can be constrained *in-situ* by the measurement
- Interesting future results coming up on the 2017-2018 CMS Run2 data:
 - A first look at these are given in my thesis defence on Tuesday November 22nd 1 pm at Chemicum A129







- Precision Limit?
- IN-SITU Systematics
- BINNING
- Consequence
- FURTHER FEATURES
- RESULTS
- SUMMARY
- Sources



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- IN-SITU Systematics
- BINNING
- Consequence
- Further Features
- RESULTS
- SUMMARY
- Sources



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- Precision Limit?
- IN-SITU Systematics
- BINNING
- Consequence
- Further Features
- RESULTS
- SUMMARY
- Sources



• The most precise m_t measures at the LHC are currently performed on the top quark pair topology, based directly on the top quark decay products

SUMMARY

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- Precision Limit?
- IN-SITU Systematics
- BINNING
- Consequenci
- FURTHER FEATURES RESULTS SUMMARY SOURCES

- These slides can be reached at tinyurl.com/hiphannu
- https://cds.cern.ch/record/2674989
- https://arxiv.org/pdf/1812.10534.pdf
- https://cds.cern.ch/record/2806509/files/TOP-20-008-pas.pdf
- https://www.precision.hep.phy.cam.ac.uk/wp-content/people/mitov/ lectures/GraduateLectures/Advanced-Statistics-Verkerke.pdf

