

**Physics Institute**

## **Event shape variables in pp collisions in CMS**

Weijie Jin

QCD@LHC 2024

**Motivation**

#### **Motivation: previous event shape measurements**

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



#### **Motivation: previous event shape measurements**

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



University of Zürich Weijie Jin

3

### **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





### **Motivation**

• Tunnelling process among discrete classical QCD vacuums which are topologically different

• A generic prediction of non-Abelian gauge theories





# **Event shape as functions of charged particle momentum**

### **Event shapes as functions of charged particle momentum**



We focus on **charged particles** ← **precise reconstruction of tracks**

Observables for measurement:

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

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

measures of momentum distributions

 $\rightarrow$  Example: transverse sphericity (detector level correspondence, to be discussed later)



1

2

Normalized Events/Bin Width

Normalized

Events/Bin Width

3

**CMS**

*Preliminary*

 $3.0 \le N_{\text{tracks}} < 160.0$ 

Anisotropic

13 TeV

Isotropic

- EPOS

 $\rightarrow$  Data  $\rightarrow$  CP1  $CUEP8M1$   $\rightarrow$  A3P

 $CP5$   $\rightarrow$  CH3

### **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

#### **The 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&stringshoving, Pythia CP5  $\alpha_s$ (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.

**Statistical uncertainty** from data

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

#### **Statistical uncertainty** from data

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

#### **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,  $p_{\overline{I}}$
- $\rightarrow$  migration function uncertainty

**Statistical uncertainty** from data

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

#### **Systematic uncertainty** from MC modelling 1. **MC statistics**

 $\rightarrow$  fluctuations in modelling

2. **Track reconstruction efficiency** uncertainty  $\rightarrow$  differences between detector simulation and truth



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

#### 4. **Mismodelling of other observables which may change detector response**

- e.g. track rapidity, particle composition,  $p_{\overline{I}}$
- $\rightarrow$  migration function uncertainty

University of Zürich Weijie Jin



 $p_T$  and  $\eta$  of the particles Not unfolded, but affect all the event shape obs.

**Statistical uncertainty** from data

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

#### **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…

**We consider variations derived from 3 separate MC models**

#### 4. **Mismodelling of other observables which may change detector response**

- e.g. track rapidity, particle composition,  $p_{\overline{I}}$
- $\rightarrow$  migration function uncertainty

 $\rightarrow$  bias

 $10^{-7}$ −6 10 −5 10  $10^{-4}$ −3 10  $10^{-2}$  $10^{-1}$ 1 10  $10^{2}$ 

0.5

1.0 Ratio

Ratio

**CMS**

*Preliminary*

 $3.0 \le N_{\text{tracks}} < 160.0$ 

Data <del>+</del>CP1  $+$  EPOS-LHC A3P <del>o C</del>P1\_trackdrop

Normalized Tracks//Bin Width

Normalized Tracks//Bin Width



13 TeV

<sub>track</sub>/dη

종

15

**CMS**

*Preliminary*  $3 \leq N_{\text{tracks}} < 160$  13 TeV

Data <del>+</del>CP1  $-$  CH3  $+$  EPOS-LHC A3P <del>o C</del>P1\_trackdrop

# **Machine-learning-based unbinned unfolding & uncertainty estimation**

### **Unfolding algorithm**



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

#### **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  $\rightarrow$ 





 $\leftarrow$  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**,



 $\leftarrow$  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





 $\leftarrow$  A typical binary classifier to distinguish two sets

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





 $\leftarrow$  We can also use the classification scores to weight **nominal MC sample** to **systematic variations**



 $\leftarrow$  A typical binary classifier to distinguish two sets

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**

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

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

#### **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



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

Example:  $Gen \rightarrow reco$  migration of transverse sphericity

#### **Mismodelling of observables used directly in unfolding**

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

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

#### **Mismodelling of observables used directly in unfolding**

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

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



#### **Mismodelling of other observables which may change detector response**

Derive the templates with two-step weighting

#### **Mismodelling of other observables which may change detector response**

Derive the templates with two-step weighting

- **Step 1**: weight the **alternative MC** to **nominal MC** at the **particle-level**
	- → output: **weighted alternative MC**
		- with migration function of alternative MC
		- particle-level distributions of nominal MC

#### **Mismodelling of other observables which may change detector response**

Derive the templates with two-step weighting

- **Step 1**: weight the **alternative MC** to **nominal MC** at the **particle-level**
	- → output: **weighted alternative MC**
		- with migration function of alternative MC
		- particle-level distributions of nominal MC
- **Step 2**: weight the **nominal MC** to the **Step 1 output** at **particle- and detector-level**
	- → output: **weighted nominal MC**
		- with migration function of alternative MC
		- particle-level distributions of nominal MC

#### **Mismodelling of other observables which may change detector response**

Derive the templates with two-step weighting

- **Step 1**: weight the **alternative MC** to **nominal MC** at the **particle-level**
	- → output: **weighted alternative MC**
		- with migration function of alternative MC
		- particle-level distributions of nominal MC
- **Step 2**: weight the **nominal MC** to the **Step 1 output** at **particle- and detector-level**
	- → output: **weighted nominal MC**
		- with migration function of alternative MC
		- particle-level distributions of nominal MC

 $Gen \rightarrow \text{reco migration}$ of spherocity







### **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

→ 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



### **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

→ 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

Unfolding results as **weighted MC events**

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



### **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

→ 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

Unfolding results as **weighted MC events**

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



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





### **Unbinned uncertainty estimation**

- **ML-based reweighting** → **Uncertainty templates** as sets of **weights on nominal MC**
- → **Continuous nuisance** parameters can be assigned to the **event-weights**
- → 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 → Stat. Unc. + Covariance**





### **Unbinned uncertainty estimation**

- **ML-based reweighting** → **Uncertainty templates** as sets of **weights on nominal MC**
- → **Continuous nuisance** parameters can be assigned to the **event-weights**
- → 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 → Stat. Unc. + Covariance**



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**
	- **→ Unc. + Covariance**

University of Zürich Weijie Jin



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

**Uncertainties+Covariance on the results**



#### **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 →** Test the closure



### **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

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**

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

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







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

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

#### **Validation: unfold the pseudo-data from Pythia CP5 tune**

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

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

Example: Unfold the Pythia **CP5** sample





 $\sigma$ /dB<sub>trac</sub> nominal refold MC: A3P EPOS gen. EPOS mig. CP1 gen. CP1 mig. CH3 gen. CH3 mig. track reco unc pseudodata: CP5 data Refold  $0.00$ 0.05  $0.10$  $0.20$  $0.25$ 0.30 0.35 0.40 0.15  $B_{\text{tracks}}$ 

2018 (13 TeV)

 $_{1\,e8}$ CMS Simulation Preliminary

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

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

#### **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 Transverse sphericity **Functions** are at a similar level

#### **Broadening unfold** v.s. **truth**

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

uncertainty decomposition

### **Validation: unfold the pseudo-data with other systematic templates**



**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 Transverse sphericity **Functions** are at a similar level

#### **Broadening unfold** v.s. **truth**

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

uncertainty decomposition

#### **Validation: unfold the pseudo-data**

Test the unfolding on **2D distributions**



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

#### **Validation: unfold the pseudo-data**

#### Test the unfolding on **2D distributions**

Example: Unfold the Pythia **CUETP8M1** sample, transverse sphericity in slices of Nch



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

#### **Validation: bottom-line test**

Information loss during unfolding

- → the distinction between the **unfolded results** & **MC truth** < the distinction between **(pseudo-)data** & **smeared MC**
- → **bottom-line test**: the **χ2** between **unfolded results** (bias & MC stat. unc.) & **MC truth**

< the **χ2** between **(pseudo-)data** & **smeared MC**

Example: **χ2** (unfold&gen-MC) / **χ2** (data&smeared MC) when unfolding CUEPT8M1 pseudo-data

2018 (13 TeV) 2018 (13 TeV) **CMS** Simulation Preliminary **CMS** Simulation Preliminary  $\frac{\chi^2(\text{unfold8genMC})}{\chi^2(\text{data8smearedMC})}$  $\frac{\chi^2(\text{unfold\&genMC})}{\chi^2(\text{data\&mearedMC})}$ thrust — thrust transverse sphericity transverse sphericity transverse thrust transverse thrust broadening broadening isotropy isotropy ≿ّ Ideal case:  $\chi^2$  ratios  $\sim$  1 mass mass  $0.4$ nparticle — sphericity  $06$ chjet\_deltaphi information loss or sphericity  $0.3$ conservative unc. estimation  $0.4$  $0.2$  $\rightarrow$  **x**<sup>2</sup> ratios < 1  $0.2$  $0.1$  $-0.06$  $0.0<sub>n</sub>$  $\overline{2}$  $\overline{3}$  $\boldsymbol{\Lambda}$  $\overline{2}$  $\overline{3}$ Iteration Iteration **<sup>χ</sup>2** ratios of 1D histograms **<sup>χ</sup>2** ratios of 2D histograms (event shape obs. in Nch slices) University of Zürich Weijie Jin

Randomly **shift nominal MC** according to systematic variations + **shift systematic templates** accordingly **Resampled pseudo-data**









Randomly **shift nominal MC** according to systematic variations + shift systematic templates accordingly **Resampled pseudo-data** unfold Deviation from nominal to sys. template:  $\overrightarrow{w_{i}}$ *θi* Random samples of nuisance parameters for each sys. unc.  $\theta_2$ ,  $\theta_3$ <sub>CP1</sub>,  $\theta_3$ <sub>EPOS</sub>,  $\theta_4$ <sub>CP1</sub>,  $\theta_4$ <sub>EPOS</sub>,  $\theta_4$ <sub>CH3</sub> ~N(0,1) Track reconstruction efficiency Mismodeling of the Mismodeling of the unfolded Mismodeling of other observables 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

![](_page_58_Figure_5.jpeg)

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

How often does the unfold cover the pseudo-data?

#### Box-plot: 0.25, 0.5 and 0.75 quantile of 50 toys **Average coverage and its 68.2% confidence interval**

![](_page_58_Figure_10.jpeg)

#### **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  $\widetilde{w}_{3A3}, \widetilde{w}_{3EPOS}, \widetilde{w}_{3CH3}$  on nominal MC

**4. Mismodel of other obs. template:** weights  $\widetilde{w}_{4A3}, \widetilde{w}_{4EPOS}, \widetilde{w}_{4CH3}$  on nominal MC

#### **Estimate systematic uncertainty with pseudo-experiments**

![](_page_60_Figure_1.jpeg)

#### **Estimate systematic uncertainty with pseudo-experiments**

![](_page_61_Figure_1.jpeg)

#### **PDF variations of MC**

![](_page_62_Figure_1.jpeg)

#### **Tune variations of MC**

#### A14 tune eigen-variation 1 and 2

![](_page_63_Figure_2.jpeg)

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

![](_page_63_Figure_4.jpeg)

#### University of Zürich Weijie Jin

### **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)

![](_page_64_Picture_14.jpeg)