

Physics Institute

Event shape variables in pp collisions in CMS

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QCD@LHC 2024

Motivation

Motivation: previous event shape measurements

Existing observations of **unexpected effects in event shapes**



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Motivation: Strange hadron production in pp collisions

Mismodeling of strangeness production in pp collisions

- Indicates the mismodeling in hadronization & potential quark-gluon plasma effects
- Affects the detector response and then the event shape measurement







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Motivation

QCD instantons

Tunnelling process among discrete classical QCD vacuums which are topologically different





Event shape as functions of charged particle momentum

Event shapes as functions of charged particle momentum



Observables for measurement:

From charged particles p_T > 0.5 GeV, $|\eta|$ < 2.4

- Charged particle multiplicity
- Invariant mass of charged particles
- Sphericity (+ transverse)
- Thrust (+transverse)
- Broadening
- Isotropy

measures of momentum distributions

 → Example: transverse sphericity (detector level correspondence, to be discussed later)



Anisotropic

🔶 Data

Width

Event

Vormalized

CMS Preliminary

3.0≤N_{tracks}<160.0

Anisotropic

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Isotropic

13 TeV

Isotropic

🔶 СР1

♦ EPOS

Data & MC

Data: Zerobias, 2018 low pileup run, O(5M) events, ~64 µb⁻¹

MC: private minimum bias simulation **without pileup** (pileup effects given in backup)

 \rightarrow minimal selections on primary vertices & tracks

Nominal samples and systematic variations

Pythia 8 CP1 (CMS), A3 (ATLAS)* EPOS-LHC Herwig 7 CH3

Different tunes, same MC model

- Regge-Gribov model, collective flow
- Different shower& hadronization models

Validations and comparisons

Pythia CP5(CMS), CUETP8M1-NNPDF3.1(CMS), A14 (ATLAS) & its variations, CUETP8M1-NNPDF2.3(CMS), CUETP8M2T4, CUETP8M2T4-rope-hadronization&string-shoving, Pythia CP5 α_{s} (FSR) variations, Pythia CP5 color-reconnection tunes

*The ATLAS A3 tune was used as nominal MC for unfolding in the strategy development and validation. Later the nominal MC was changed to CMS CP1 tune for the data unfolding.

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Statistical uncertainty from data

- \rightarrow fluctuations in the NN parameters
- \rightarrow fluctuations of the unfolding output

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Systematic uncertainty from MC modelling 1. MC statistics

 \rightarrow fluctuations in modelling

2. Track reconstruction efficiency uncertainty

 \rightarrow differences between detector simulation and truth

3. Mismodelling of observables used directly in unfolding

e.g. charged particle multiplicity, sphericity... \rightarrow bias

4. Mismodelling of other observables which may change detector response

- e.g. track rapidity, particle composition, $\ensuremath{p_T}$
- \rightarrow migration function uncertainty

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 p_T and η of the particles Not unfolded, but affect all the event shape obs.

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We consider variations derived from 3 separate MC models

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 \rightarrow bias



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Machine-learning-based unbinned unfolding & uncertainty estimation

Unfolding algorithm



* <u>https://arxiv.org/abs/1911.09107</u> <u>https://arxiv.org/abs/2105.04448</u>

Multifold *:

- **Input**: values of 8 observables for every event in simulation and data
- **Output**: reweighted simulated events approximating data

 \rightarrow The result are **unbinned** weighted events, although we show binned histograms for visualisation

Two steps of unbinned reweighting:

- 1. Weight MC to data at detector level
- 2. Weight original MC to reweighted MC at generator level Extra 2 steps added to deal with the selection efficiency and signal acceptance
 - \rightarrow repeat in **iterations**

Unbinned weighting for uncertainty estimation



← A typical binary classifier to distinguish two sets



 \leftarrow A typical binary classifier to distinguish two sets

What it actually did: learn the differences in the distributions \rightarrow





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 \leftarrow We can use the classification scores to weight MC to data,



 \leftarrow A typical binary classifier to distinguish two sets

What it actually did: learn the differences in the distributions \rightarrow





← We can use the classification scores to weight MC to data

Event-wise unfolding \rightarrow the result independent of binning

The actual unfolding in iterations:

- Step 1: weight MC to data, at detector level
- Step 2: pull back the weights to particle(truth) level





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What it actually did: learn the differences in the distributions \rightarrow





← We can also use the classification scores to weight nominal MC sample to systematic variations



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Event-wise uncertainty template \rightarrow unbinned unfolding uncertainty & covariance

Track reconstruction efficiency uncertainty

- Step1: Randomly drop 2.1%(1%) tracks with pT<20 GeV (>20 GeV) in nominal MC*
- Step2: weight the nominal MC to Step1 output at particle- and detector-level

* The uncertainty of track reco. eff. is given by D* analysis: <u>https://cds.cern.ch/record/2810814/</u> University of Zürich Weijie Jin

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Example: Gen \rightarrow reco migration of transverse sphericity

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Mismodelling of observables used directly in unfolding

Derive the templates by **weighting nominal MC** to **alternative MC** at the **particle-level**

- \rightarrow **ML-based** unbinned weighting
- \rightarrow output: weighted nominal MC events
 - same particle-level distribution as alternative MC
 - keeps the gen. \rightarrow reco. migration of the nominal MC

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Mismodelling of other observables which may change detector response

Derive the templates with two-step weighting

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Example: Gen \rightarrow reco migration of spherocity





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Unfolding results

Simultaneously unfold the 8 variables for ML-based weighting

Add a variable to the unfolding:

Methods based on **binned** histograms:

Add another dimension in binning

 \rightarrow require **higher statistics**

 \rightarrow more **computation** in simulation and unfolding

This method:

Add **a feature** in the ML training and evaluation \rightarrow much easier to scale up the dimensions



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Unfolding results as weighted MC events

Customise binning and variable choices are supported with the event-wise unfolded data



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1D visualisation of **charged particle invariant mass** distribution



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Unbinned uncertainty estimation

ML-based reweighting → Uncertainty templates as sets of weights on nominal MC

- \rightarrow Continuous nuisance parameters can be assigned to the event-weights
- \rightarrow Uncertainty covariance can be estimated from toy experiments
 - Unfold with "bootstraps" of MC with variations of nuisance parameters → Syst. Unc + Covariance
 - Unfold with "bootstraps" of resampled data \rightarrow Stat. Unc. + Covariance





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Example: correlation of the syst. unc. of sphericity

The way to improve the usability of **unfolded results**

- Publish the unbinned results on event-level
- Publish the **weight sets** from **toy experiments**
 - \rightarrow Unc. + Covariance

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Interpretation of results



The **data** tends to be **more isotropic** than all the **MC** predictions



The data is more accumulated in the middle Nch region (~20)

Interpretation of results



Summary

- Minimum bias collisions may be the home of interesting physics at the LHC
 - Observables that are not described by existing models \rightarrow QGP or others?
 - Could be contributed by QCD instantons ← topological effects of non-abelian gauge fields
- Event shapes are important signatures of these physics effects
- We present a measurement of these event shape observables in CMS
 - Unbinned high-dimensional unfolding based on machine-learning models
 - Unbinned uncertainty estimation based on pseudo-experiments
 - Validations provided: pseudo-data unfolding, bias & coverage test, bottom-line test (backup)
 - The unfolding method is also used in an ATLAS measurement of Z+jets kinematics arxiv:2405.20041
- Unfolding results as weighted MC events
 - Unbinned events \rightarrow further usage of data does not depend on binning
 - Visualised by 1D or 2D histograms
 - Correlations of the uncertainties are provided (visualised by 2D histograms)
 - Data is more isotropic than all the MC variations, especially in mid-Nch region



Validation: unfold the pseudo-data from Pythia A14 tune

Alternative MC from Pythia A14, CP5 and CUETP8M1 tunes → pseudo-data

Unfold the **pseudo-data** with **nominal MC** and the **systematic templates** \rightarrow Test the closure



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Example: Unfold the Pythia A14 sample (plots of other observables, reco-level plots, efficiency and acceptance in backup)



Validation: unfold the pseudo-data from Pythia CP5 tune

Particle-level

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Detector-level MC, unfold, and pseudo-data truth MC, refold, and pseudo-data broadening at iteration 2 broadening at iteration 2

σ/dB_{track} nominal refold MC: A3P EPOS gen. EPOS mig. CP1 gen. CP1 mig. CH3 gen. CH3 mig. track reco. unc. pseudodata: CP5 data Refold 0.05 0.20 0.25 0.30 0.35 0.40 0.00 0.10 0.15 **B**_{tracks}

2018 (13 TeV)

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1e8CMS Simulation Preliminary

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Example: Unfold the Pythia CP5 sample







Particle-level MC, unfold, and pseudo-data truth broadening at iteration 2 Weijie Jin

Detector-level **MC**, **refold**, and **pseudo-data** broadening at iteration 2 25

Validation: unfold the pseudo-data with other systematic templates



Particle-level **MC**, **unfold**, and **pseudo-data truth**

Systematic templates derived from EPOS, **Pythia CP1, Herwig CH3**

Systematic templates derived from EPOS, **Pythia A14, Pythia CUETP8M1**

Robustness test of MC choices for systematic templates

- The unfolding from alternative systematic templates also recovers the truth
- Uncertainties from gen-bias & migration functions are at a similar level

Broadening unfold v.s. truth

Transverse sphericity **unfold** v.s. **truth**

Transverse sphericity uncertainty decomposition

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Validation: unfold the pseudo-data

Test the unfolding on 2D distributions



2D test also shows closure between unfolding results and the pseudo-data truth

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Validation: unfold the pseudo-data

Test the unfolding on 2D distributions

Example: Unfold the Pythia CUETP8M1 sample, transverse sphericity in slices of N_{ch}



2D test also shows closure between unfolding results and the pseudo-data truth

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Validation: bottom-line test

Information loss during unfolding

- → the distinction between the unfolded results & MC truth < the distinction between (pseudo-)data & smeared MC
- \rightarrow bottom-line test: the χ^2 between unfolded results (bias & MC stat. unc.) & MC truth

< the **x**² between (pseudo-)data & smeared MC

Example: χ^2 (unfold&gen-MC) / χ^2 (data&smeared MC) when unfolding CUEPT8M1 pseudo-data

2018 (13 TeV) 2018 (13 TeV) **CMS** Simulation Preliminary **CMS** Simulation Preliminary X²(unfold&genMC) X²(data&smearedMC) C0 50 50 50 50 thrust thrust transverse sphericity transverse sphericity transverse_thrust transverse_thrust broadening broadening isotropy isotropy Ideal case: χ^2 ratios ~ 1 mass mass 0.4 nparticle sphericity 0.6 chjet_deltaphi sphericity information loss or 0.3 conservative unc. estimation 0.4 $\rightarrow \mathbf{x}^2$ ratios < 1 0.2 0.2 0.1 0.0 0.0L 2 3 2 3 4 4 Iteration Iteration **x**² ratios of 2D histograms χ^2 ratios of 1D histograms (event shape obs. in Nch slices) $^{28}_{28}$ University of Zürich Weijie Jin

Randomly **shift nominal MC** according to systematic variations uses **shift systematic templates** accordingly



Resampled pseudo-data







Randomly **shift nominal MC** according to systematic variations unfold **Resampled pseudo-data** + shift systematic templates accordingly Mismodeling of the Mismodeling of other observables Track reconstruction efficiency observables to be unfolded Random samples of nuisance parameters for each sys. unc. θ_2 , θ_{3CP1} , θ_{3EPOS} , θ_{3CH3} , θ_{4CP1} , θ_{4EPOS} , $\theta_{4CH3} \sim N(0,1)$ Deviation from nominal to sys. template: $\overrightarrow{W_i}^{\theta_i}$ Poisson(1) weight on MC events (MC stat. unc.) Multiply the weights for all the sys. unc. sources











Unfold pseudo-data with toy experiments of uncertainty variations

Bias test:

Bias of the unfolding results compared to pseudo-data truth

Box-plot: 0.25, 0.5 and 0.75 quantile of 50 toys



Example: unfolding CUETP8M1 pseudo-data Transverse sphericity distribution at iteration 2 Coverage test:

How often does the unfold cover the pseudo-data?

Average coverage and its 68.2% confidence interval



Estimate systematic uncertainty with pseudo-experiments

1.MC statistics templates: random **Poisson(1) weights** on MC

2. Track reco. eff. template: weights $\overrightarrow{w_2}$ on nominal MC

3. Mismodel of obs. for unfolding template weights $\overrightarrow{w}_{3A3}, \overrightarrow{w}_{3EPOS}, \overrightarrow{w}_{3CH3}$ on nominal MC 4. Mismodel of other obs. template: weights $\overrightarrow{w}_{4A3}, \overrightarrow{w}_{4EPOS}, \overrightarrow{w}_{4CH3}$ on nominal MC

Estimate systematic uncertainty with pseudo-experiments



Estimate systematic uncertainty with pseudo-experiments



PDF variations of MC



Tune variations of MC

A14 tune eigen-variation 1 and 2



A14 tune eigen-variation 3a, 3b, 3c



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Estimation of systematic uncertainty

Binned unfolding:

- Systematic templates as alternative MC histograms
- Nuisance parameters quantify the deviation from nominal MC to systematic template histograms

Extrapolate to unbinned unfolding:

- Systematic templates as alternative weights on nominal MC events (nominal: weight=1)
- Nuisance parameters quantify the deviation from the nominal weight 1 to the alternative weights

Aim in systematic uncertainty estimation:

- Construct the templates as weights on nominal MC events
- Continuous nuisance parameters applied on the weights
 - \rightarrow continuous deviation from nominal MC to systematic templates
 - \rightarrow enables uncertainty estimation with pseudo-experiments (unfolding with "bootstrap" MC)

