Unfolding
– Comparison ATLAS/CMS –

LHC TOP WG meeting 14-15 Nov 2019, CERN

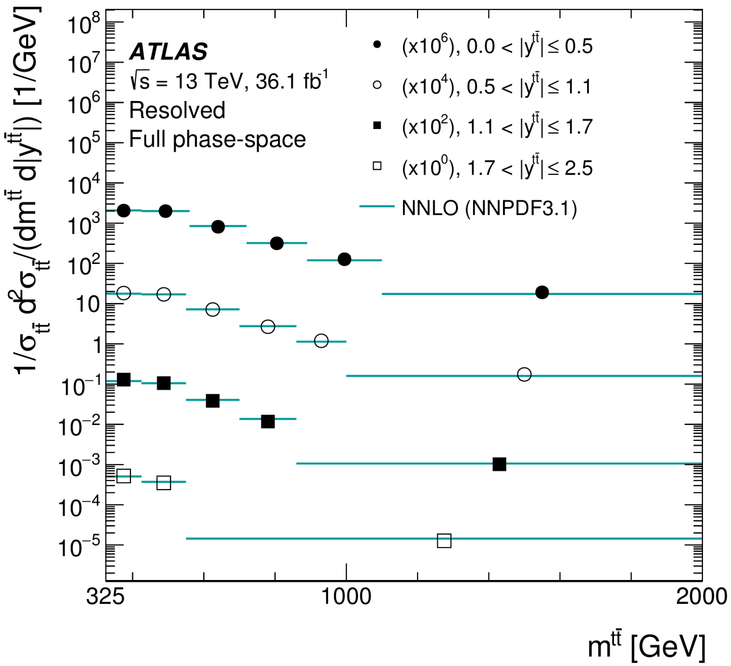
Olaf Behnke (DESY)

Tip: overview talk on unfolding methods in HEP by M. Kuusela

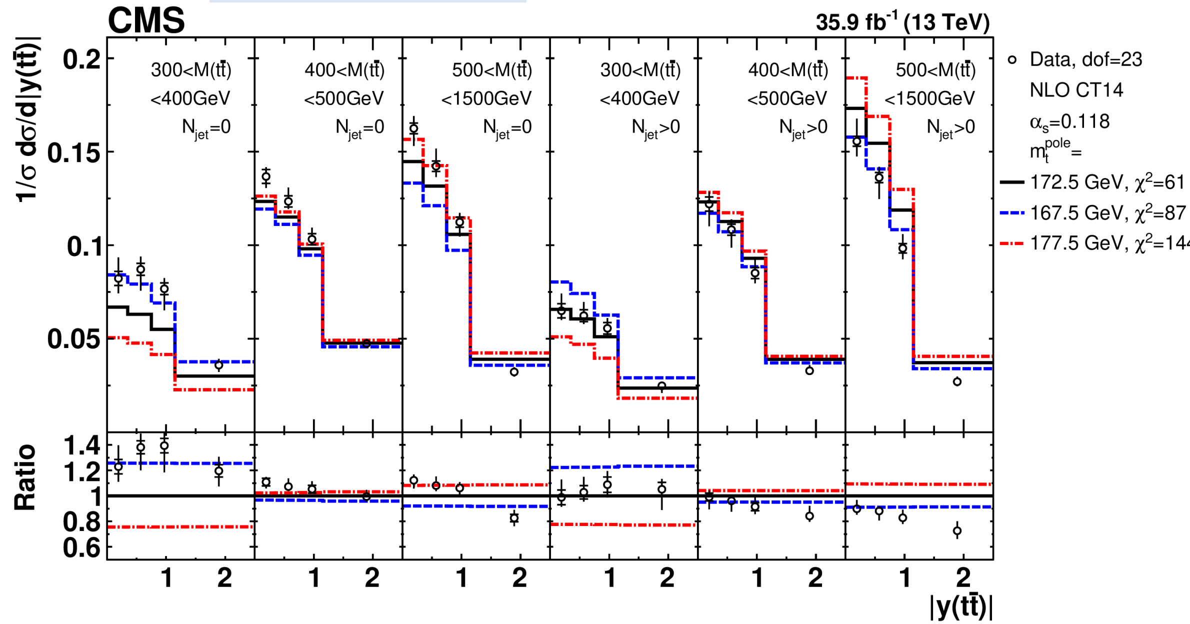
https://indico.desy.de/indico/event/22731/session/5/contribution/24/material/slides/0.pdf

Precision $d\sigma^{tt}/dx$ measurements with 2016 data

Lepton+jet arXiv:1908.07305



Dilepton arXiv:1904.05237



CMS lepton+jet paper: Phys. Rev. D 97, 112003 (2018)

- → Measurements reach few percent uncertainties
- → Highly sensitive to gluon PDF, α_s and m_t
- → Use different statistical tools for detector corrections (=unfolding), lets compare them

Compare $d\sigma^{t\bar{t}}/dx$ measurements

	ATLAS lepton+jets 2015/16, 36 fb^{-1} arXiv:1908.07305	CMS Dilepton 2016, 36 fb^{-1} arXiv:1904.05237
Unfolding Tool	D'Agostini iterative arXiv:1010.0632 via RooUnfold arXiv:1105.1160	TUnfold JINST 7 (2012) T10003
Regularisation	Early stopping after few iterations	Tikhonov curvature
Statistical uncertainties	Pseudo experiments	Error propagation
Model uncertainties	Unfold alternative MCs with nominal MC	Unfold data with alternative MC

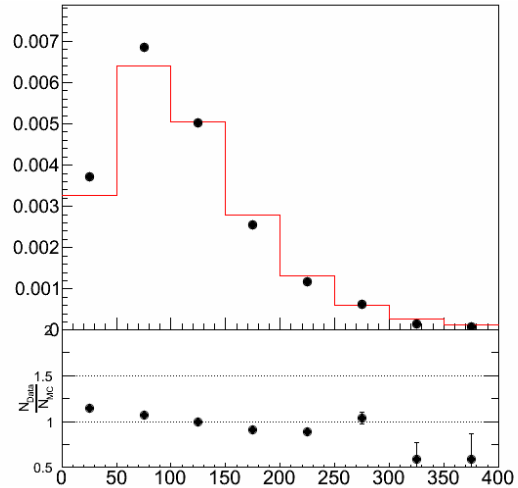
→ Lets take a closer look

Unfolding of λ

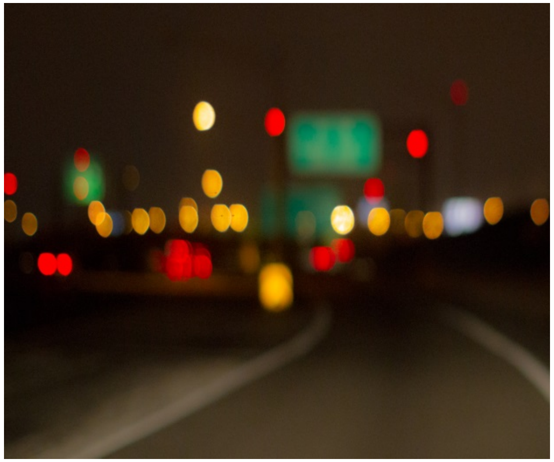
Detector effects + background

Smeared space

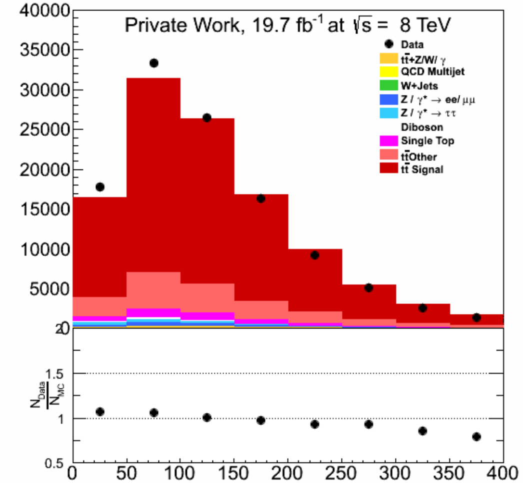
True level



λ



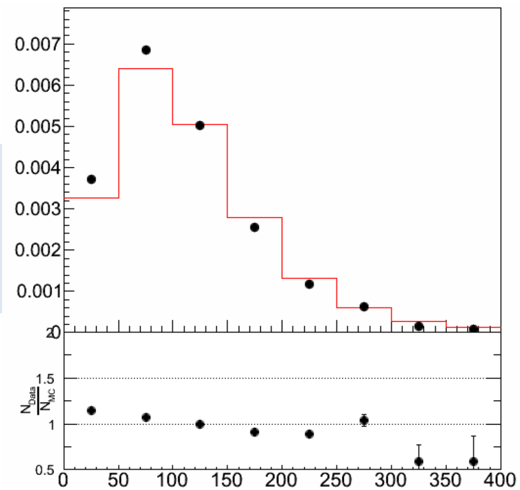
$K\lambda + b$



$y + b$

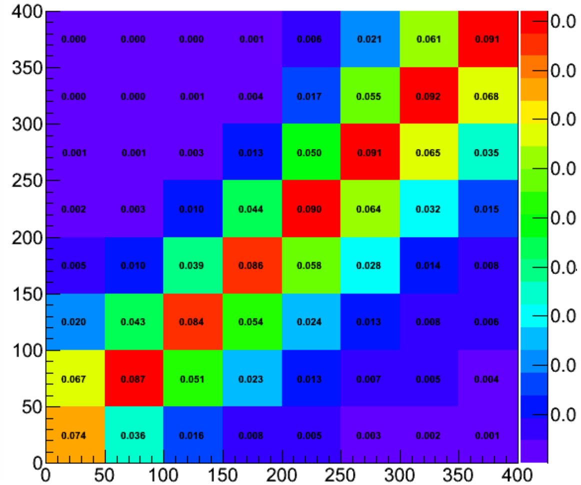
Unfolding of λ

True level



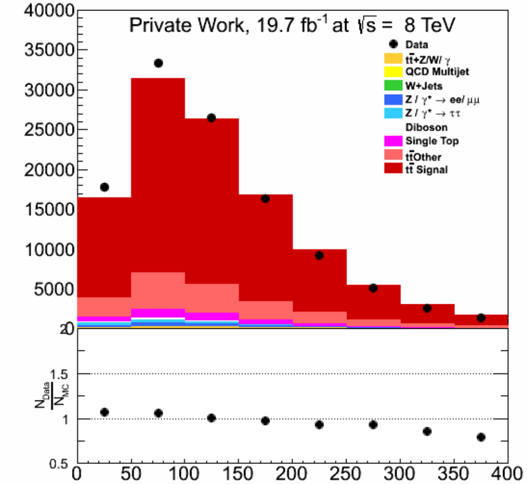
λ

Detector effects + background



Kλ + b

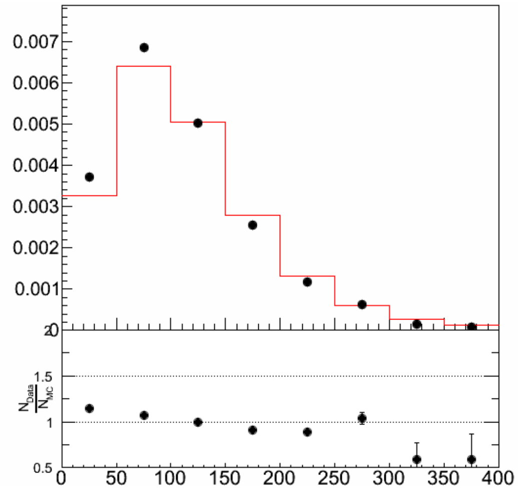
Smeared space



y + b

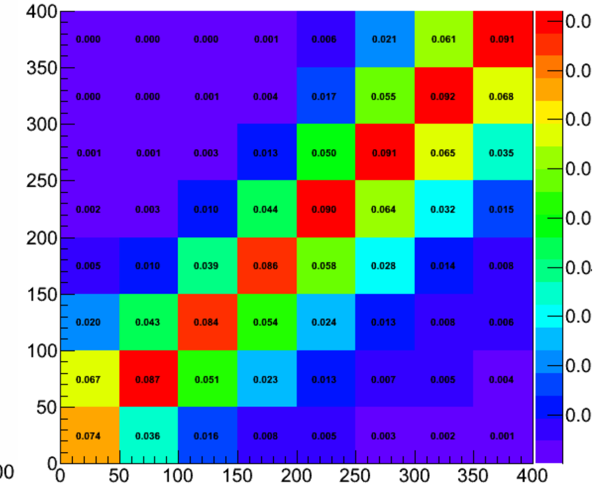
Unfolding of λ

True level



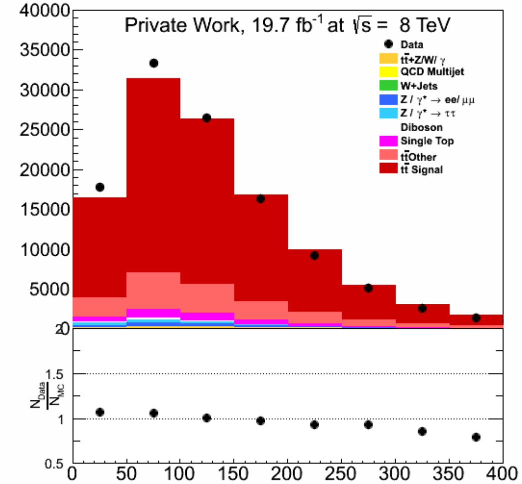
λ

Detector effects + background



Kλ + b

Smeared space



y + b

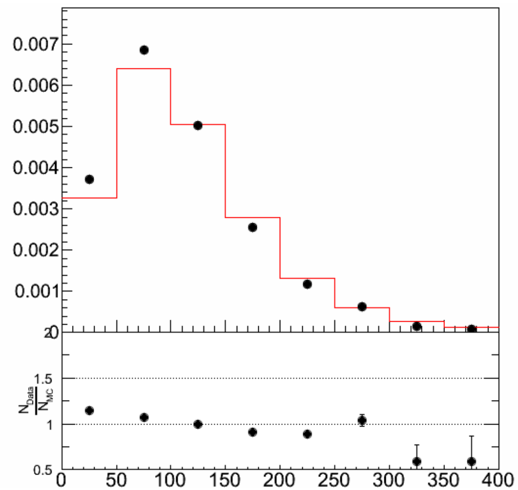
Unfolding means estimating λ from D=y+b

Unfolding of λ

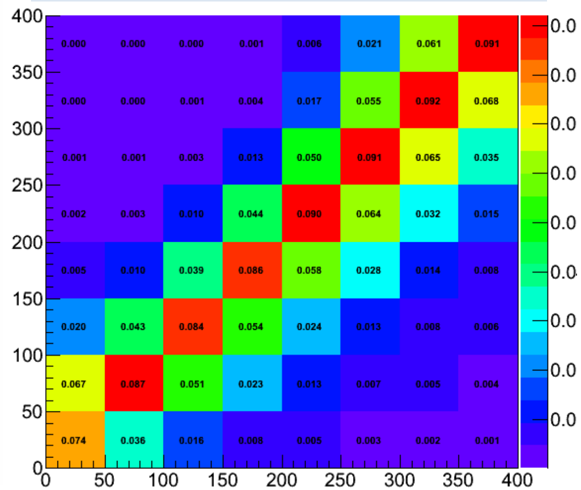
Detector effects + background

Smeared space

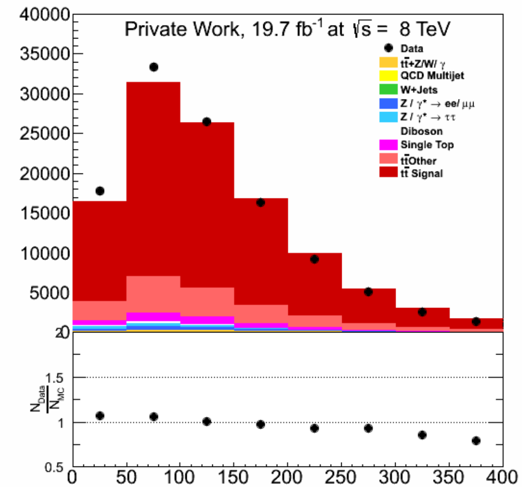
True level



λ



$K\lambda + b$



$y + b$

Max. Likelihood solution gaussian approximation

Same # of λ and y bins: $\lambda = K^{-1} y$

More y bins: minimize $\chi^2 = [\mathbf{y} - \mathbf{K}\lambda]^t \, \mathbf{V_y}^{-1} \, [\mathbf{y} - \mathbf{K}\lambda]$

Often instable high frequency components of unfolded $\lambda \rightarrow$ regularisation

TUnfold:

$$\chi^2 = [\mathbf{y} - \mathbf{K}\lambda]^t \, \mathbf{V_y}^{-1} \, [\mathbf{y} - \mathbf{K}\lambda] \; + \boldsymbol{\tau}^2 ||\mathbf{L}(\lambda - \lambda_\mathbf{0})||^2$$

Bias vector

Regularisation strength

Matrix: unity, 1st or 2nd derivatives

Regularisation strength criterion

should use objective criteria such as Akaike information, Cross validation and numerous others

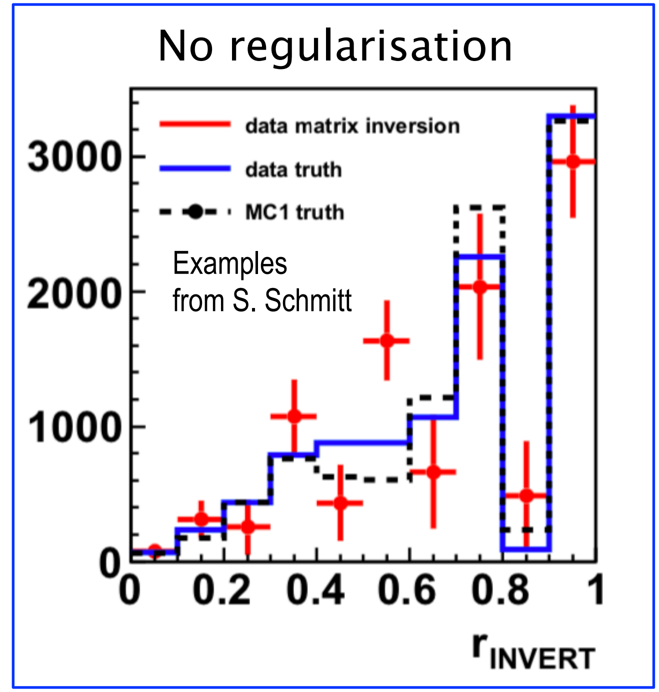
TUnfold:

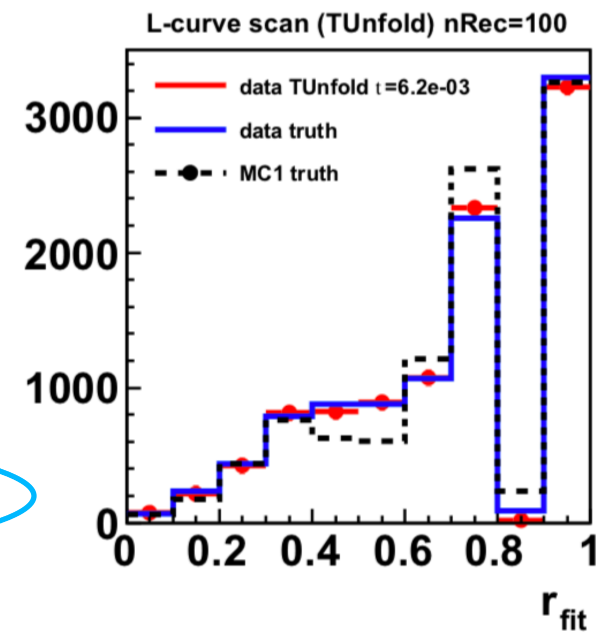
$$\chi^2 = [\mathbf{y} - \mathbf{K}\lambda]^t \mathbf{V_y}^{-1} [\mathbf{y} - \mathbf{K}\lambda] \; + \boldsymbol{\tau}^2 ||\mathbf{L}(\lambda - \lambda_0)||^2$$

Two criteria available for choosing $\boldsymbol{\tau}$:

1. L-curve: balancing the two χ^2 terms - - - - - - →
2. Minimizing average global correlation

Do we really always need regularisation?





https://indico.desy.de/indico/event/9288/contribution/9/material/slides/0.pdf

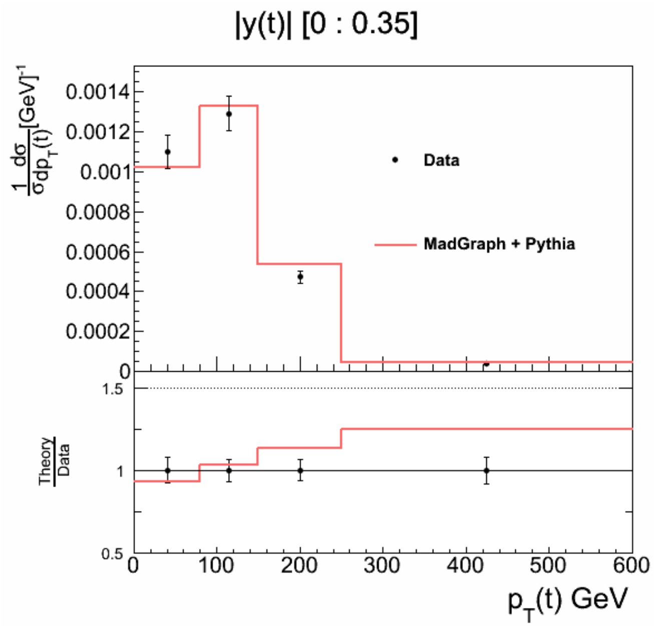
Unfolding without regularisation

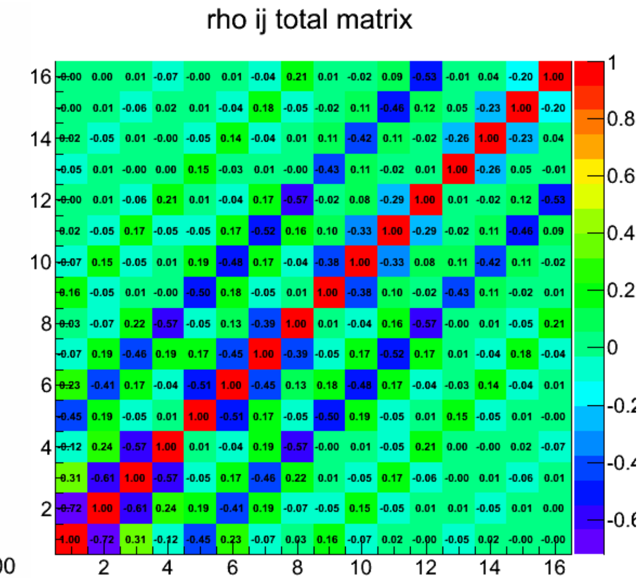
CMS: $d\sigma^{tt}(p_T(t),y(t))$

PhD thesis
I. Korol, DESY
Uni Hamburg

$p_T(t)$ vs $y(t)$

$\tau = 0$





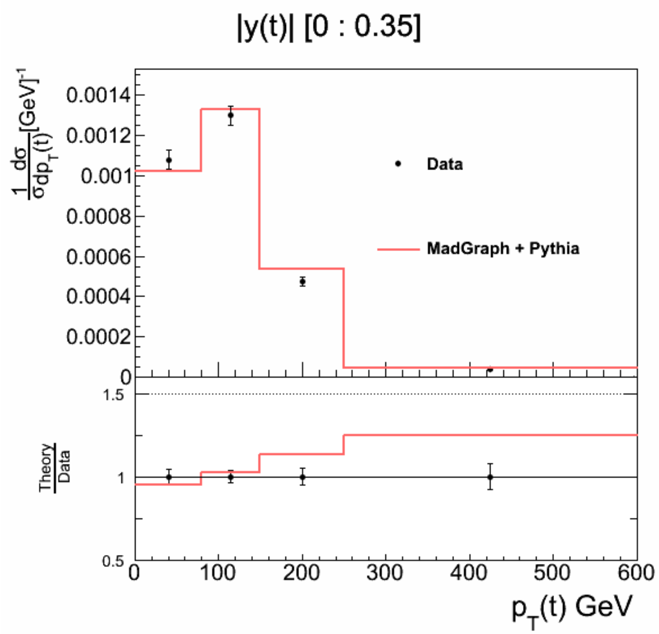
$$\rho_{ij} = \frac{V_{ij}}{\sqrt{V_{ii}V_{jj}}}$$

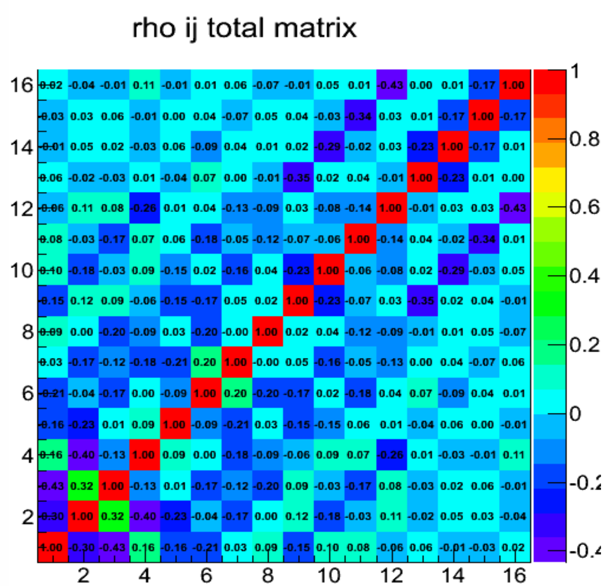
with V = covariance matrix from unfolding

→ Looks ok

$\tau = 0.0006$ from min. global correlation

$$\sum_i \sqrt{1 - \frac{1}{V_{ii}V^{-1}_{ii}}}$$





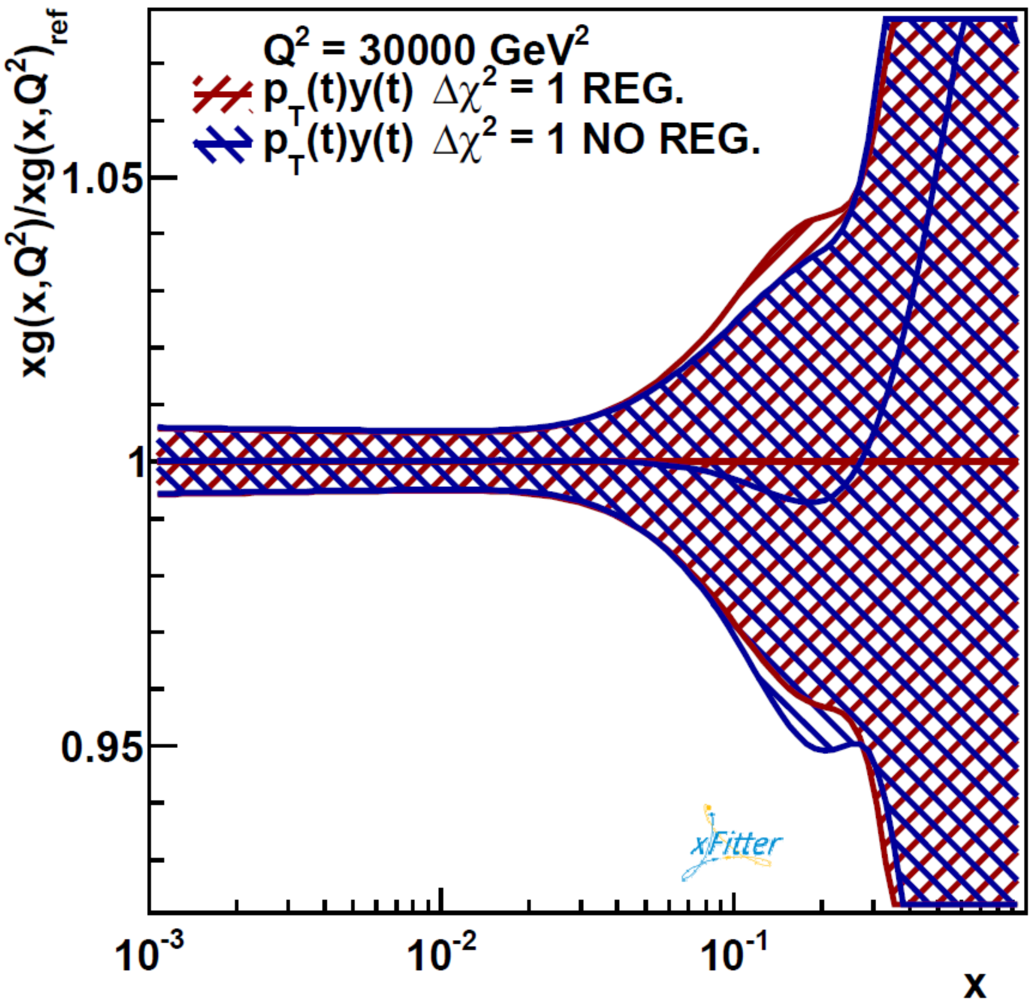
→ Correl. spread out

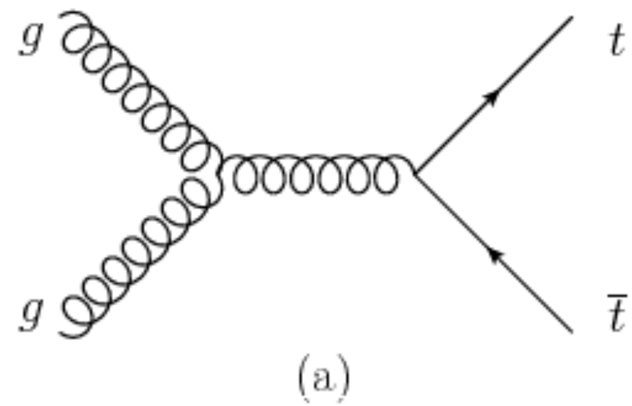
CMS Results published in EPJC 77 (2017) 459

Regularisation effect →final PDF fit

PhD thesis I. Korol, DESY Uni Hamburg
+ private work Oleksandr Zenaiev

Add $d\sigma^{tt}(m_{tt}, y_{tt})$ to proton PDF fit → constrain g(x) at high x





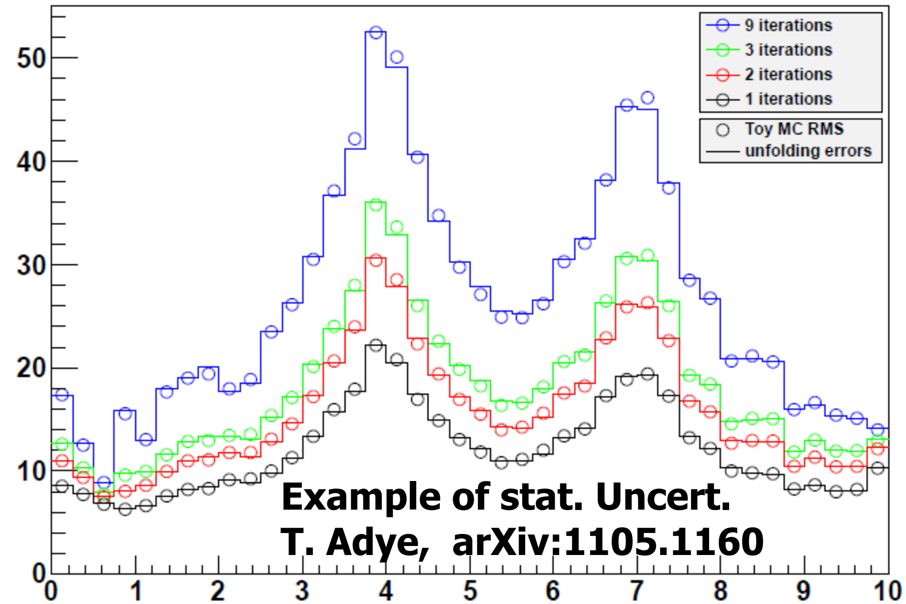
→ rather small effect

D'Agostini iterative unfolding arXiv:1010.0632

iteration index

$$\lambda_j^{(k+1)} = \frac{\lambda_j^{(k)}}{\sum_{i=1}^{n} K_{ij}} \sum_{i=1}^{n} \frac{K_{ij} y_i}{\sum_{l=1}^{p} K_{il} \lambda_l^{(k)}}, \quad j = 1, \ldots, p$$

- Biased towards $\lambda_j^{(0)}$ = Signal MC, inheriting lack of high frequencies
- Converges slowly to unregularized max. likelihood estimation
- Statistical uncertainties attractively small but grow with k (as bias ↘)
- When to stop iteration? (Default in RooUnfold: 4) Need to tune for each analysis! **Some analysis "It was found that after 80 iterations the unfolding bias is small enough as well as the Poisson-induced stat. fluctuations do not yet contribute."**

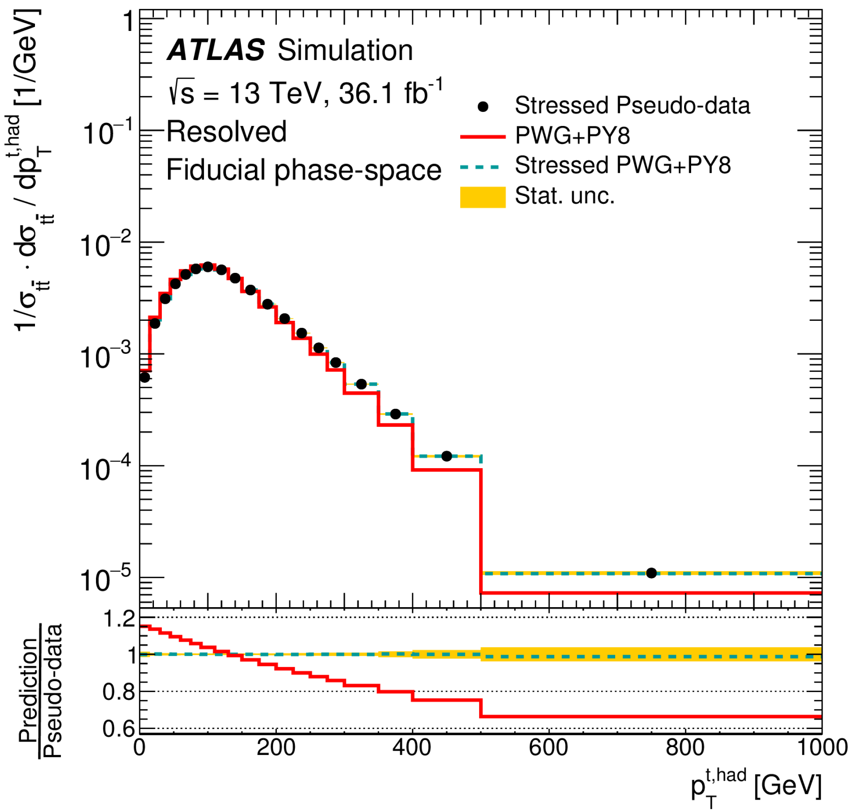


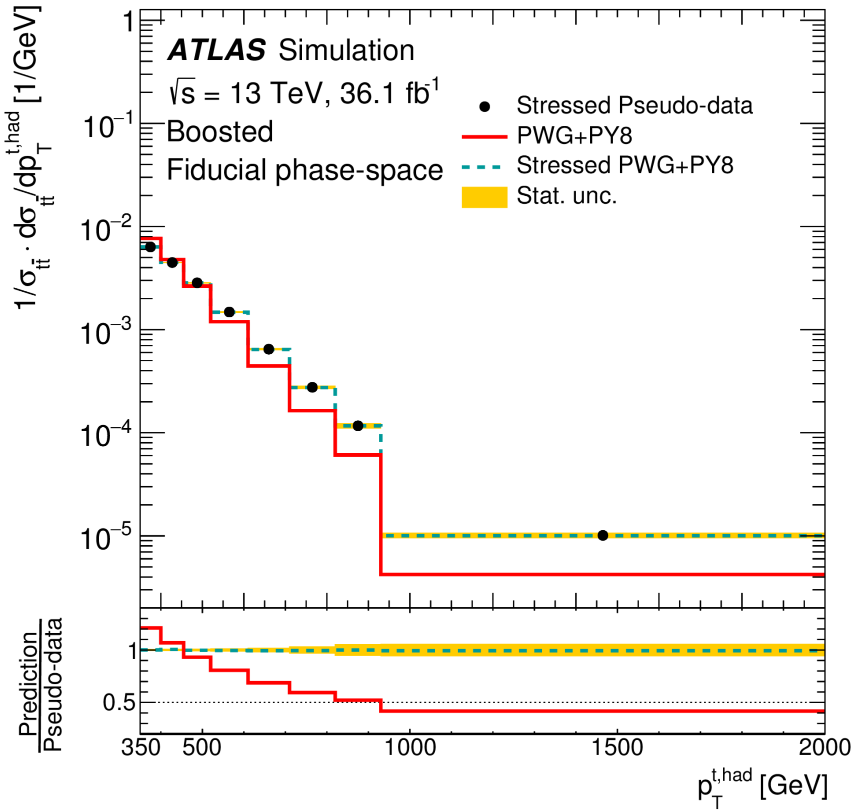
Example of stat. Uncert.
T. Adye, arXiv:1105.1160

How can we check/control biases? → See following slides

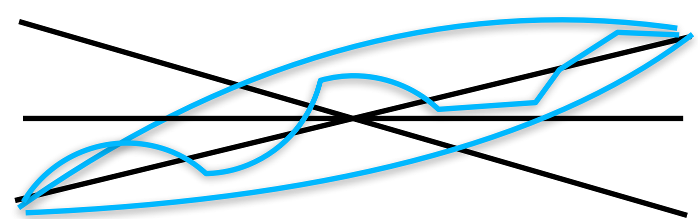
ATLAS lepton+jets: *Stress tests*

Unfold MC $p_T^{t,had}$ spectra, reweighted by straight line





🙂 Stressed spectra recovered within uncertainties
→ How far should one stress?

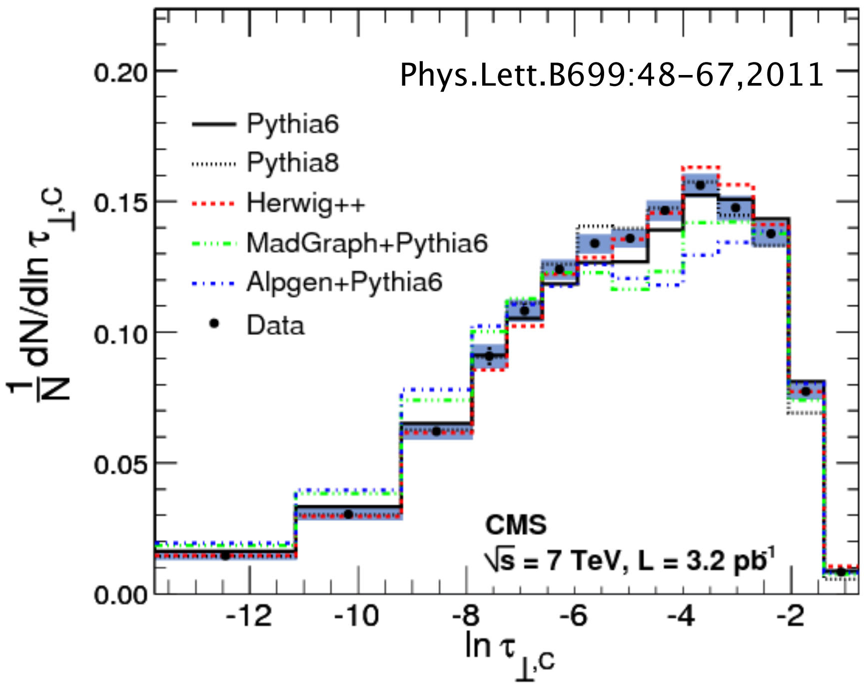


Bottomline test

Idea: Comparing theory models to unfolded data should NOT be more discriminative than comparing folded theories to detector data

→ assess with data-model χ^2 tests at both levels (stat. uncert. only)

Hadronic event shape analysis example with SVD unfolding



Material from talk M. Weber, PHYSTAT 2011

MC Generator	χ^2 values between data and smeared mc	χ^2 values between unfolded data and Gen mc
PYTHIA6	421	398
HERWIG++	211	200
MADGRAPH	2590	2570
ALPGEN	3860	3860

➡ Chi2 order is the same before and after unfolding, values are similar

🙂 No sign of too strong regularisation in this example

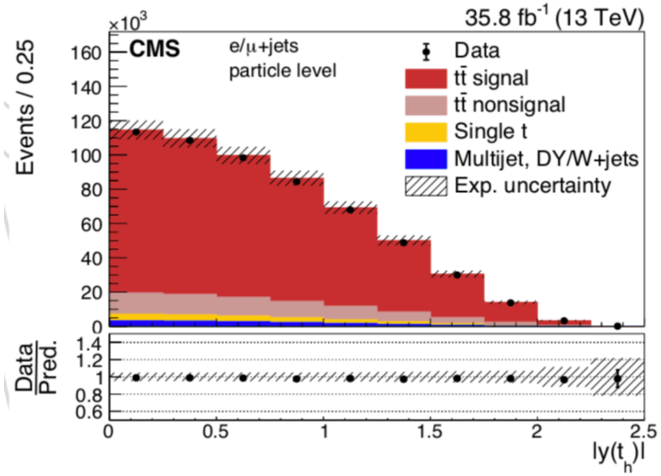
Bottomline test in CMS lepton+jets tt analysis

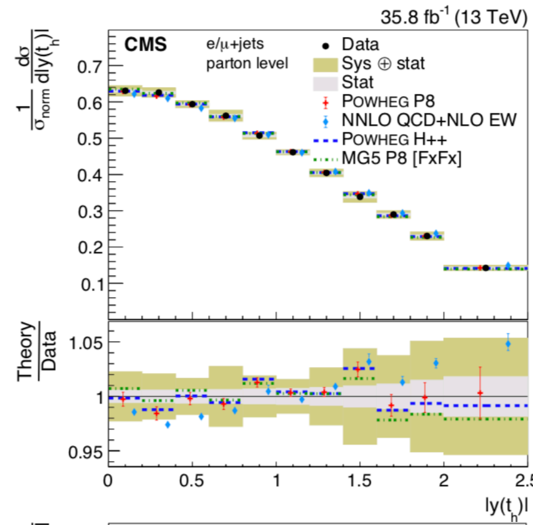
D’Agostini unfolding

y(t) at det. level

y(t) unfolded to parton level

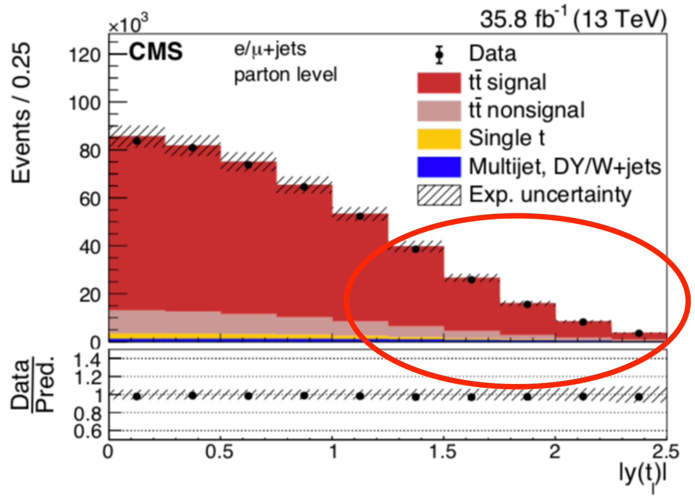
t → bjj’

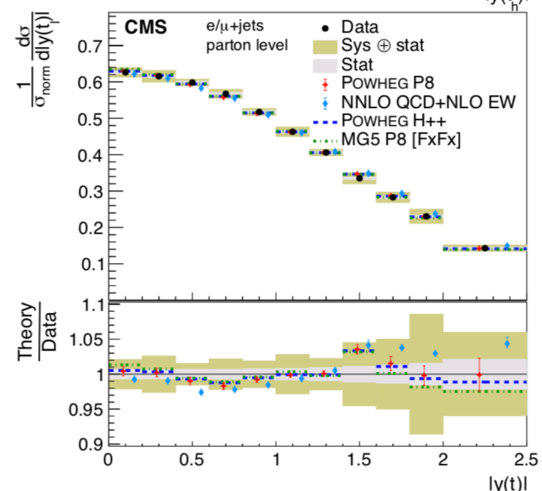




Need ~ 5 iterations to have $\chi^2_{\text{data-models}}$ similar at both levels

t → blν





Need ~ 50 iterations to have $\chi^2_{\text{data-models}}$ similar at both levels

Phys. Rev. D 97, 112003 (2018)

→ Number of needed iterations depend on bin-size/resolution
→ Don’t use blindly the RooUnfold default of 4 iterations

Statistical uncertainties

ATLAS Lepton+jet

- using sampling techniques (pseudo experiments)
- for data, signal and background MCs

+ Flexible, can also handle correlations between different unfolded spectra

CMS Dilepton

- using TUnfold errorpropagation
- for data, signal and background MCs

+ Fast

Generator model uncertainties of response matrix

ATLAS Lepton+jet

- Unfold alternative Signal MCs using the nominal MC for detector corrections (fixed response matrix)

+ Avoid effects from data statistical fluctuations

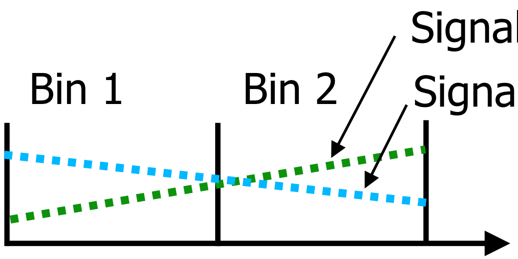
− Assume signal MC ≅ signal data

CMS Dilepton

- Unfold data with using alternative Signal MCs for detector corrections (varied response matrices)

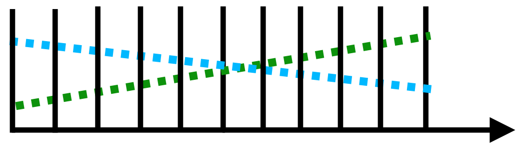
Wide bins and model systematics

M. Kuusela

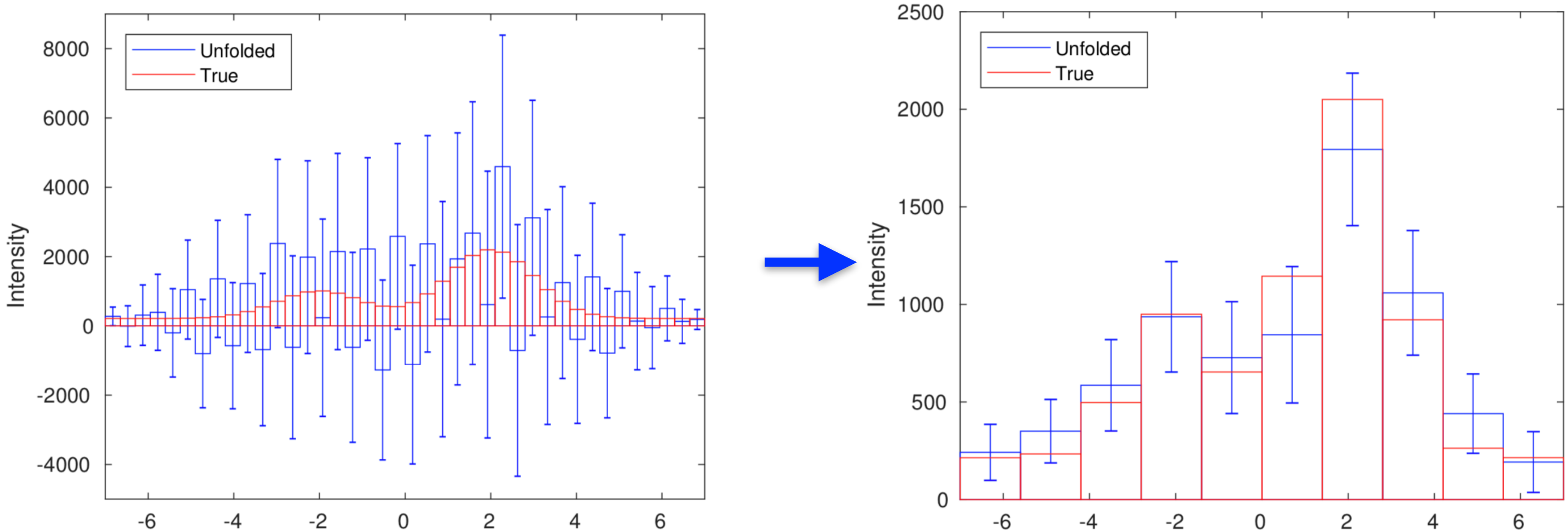


Different distributions within bins
→ Different response matrices
→ Model Systematics

Reduced effects within smaller bins



- Idea: unfold with fine bins and then aggregate results in wide bins



→ Improved modelling systematics, as detailed in talk
https://indico.desy.de/indico/event/22731/session/5/contribution/24/material/slides/0.pdf

Summary

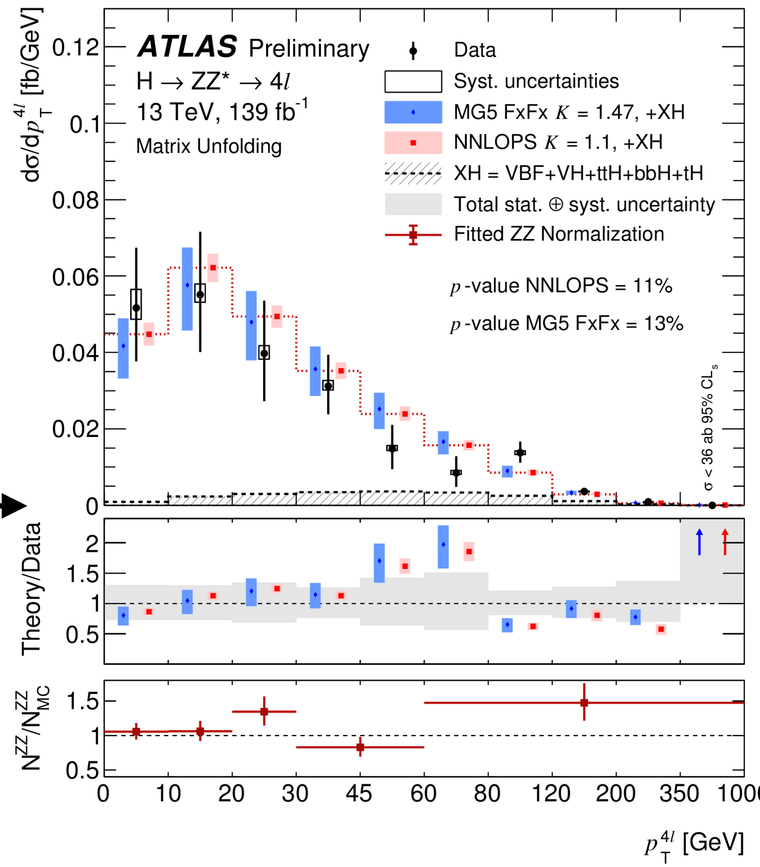
- ✓ New levels of precision (few %) reached in ATLAS and CMS unfolded $d\sigma^{tt}/dx$ with 2016 data

- ✓ Several powerful unfolding tools available: TUnfold, SVD, D'Agostini, Full Bayes and more

- ✓ Need careful optimisation of binning, regularisation and *closure and bias tests (e.g. bottomline* test)*

- ✓ Outlook: Will probably see more profile likelihood based unfoldings →

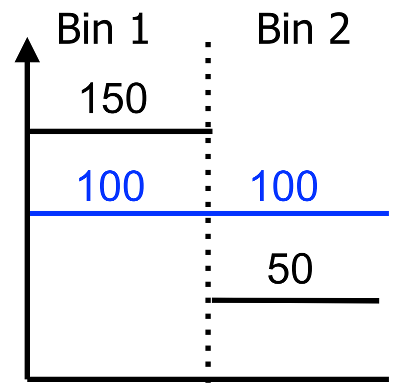
ATLAS-CONF-2019-025



Appendix

Unfolding with removing ‘bad’ events from Response Matrix

Invented example: compare two bin event counts to theory:



Theory prediction at gen level: (150, 50)

Data true values at gen level: (100, 100)

Response Matrix:

Good events: $K_G = \begin{pmatrix} 0.6 & 0. \\ 0. & 0.6 \end{pmatrix}$ Bad events: $K_B = \begin{pmatrix} 0.2 & 0.2 \\ 0.2 & 0.2 \end{pmatrix}$

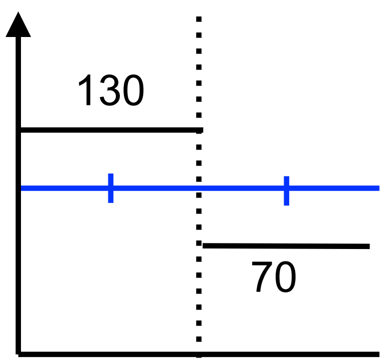
Fold theory to detector level: (130, 70)

<Data> at detector level: (100, 100)

Take example: observed data events (100,100):

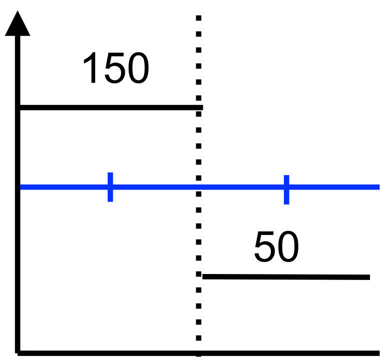
1. Correct for good events fraction $\rightarrow$ (60,60)
2. Unfold to gen level with $K_G^{-1} \rightarrow$ (100,100)

Det. level:



$\chi^2_{\text{data-theory}}$
$= 9^2 + 9^2 = 18$

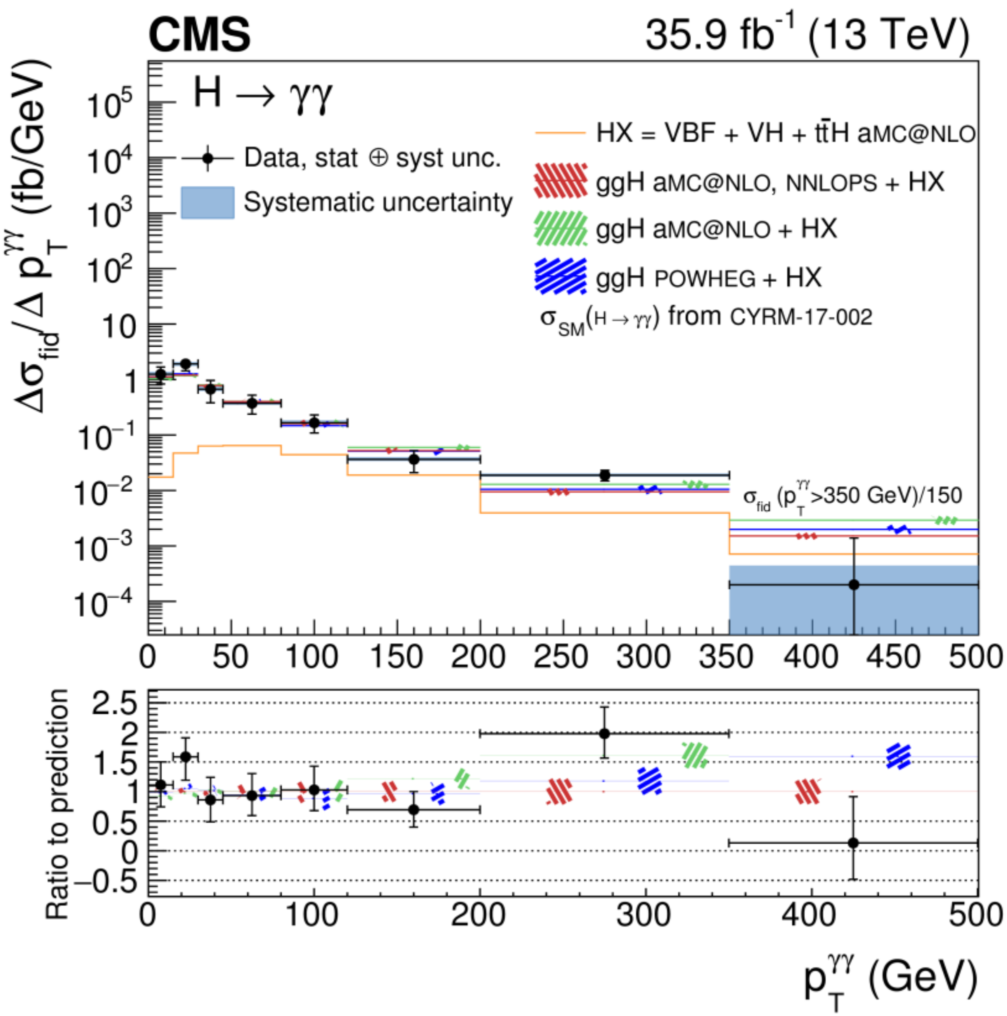
Unfolded level:



$\chi^2_{\text{data-theory}}$
$= 25^2 + 25^2 = 50$

→ Fails Bottomline test

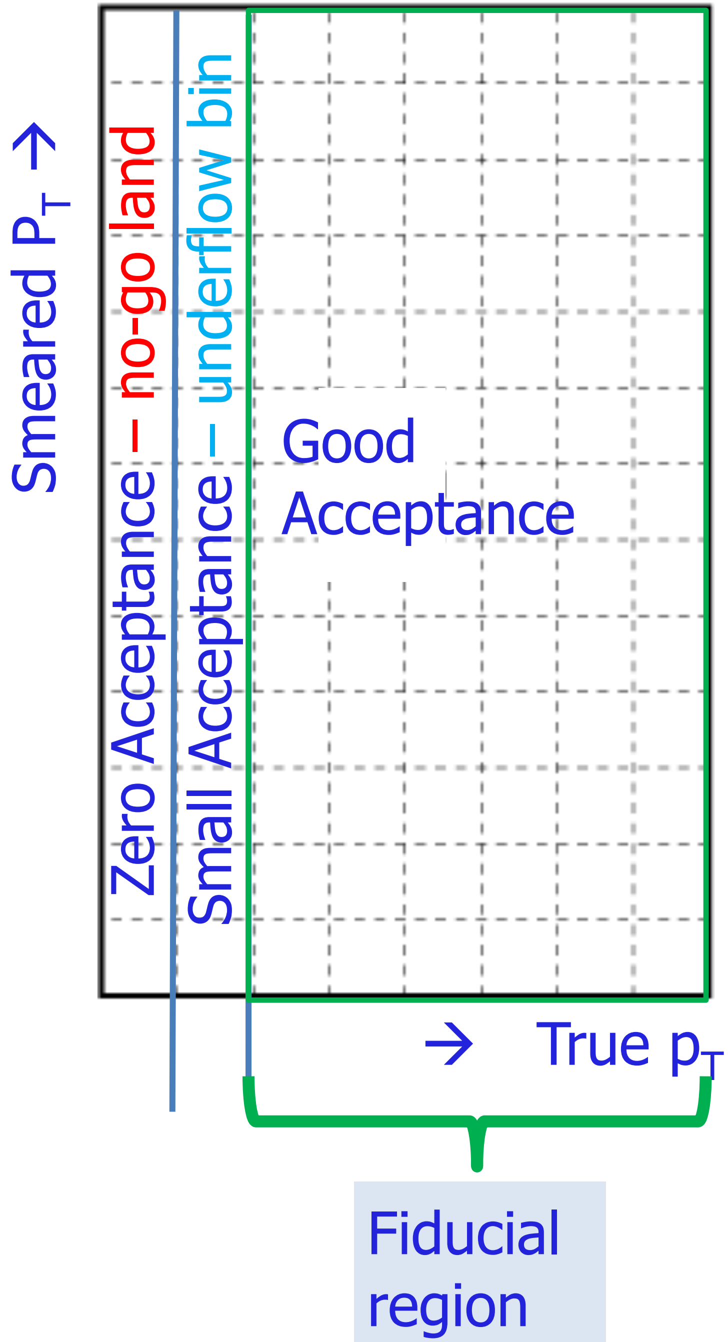
CMS example for profile likelihood unfolding



JHEP 01 (2019) 183

Performed with Higgs combine tool

https://cms-analysis.github.io/HiggsAnalysis-CombinedLimit/



Underflow bins and 2d-TUnfolding

Example: top p_T cross sections

Include underflow bin(s) in unfolding and publish results in fiducial region
→ minimizes MC model systematics for migrations in- and out fiducial range

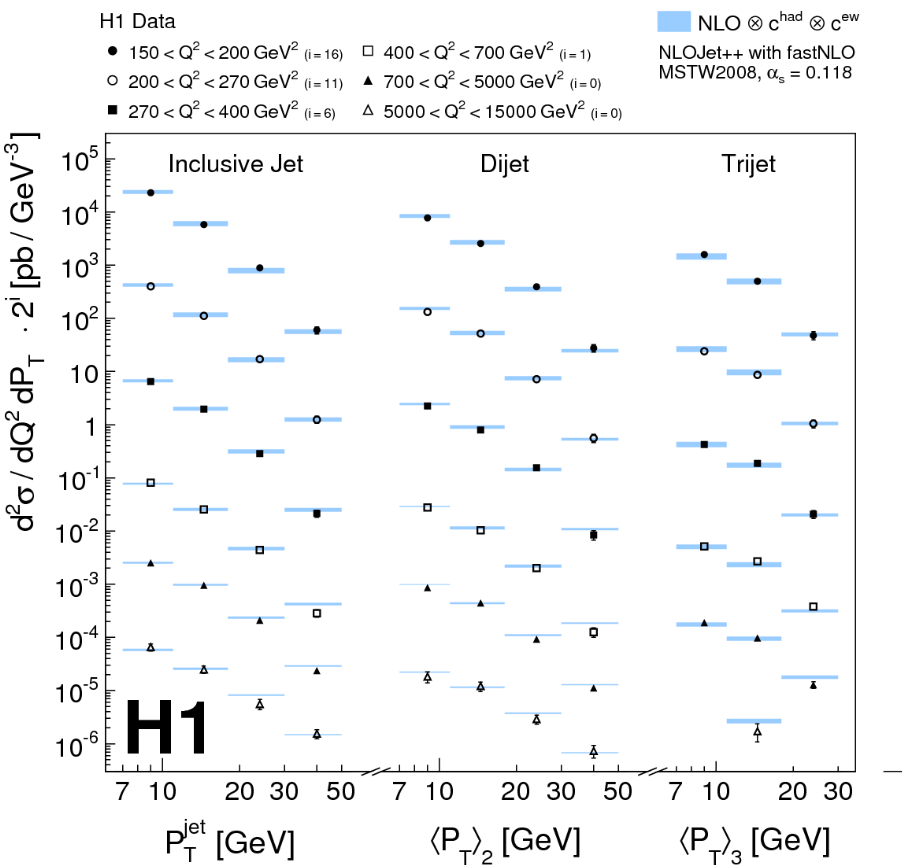
Other fiducial cuts, e.g rapidity y of top
→ useful to include for unfolding of p_T also underflow bin in y (and for any other fiducial cut variable)

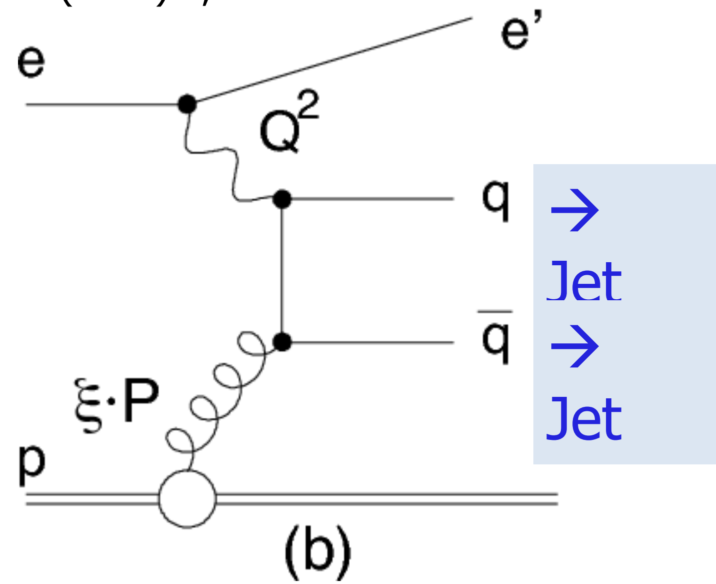
→ TUnfold provides multi-dimensional unfolding with automated internal mapping to 1d-arrays

H1 TUnfolded jet cross sections

EPC C75 (2015) 2, 65

	Extended analysis phase space	Measurement phase space for jet cross sections
NC DIS phase space	$100 < Q^2 < 40\,000\ \mathrm{GeV}^2$ $0.08 < y < 0.7$	$150 < Q^2 < 15\,000\ \mathrm{GeV}^2$ $0.2 < y < 0.7$
Jet polar angular range	$-1.5 < \eta^{\mathrm{jet}}_{\mathrm{lab}} < 2.75$	$-1.0 < \eta^{\mathrm{jet}}_{\mathrm{lab}} < 2.5$
Inclusive jets	$P_{\mathrm{T}}^{\mathrm{jet}} > 3\ \mathrm{GeV}$	$7 < P_{\mathrm{T}}^{\mathrm{jet}} < 50\ \mathrm{GeV}$
Dijets and trijets	$3 < P_{\mathrm{T}}^{\mathrm{jet}} < 50\ \mathrm{GeV}$	$5 < P_{\mathrm{T}}^{\mathrm{jet}} < 50\ \mathrm{GeV}$ $M_{12} > 16\ \mathrm{GeV}$



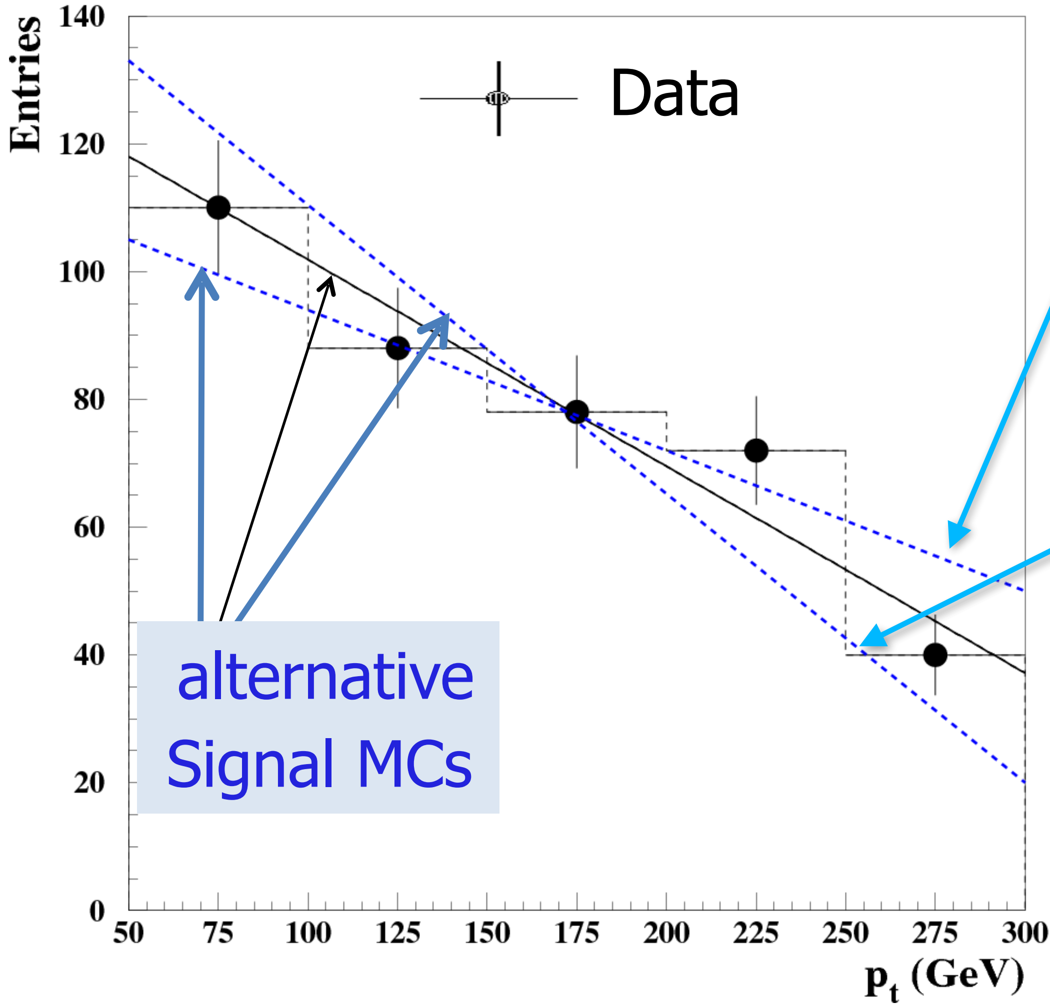


→ Simultaneously unfolded 1,2 and 3 jet event cross sections

→ Among the worldwide most precise jet measurements

→ Unfolding effort pays off

Wide bins and model systematics



Generator events more uniformly distributed in bin

More generator events at low bin edge

→ Different response matrices K

→ Contributes to model systematics