PROCEEDINGS OF SCIENCE

Measurement of event shape variables in pp collisions

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Inclusive event shape distributions, as well as event shapes as a function of charge particle multiplicity are extracted from CMS low-pileup and compared with predictions from various generators. Multidimensional unfolded distributions are provided, along with their correlations, using state-of-the-art machine-learning unfolding methods.

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1. Introduction

Recent measurements of global event observables in proton-proton (pp) collisions, such as the correlations between outgoing particles[2, 3] and the multiplicity of strange hadrons[4], underscore the challenges in accurately modeling these collisions. An attempt to describe these observations include models involving non-perterbative effects. This motivates to study observables sensitive to non-perturbative effects using minimum-bias pp collision events. In this analysis a total of eight observables are studied which are related to the overall kinematics of the events, also known as event shapes[5]. These obserbables are:

- **Particle multiplicity:** N
- **Total invariant mass:** $\sqrt{s}$
- **Sphericity:** measure of how isotropically the momenta are distributed: $S^{\alpha\beta} = \frac{\sum_i p_i^\alpha p_i^\beta}{\sum_i |p_i|^2}$
- **Thrust:** measure of how highly collimated the momenta in an event along one particular axis: $\tau = 1 - \max_{\vec{n}} \frac{\sum_i p_i^\alpha p_i^\beta}{\sum_i |p_i|^2}$
- **Broadening:** measure of the fraction of energy perpendicular to the thrust axis
- **Transverse sphericity:** the sphericity in the transverse plane
- **Transverse thrust:** the thrust in the transverse plane
- **Isotropy:** measure of how isotropically energy is distributed in an event

2. Event Selection

Analysis is performed using charged hadrons without clustering into jets. Few basic selecions are applied, which requires the events to have a primary vertex within $\pm 2(\pm 24)$ cm around the nominal interaction point along transverse (longitudinal) beam direction, the transverse momentum of the track should be more than 0.5 GeV and the track needs to be within tracker acceptance ($|\eta| < 2.5$).

3. Unfolding

We use the Multifold machine learning-based unfolding procedure, which performs unbinned, multidimensional unfolding and employs iteration as the method of regularization [6, 7]. Similar to Richardson-Lucy or Iterative Bayesian Unfolding (IBU), Multifold extends these concepts using neural networks to estimate likelihood ratios. The classifier's likelihood ratio is used to reweight events in an unbinned way.

The unfolding uses multiple reweighting steps on each iteration, first correcting the simulation towards the data at detector level, then correcting the original simulation towards this corrected simulation at the particle level. Additional sub-steps are also employed to account for acceptance and efficiency effects[7].

The unfolding procedure is iterated multiple times, with iteration serving as a form of regularization. Fewer iterations provide stronger regularization and bias towards the input simulation. The number of iterations was determined using goodness-of-fit tests on pseudodata, ensuring no significant improvement with additional iterations. Bias and coverage properties stabilized quickly, with no notable changes after two iterations.

For every event, the neural network is provided with the values of all observables being unfolded, such that all observables are simultaneously unfolded, and their correlations are taken into account.

The classification network has three fully connected layers with 100 nodes each, using cross-entropy as the loss function. Training is done with 80% of the sample, while 20% is used for validation. Early stopping is used, where the training is stopped after no improvement in the loss function is seen for 10 epochs on the validation sample. Then the network parameters are taken from the last epoch that showed improvement in the training.

The nominal MC simulated events are given uniform weights, normalizing them to the total inelastic cross section for 13 TeV pp collisions. All MC samples are weighted so that the sum of weights matches the nominal MC sample for events passing particle-level selections. In each reweighting step of the training, the program uses balanced weights between the set to be weighted and the target, so that the weighting function from the machine-learning model is based only on the shape differences between the distributions of the two sets. The weights from the unfolding are multiplied to the previous ones in each iteration.

The final result of the unbinned unfolding is a set of reweighted MC events, estimating the probability density of real data in phase space. These are binned to produce histograms of the differential cross section for key observables.

To validate the unfolding, alternative simulated samples were treated as pseudodata. Visual checks, goodness-of-fit tests, and a bottomline test confirmed the improved description of pseudodata without introducing artificial discriminating power. Frequentist bias and coverage tests showed bias near zero, well within the overall uncertainty, with no cases of undercoverage.

4. Uncertainties

Several sources of uncertainties have been taken into account:

- **MC modelling:** MC modeling can affect unfolded measurements in two main ways. First, it can result in a regularization bias, and second, it may give rise to detector response mismatch. The regularization bias depends on the choice of the nominal MC model. To estimate the effect of this systematic uncertainty, alternative templates are estimated by weighting the nominal MC to the alternative MC samples from other tunes or generator at the particle level. The resulting reweighted nominal sample has the same particle-level distributions as the alternative MC but keeps the same migration function as the nominal ones.

  To estimate the uncertainty related to the detector response mismatch, templates are estimated by first weighting the alternative MC samples to the nominal MC samples at the particle level, and then performing a particle-level and detector-level weighting from the nominal MC to the output of the previous step. The resulting weighted samples have the same particle-level distributions as the nominal MC and the same migration function as the alternative MC.

We use multiple MC models (PYTHIA tune, EPOS, HERWIG) to assess these uncertainties.

- **Track reconstruction efficiency:** To estimate the effect of this uncertainty to the event shape measurement, we randomly drop 2.1% of the tracks with $p_T < 20$ GeV and 1% of those with $p_T > 20$ GeV in the MC[8].
- **Statistical uncertainty of the simulated model:** The statistical uncertainty of the MC sample leads to a systematic uncertainty in the unfolding results. This uncertainty is estimated by the same Bootstrapping method that is used in estimating the uncertainty from data statistics.

To address uncertainties from MC regularization bias, migration function, and track reconstruction, we use weights derived from alternative MC samples. These weights are adjusted based on a continuous nuisance parameter θ, with a formula:

$$w_i(\theta) = w_{nom}(w_i(1)/w_{nom})^{\theta} \quad (1)$$

where w_{nom} is the weight of the nominal MC events, and $w_i(1)$ is the weight for the systematic uncertainty template.

Total uncertainty and covariance matrices are estimated via toy experiments with weighted nominal MC and data, simulating template fluctuations. For statistical uncertainties, Poisson(1) weights are used. For systematic uncertainties, nuisance parameters $\theta_j \sim \mathcal{N}(0, 1)$ are generated for each template. The overall weight for each MC event in a toy experiment combines weights from all systematic sources.

The systematic uncertainties on the results are larger than the statistical uncertainties for the chosen binnings in this paper. For 1-dimensional distributions, the typical uncertainty is $O(5\%)$, depending on the kinematic bin, whereas the statistical uncertainties are significantly less than 1%.

5. Results

Figure 1 shows the one-dimensional projections of charged-particle multiplicity and their invariant mass, sphericity, thrust and the distribution of sphericity in the slices of charged-particle multiplicity. It can be seen that none of the generator describe the data completely. For the charged particle multiplicity and their invariant mass, all generator overestimate data at low multiplicity region, under estimate at intermediate value and the consistency is broken at high multiplicity and mass. Other event-shape observables show a consistent trend where the unfolded data are more isotopic than the simulation. From the sphericity distribution we can see that the Data-MC discrepancy is largest in the middle of the charged-particle multiplicity region. Other observables also show similar trend. The discrepancy sustains under variations of PDF, generator, UE tune, color-reconnection models, α_S (FSR).

6. Conclusion

A measurement of event shapes in minimum bias proton-proton collisions at a centre-of-mass energy of 13 TeV has been presented. Low pileup data collected with the CMS detector in 2018

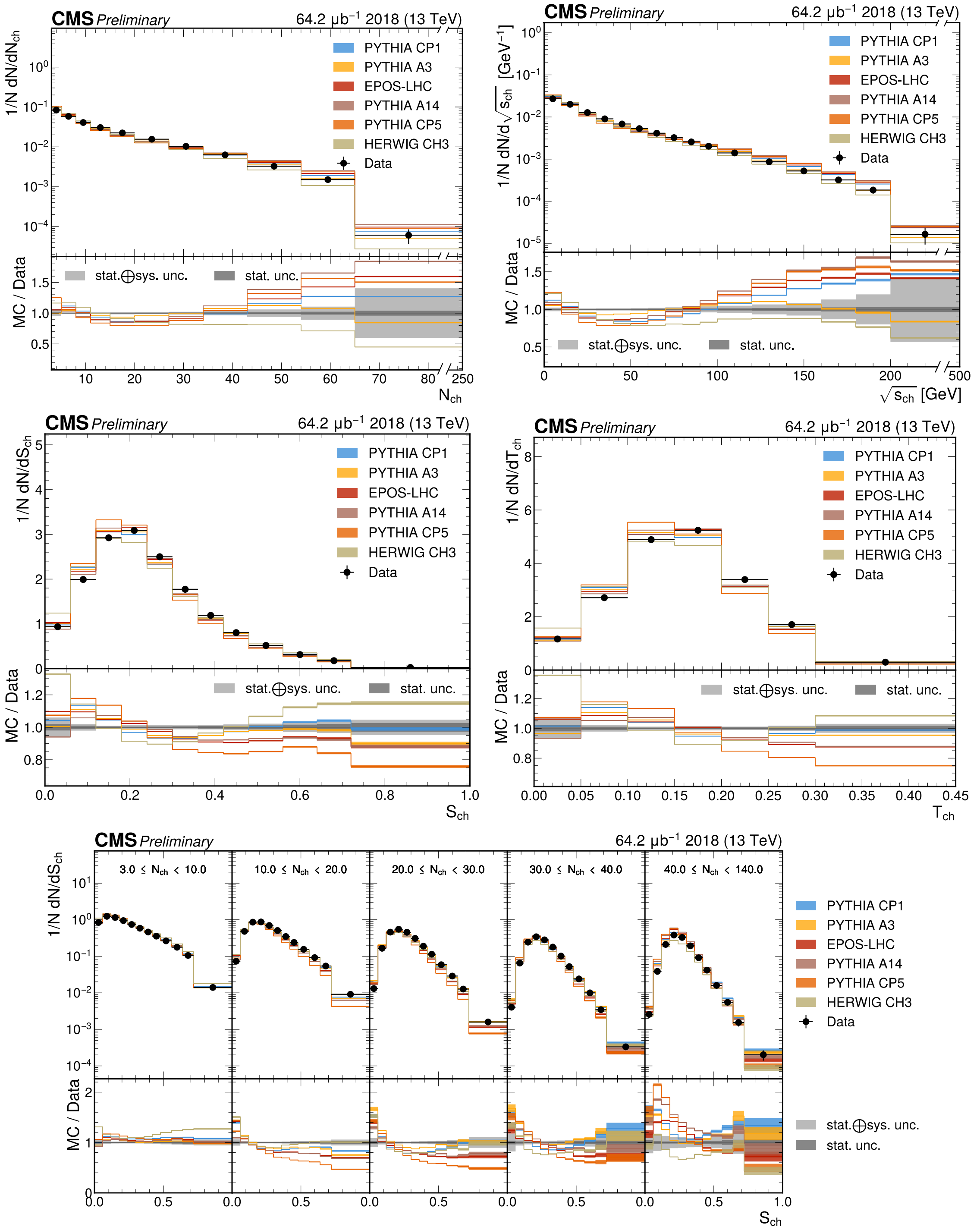

Figure 1: The 1-d unfolded results for the particle multiplcity (upper left), invariant mass (upper right), sphericity (middle left), thrust (middle right) and the unfolded distributions of sphericity (lower) in slices of charged particle multiplicity compared to the nominal MC from PYTHIA CP1 tune and MC predictions from the PYTHIA A14, CP5, A3 tunes, the EPOS generator and the HERWIG CH3 tune.

were used, and the kinematics of reconstructed tracks were used to unfold the distributions to the level of stable charged particles. The results show a consistent trend of mismodelling event shapes common across all simulation configurations considered. An unbinned multi-dimensional unfolding algorithm was used to provide these results.

These event-shape observables are important in probing soft and non-perturbative effects in quantum chromodynamics at the LHC. The unfolded data should be used by the community to improve and develop proton-proton collision models, as it will be critical for understanding phenomena such as quark-gluon plasma and topological effect in non-abelian gauge theories.

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