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Measurement of jet track functions in pp collisions at $\sqrt{s} = 13$ TeV with the ATLAS detector

The ATLAS Collaboration

Measurements of jet substructure are key to probing the energy frontier at colliders, and many of them use track-based observables which take advantage of the angular precision of tracking detectors. Theoretical calculations of track-based observables require 'track functions', which characterize the transverse momentum fraction r_q carried by charged hadrons from a fragmenting quark or gluon. This letter presents a direct measurement of r_q distributions in dijet events from the 140 fb^{-1} of proton–proton collisions at $\sqrt{s} = 13$ TeV recorded with the ATLAS detector. The data are corrected for detector effects using machine-learning methods. The scale evolution of the moments of the r_q distribution is sensitive to non-linear renormalization group evolution equations of QCD, and is compared with analytic predictions. When incorporated into future theoretical calculations, these results will enable a precision program of theory-data comparison for track-based jet substructure observables.

1 Introduction

Jets are collimated streams of hadrons resulting from the fragmentation of high energy quarks and gluons. The wide range of energy scales probed during jet formation provides a unique experimental window into the dynamics of Quantum Chromodynamics (QCD) in both perturbative and non-perturbative regimes of the strong coupling. The experimental study of jets has greatly expanded in the last decade with the ability to measure correlations between multiple particles produced in the same identified jet, a field referred to as jet substructure [1, 2]. Jet substructure has provided numerous new ways to study the dynamics of the Standard Model and to search for new phenomena [2].

The theoretical understanding of jets is based on the combination of perturbation theory and non-perturbative functions characterizing the hadronization process, which are universal in the context of factorization. The most well-known examples of such a universal non-perturbative object are fragmentation functions [3], which describe the energy distribution of single hadrons arising from the fragmentation of quarks and gluons. These functions cannot currently be calculated from first principles, and therefore must be determined by experiment. The broad program of fragmentation-function measurements [4] has been extremely successful, enabling the theoretical understanding of a wide variety of collider physics processes. However, fragmentation functions are single-hadron observables, and therefore do not incorporate the correlations in the hadronization process necessary for the understanding of modern jet substructure observables.

Among the many functions characterizing the hadronization process, those describing the fragmentation into electrically charged hadrons, which are identified as tracks in the detector, are particularly important. Tracking detectors have better angular granularity, enabling measurements at small angular scales within jets. Track-based measurements have been key to enabling a precision jet substructure program at the Large Hadron Collider (LHC) by the ATLAS [4–9], CMS [10, 11], ALICE [12–15] and LHCb [16, 17] experiments.

The interpretation of track-based jet substructure measurements requires an understanding of the correlated fragmentation of quarks and gluons into charged hadrons. This is described by universal non-perturbative functions called track functions [18, 19], which describe the energy distribution of charged hadrons arising from fragmenting quarks or gluons. These functions are multi-hadron observables. Experimentally, track functions can be determined [20] from a measurement of the the transverse-momentum (p_{T}) fraction in tracks in high-energy jets denoted by $r_q = p_{\mathrm{T}}^{\mathrm{charged}}/p_{\mathrm{T}}^{\mathrm{all}}$, where $p_{\mathrm{T}}^{\mathrm{all}}$ is the p_{T} of the jet and $p_{\mathrm{T}}^{\mathrm{charged}}$ is the p_{T} of the sum of charged particles within the jet. The first moment of this distribution, $\langle r_q \rangle \sim 2/3$ due to approximate isospin symmetry, is described by standard fragmentation functions, and is a fundamental property of the strong force that has been utilized by a multitude of experiments for calibration and precision studies [21]. The higher moments of the distribution encode interesting correlations in the hadronization process, and have not previously been measured. In addition to their explicit values, which are an important ingredient for precision jet substructure calculations using tracks [22, 23], their scale evolution provides a test of QCD beyond the DGLAP paradigm [24–26], yielding interesting insights into the non-linear renormalization group evolution of correlations in the hadronization process [27–30].

This paper presents a measurement of the energy distribution of tracks in identified high-p_{T} jets, using the full Run 2 dataset of proton–proton (pp) collisions at $\sqrt{s} = 13$ TeV recorded with the ATLAS detector at the LHC, corresponding to an integrated luminosity of 140 fb^{-1}. The measurement is performed differentially in r_q and in different regions of jet p_{T} and for different rapidity-ordering of a dijet system (*i.e.,* for more-central *vs.* more-forward jets). These distributions are used to extract the moments of r_q as a function of the jet p_T. The data are corrected for detector effects using Iterative Bayesian Unfolding (IBU) [31–33] and a machine learning-based method called OmniFold [34, 35] is employed as a novel data-driven correction for binning artifacts in the moment extractions.

2 ATLAS Detector

The ATLAS experiment [36] at the LHC is a multipurpose particle detector with a forward–backward symmetric cylindrical geometry and a near 4π coverage in solid angle.[1] It consists of an inner tracking detector surrounded by a thin superconducting solenoid providing a 2 T axial magnetic field, electromagnetic and hadronic calorimeters, and a muon spectrometer. The inner tracking detector covers the pseudorapidity range $|\eta| < 2.5$. It consists of silicon pixel, silicon microstrip, and transition radiation tracking detectors. Lead/liquid-argon (LAr) sampling calorimeters provide electromagnetic (EM) energy measurements with high granularity within the region $|\eta| < 3.2$. A steel/scintillator-tile hadronic calorimeter covers the central pseudorapidity range ($|\eta| < 1.7$). The endcap and forward regions are instrumented with LAr calorimeters for EM and hadronic energy measurements up to $|\eta| = 4.9$. The muon spectrometer surrounds the calorimeters and is based on three large superconducting air-core toroidal magnets with eight coils each. The field integral of the toroids ranges between 2.0 and 6.0 T m across most of the detector. The muon spectrometer includes a system of precision tracking chambers up to $|\eta| = 2.7$ and fast detectors for triggering up to $|\eta| = 2.4$. The luminosity is measured mainly by the LUCID–2 [37] detector, which is located close to the beampipe. A two-level trigger system is used to select events [38]. The first-level trigger is implemented in hardware and uses a subset of the detector information to accept events at a rate close to 100 kHz. This is followed by a software-based trigger that reduces the accepted rate of complete events to 1.25 kHz on average depending on the data-taking conditions. A software suite [39] is used in data simulation, in the reconstruction and analysis of real and simulated data, in detector operations, and in the trigger and data acquisition systems of the experiment.

3 Simulated event samples

Samples of Monte Carlo (MC) simulated dijet events are used to perform the unfolding and compare with the corrected data. Pythia 8.230 [40, 41] is used as the nominal MC generator for this analysis, and is also referred to here as the 'nominal' simulation. Samples of $2 \to 2$ dijet events were simulated at leading-order (LO) in QCD using the A14 tune [42], the Lund string hadronisation model and the NNPDF2.3lo [43] parton distribution function (PDF) set. The Pythia parton shower (PS) algorithm uses a dipole-style p_T-ordered evolution, and its renormalisation and factorisation scales were set to the geometric mean of the squared transverse masses of the outgoing particles. EvtGen [44] was used to model decays of heavy-flavour hadrons.

Two sets of Sherpa 2.2.5 [45] dijet events were simulated with the default AHADIC cluster hadronisation model [46] or with the Sherpa interface to the Lund string hadronisation model as implemented in

[1] ATLAS uses a right-handed coordinate system with its origin at the nominal interaction point (IP) in the centre of the detector and the z-axis along the beam pipe. The x-axis points from the IP to the centre of the LHC ring, and the y-axis points upwards. Cylindrical coordinates (r, ϕ) are used in the transverse plane, ϕ being the azimuthal angle around the z-axis. The pseudorapidity is defined in terms of the polar angle θ as $\eta = -\ln\tan(\theta/2)$. Angular distance is measured in units of $\Delta R \equiv \sqrt{(\Delta\eta)^2 + (\Delta\phi)^2}$.

Pythia 6.4, and its decay tables. These samples include LO matrix element calculations for $2 \to 2$ processes, and use the Sherpa parton shower algorithm based on Catani–Seymour dipole subtraction [47]. The CT14nnlo next-to-next-to-leading-order (NNLO) PDF [48] set is used for matrix element calculations and CT10 is used for multi-parton interactions (MPI) [49].

A sample of Herwig 7.1.3 [50–52] multijet events was generated with the MMHT2014nlo PDF set [53], default cluster hadronisation model and the default angle-ordered PS. This sample models $2 \to 2$ matrix elements with NLO accuracy and $2 \to 3$ matrix elements with LO accuracy. The parton shower was matched to the matrix element calculation using the MC@NLO matching scheme [54, 55], and the p_{T} of the leading jet is taken as the renormalisation scale.

All generated events used in the unfolding and its associated uncertainties were passed through a full detector simulation [56] based on Geant4 [57] and overlaid with simulated minimum-bias interactions generated using Pythia 8 with the A3 tune [58] and NNPDF2.3lo PDF set [43] to represent the effect of multiple pp interactions in the same and neighboring bunch crossings ('pile-up'). The distribution of the average number of pile-up interactions in simulation was reweighted during data analysis to match that observed in Run 2 data. Additional details of the MC samples used in this measurement may be found in Ref. [59].

4 Event reconstruction and selection

Detector-level inner-detector tracks are required to have $p_{\mathrm{T}} > 500$ MeV, to be associated with the primary vertex with the largest sum of track p_{T}^2 in the event, and to satisfy 'loose' quality criteria [60]. At particle-level, charged hadrons (and leptons produced through secondary decays) are required to have $p_{\mathrm{T}} > 500$ MeV. Tracks (charged hadrons) within $\Delta R = 0.4$ of the cores of selected detector-level (particle-level) jets are clustered using the anti-k_t algorithm [61] as implemented in FastJet [62] in order to obtain the jet p_{T} originating only from charged particles, *i.e.* $p_{\mathrm{T}}^{\mathrm{charged}}$.

Detector-level jets are reconstructed from particle-flow objects [63] using the anti-k_t algorithm with radius parameter $R = 0.4$ [61, 62], which combine measurements from the ATLAS inner detector and calorimeter systems to improve the jet energy resolution (JER) and the jet reconstruction efficiency, especially for low-p_{T} jets. The jet energy scale (JES) is calibrated so that, on average, the detector-level jet energy is the same as that of the corresponding particle-level jets [64]. These jets are 'cleaned' to remove those originating from detector noise, cosmic rays and beam-induced processes [65]. Merging pixel clusters within the dense core of jets at detector-level may degrade the track parameter resolution and decrease the track reconstruction efficiency. These effects are mitigated with the use of stacked neural networks that assist with ambiguity-solving during track reconstruction by splitting clusters of pixel charges [66–70]. Particle-level jets are reconstructed in MC generated events without detector simulation. All particles with a laboratory-frame lifetime τ such that $c\tau > 10$ mm are used, except those particles that are expected to leave no or negligible energy depositions in the calorimeter (*i.e.* neutrinos or muons).

Events in data are selected using single-jet triggers [38, 71] and the highest two p_{T} jets are analyzed. The leading and subleading jets are selected for the measurement at both detector- and particle-level, and are required to satisfy $p_{\mathrm{T}}^{\mathrm{leading}} > 240$ GeV and $p_{\mathrm{T}}^{\mathrm{leading}} < 1.5 \times p_{\mathrm{T}}^{\mathrm{subleading}}$. This balance requirement simplifies the interpretation of the final state in terms of a $2 \to 2$ scattering process. Both jets must be completely within the inner detector acceptance ($|\eta_{\mathrm{jet}}| < 2.1$).

5 Unfolding procedure

The selected data are unfolded to correct for detector bias, resolution, and acceptance effects by applying IBU [33] with two iterations implemented in RooUnfold [72]. The MC generator used to unfold the data is Pythia 8.230, and the total number of iterations is chosen to minimize the total uncertainty. The unfolding procedure corrects the r_q constructed from detector-level objects to particle level, where the same kinematic requirements are imposed on particle-level jets as on detector-level jets.

Particle-level jets not passing the detector-level kinematic requirements, and detector-level jets not passing the particle-level requirements, are accounted for with efficiency and purity corrections, respectively. Purity corrections are applied before the regularized inversion of the response matrix, and efficiency corrections are applied afterwards. One additional low jet p_{T} bin is included in the unfolding matrix so migrations into that bin take the place of (much of) the inefficiency. The jet p_{T}, r_q, and η region are unfolded simultaneously, where the η region of the two selected jets (denoted 'Forward η bin' and 'Central η bin', respectively). The binning of the jet p_{T} and of the r_q distribution is chosen such that the migrations in the unfolding matrix are typically less than 60%. The migrations are smallest at low r_q and low jet p_{T}, with larger migrations in the higher p_{T} bins where the track p_{T} resolution degrades. For each jet p_{T} bin, the unfolded distribution is normalized to the number of jets in that bin.

6 Uncertainties

Statistical and systematic uncertainties originating from several different sources are considered in this measurement. Different sources of uncertainty are always treated independently.

The statistical uncertainties due to the finite statistics of the data and simulated event samples are evaluated from 100 pseudo-experiments using the bootstrap method [73]. The data and simulation statistical uncertainties are typically subdominant. The statistical uncertainty from data is larger than that originating from MC samples throughout the measurement.

Theoretical uncertainties arise mainly from the accuracy of jet fragmentation modeling, as these discrepancies can modify the unfolding efficiency/purity corrections and the response matrix. The unfolding is repeated using the Pythia 8 prior and a response matrix constructed using the Sherpa 2.2.5 AHADIC sample instead of the nominal Pythia 8 one. The difference between this result and the nominal one is taken as a systematic uncertainty. This uncertainty is typically $\sim$ 5% in the tails of r_q, and $\sim$ 2% in the bulk of the r_q distribution, and is one of the dominant sources of uncertainty for large r_q values in the higher bins of jet p_{T} (beginning at $p_{\mathrm{T}} > 600$ GeV).

Experimental systematic uncertainties are evaluated by propagating variations from different sources through the unfolding procedure to find the difference between the varied and nominal results. Uncertainties on the jet energy scale and resolution are determined using a mixture of simulation-based and in situ techniques [64]. Uncertainties due to differences between the gluon-initiated jet energy response of different MC generator setups have also been reduced ('jet flavor response' in Ref. [64]) by performing more granular comparisons of the effect of different parton shower and hadronization models on the jet response as documented in Ref. [74]. These uncertainties cause the migration of jets into or out of the fiducial acceptance and modify the denominator of the r_q observable, typically accounting for uncertainties around 2% in total, but reaching up to 3.5% in some bins. Uncertainties related to the reconstruction of isolated tracks and tracks within dense environments are considered by modifying the measured p_{T} of individual tracks or removing them from the event [66, 75]. The tracking uncertainty is the largest source of uncertainty for r_q for all but the highest jet p_{T} bin. The dominant uncertainty in this category is related to the inclusive tracking efficiency. This uncertainty is largest for small values of r_q and is up to 8% in the more central η bin and 12% in the more forward η bin. Potential biases arising due to differences between disabled modules of the Tile calorimeter during certain data-taking periods between the data and simulation are evaluated. This is done by repeating the measurement with a veto on jets directed at any disabled modules in both data and simulation, and comparing this result to the nominal result. These uncertainties are typically between $2-3$%, with the largest impact at lower values of r_q. An uncertainty is added to cover unfolding regularization biases, which is determined by unfolding the detector-level Pythia distribution after it is reweighted based on a comparison of the corresponding simulated detector-level distribution and the detector-level data prior [76]. This uncertainty is largest for small values of r_q and increases with the jet p_{T}. This uncertainty is typically subdominant, but in the highest jet p_{T} bin, it is the dominant source of uncertainty, reaching up to 12%. Uncertainties related to the overlaid pileup events amount to an error of less than 1% throughout the measurement.

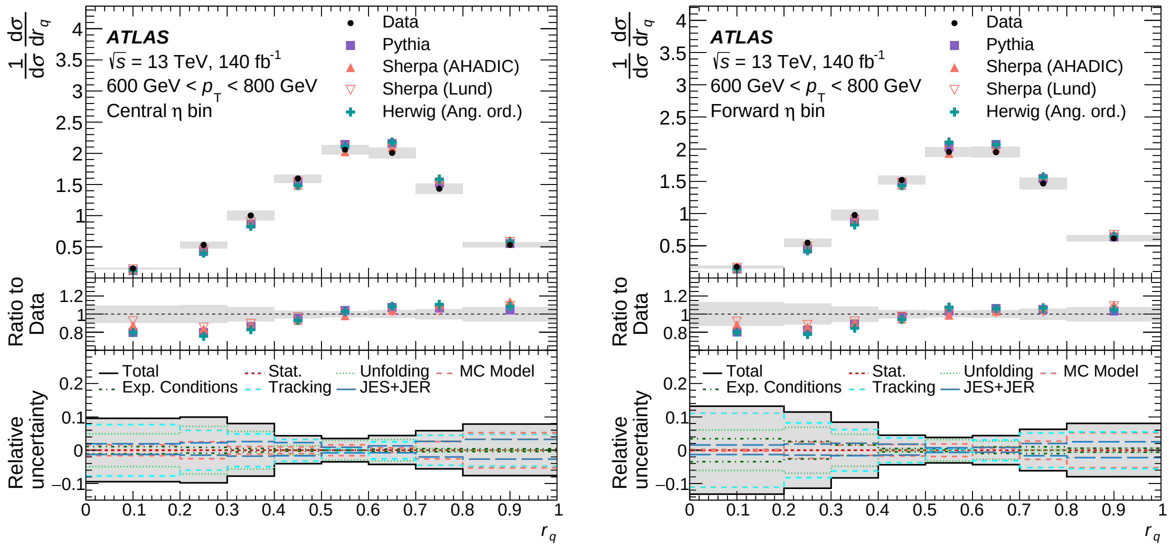
7 Results

The measured cross-section as a function of r_q is shown for a representative bin of jet p_{T} from 600–800 GeV, for the central and forward regions in Figure 1. These measured distributions are compared to predictions from several MC generators, which typically agree with the data within uncertainties. The different MC predictions show the same trends, tending to underestimate the cross-section at low values of r_q and overestimate the cross-section at high values. These trends are consistent across all measured p_{T} bins.

The r_q distributions are used to extract the moments, $\mathrm{E}[X^n]$, as a function of the jet p_{T}. These moments are shown in Figure 2, and are found to evolve slowly with the jet p_{T}. The binning of r_q introduces artifacts in the moment extraction, and these are corrected for using a data-driven method based on the OmniFold algorithm [34, 35]. In this method, the unbinned data are unfolded using OmniFold, and multiplicative correction factors are determined by comparing the moments with and without the binning. This improves upon the MC-based binning corrections that have been applied in previous measurements [4, 6] by directly utilizing the data for the correction. The correction factors are applied to all moments extracted from the r_q distribution accordingly, after each systematic variation, where the magnitudes of the correction factors range from 0.92 to 1. This approach is conservative, as it preserves the absolute uncertainty of each systematic variation on the uncorrected distribution following the binning correction.

The extracted moments of the r_q distribution can be expressed in terms of the cumulants of the distribution, κ_n, which can be written in terms of the central moments $\mu_n = \mathrm{E}[(X - \mathrm{E}[X])^n]$, as $\kappa_2 = \mu_2$, $\kappa_3 = \mu_3$, $\kappa_4 = \mu_4 - 3\mu_2^2$, $\kappa_5 = \mu_5 - 10\mu_3\mu_2$, and $\kappa_6 = \mu_6 - 15\mu_4\mu_2 - 10\mu_3^2 + 30\mu_2^3$ [20, 77]. The energy dependence of the relationship between pairs of these cumulants is theoretically determined by non-trivial renormalization group flows (RG flows) that govern the scale dependence of correlations in the hadronization process. Physically, the track function depicts not only the energy fraction of the initial hard parton converted into all the charged hadrons, but also the correlations among them [18]. One prediction of this theory is that as the energy increases, the cumulants should converge towards some fixed values that depend on the quark-/gluon-initiated jet composition (the cumulants for demixed quark-/gluon-initiated jet r_q distributions should converge to 0).

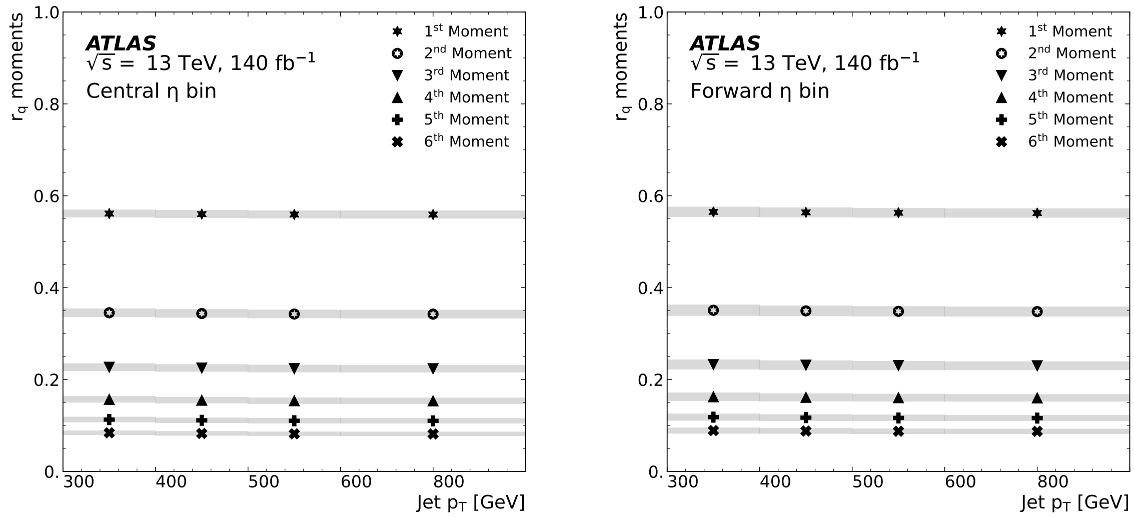
Figure 3 shows the relationship between selected pairs of cumulants extracted from the unfolded data distributions and compared to an analytical QCD prediction at next-to-leading-logarithm (NLL) of the RG



(a)

(b)

Figure 1: The unfolded central (a) and forward (b) normalized differential cross-sections as a function of r_q for data compared to predictions from several MC generators. The grey uncertainty band shows the combined statistical and systematic uncertainties on the measurement. The bottom panel shows the breakdown of the uncertainties grouped by their sources. In particular, the 'Exp. Conditions' group includes uncertainties related to the overlaid pileup events and potential biases due to differences between disabled modules of the Tile calorimeter.



(a)

(b)

Figure 2: The first six moments of the unfolded (a) central and (b) forward r_q distributions in jet p_{T} bins. The grey uncertainty band shows the combined statistical and systematic uncertainties on the measurement.

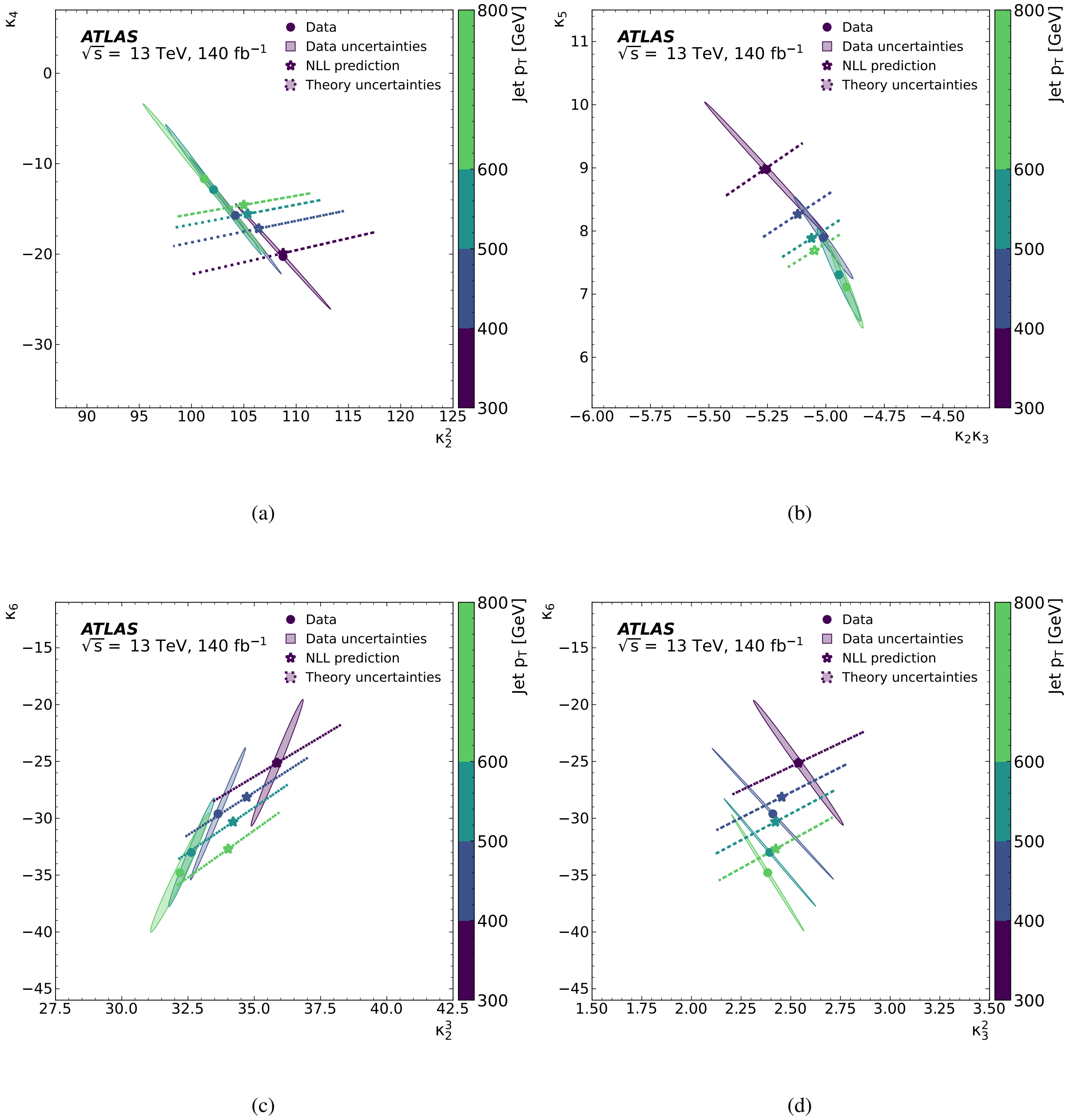


Figure 3: Non-trivial RG flow relationship between higher-order cumulants and products of lower-order ones coming from the non-linearity of the track function evolution. The relationship between (a) κ_4 and κ_2^2, (b) κ_5 and $\kappa_2\kappa_3$, (c) κ_6 and κ_2^3, and (d) κ_6 and κ_3^2 are shown for different bins of the particle-level jet p_{T}. The ellipses correspond to the 68% confidence regions based on the combined statistical and systematic uncertainty (data with solid boundaries) and scale variations (theory with dotted boundaries).

flow provided by the authors of Ref. [20]. The NLL predictions perturbatively evolve the track function distribution using data in the lowest p_{T} bin as the initial condition, meaning that the direction of flow can be compared, but not each measurement individually. Due to the strong correlations in uncertainties between the cumulants, the 68% confidence regions for each measurement have a highly elliptical shape for both theory and experiment. Binning corrections for the cumulants are derived using the same method as for the moments. While these corrections tend to be close to 1, they can be much larger or smaller for some of the higher cumulants.

Comparing the shapes of the flows between data and theory provides a direct test of non-linear renormalization group flows during jet formation. The results in Figures 3(a)–3(d) show good data-theory agreement and are consistent with the picture of flow towards a fixed point. This is seen by the fact that the moments evolve more slowly at higher momentum scales. The convergence may be better tested at even higher momentum scales.

8 Conclusions

This paper presents a measurement of the differential cross-section of the transverse momentum fraction r_q carried by charged hadrons of jets, and the scale dependence of its moments. The measurement is performed on an inclusive selections of dijet events, using a dataset corresponding to an integrated luminosity of 140 fb^{-1} of proton–proton collisions at $\sqrt{s} = 13$ TeV recorded with the ATLAS detector at the LHC. Jets are reconstructed using the anti-k_t algorithm with $R = 0.4$, and their associated charged-particle tracks are used to measure the unfolded single-differential cross-section of r_q, the observable of interest. The moments of this distribution are extracted, which are used to construct the lower-order cumulants and their relationships. This measurement of the r_q distribution enables the determination of universal track functions, which are a necessary component in providing theoretical calculations of jet substructure observables using charged particles. This paves the way towards theoretical precision for a new class of observables that will enable further studies of jet formation and the strong interaction.

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Appendix

A Quark and gluon interpretation

A statistical demixing of the quark- and gluon-like cross-sections is performed, following the demixing strategy outlined in Ref. [4]. Since the shape of the r_q distribution for a given jet p_{T} depends on the flavor of the initiating parton but not η, the quark and gluon distributions may be inferred from the measurements of the central and forward distributions using: $h_i^F = f_Q^F h_i^Q + f_G^F h_i^G$ and $h_i^C = f_Q^C h_i^Q + f_G^C h_i^G$, where h_i is one bin of the histogram, F and C denote the forward and central regions, and Q and G represent quark or gluon respectively.

The quark and gluon fractions for the more forward and more central jets are obtained from the nominal Pythia 8 MC event sample,[2] and are shown in Figure 4. By taking these fractions from an MC prediction, this results in a model-dependence, and so an additional uncertainty is applied to account for differences in the predicted quark and gluon fractions across different theoretical models.

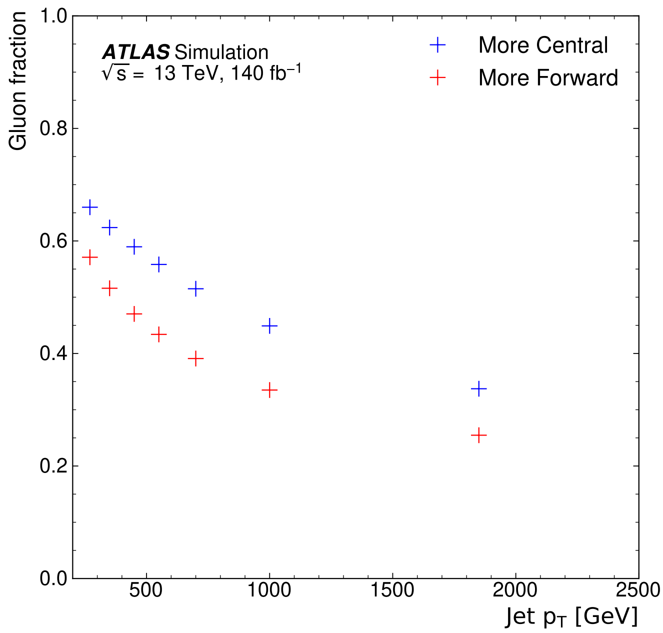
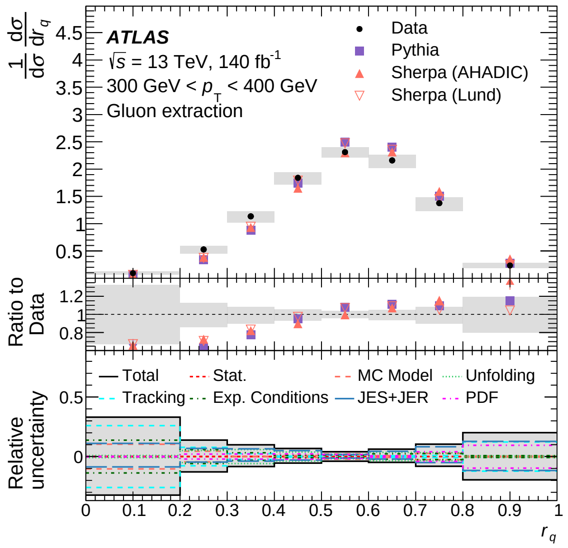


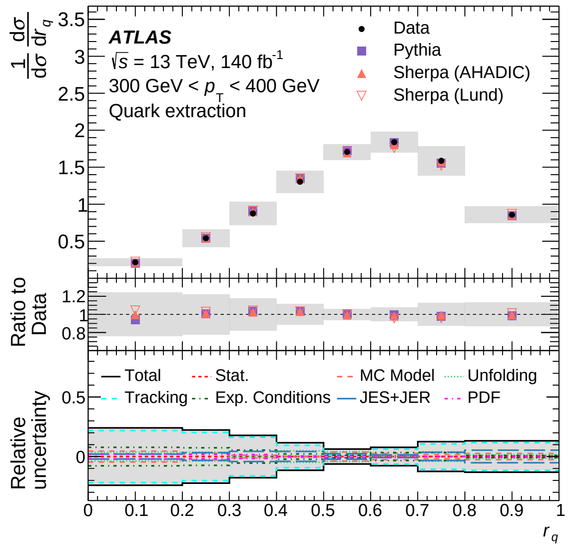
Figure 4: The gluon fraction obtained from the nominal Pythia 8 MC event sample for the more forward and more central of the two dijets as a function of the jet p_{T}. The cross markers do not include uncertainties in this plot.

The demixed quark and gluon interpretation of r_q are shown in Figure 5 for two representative jet p_{T} bins. In general, the agreement between data and MC is similar to the agreement with the measured cross-sections, with larger discrepancies for the gluon extraction than for the quark extraction. The statistically demixed gluon-initiated jets have a slightly narrower r_q distribution than that found for quark-initiated jets due to the

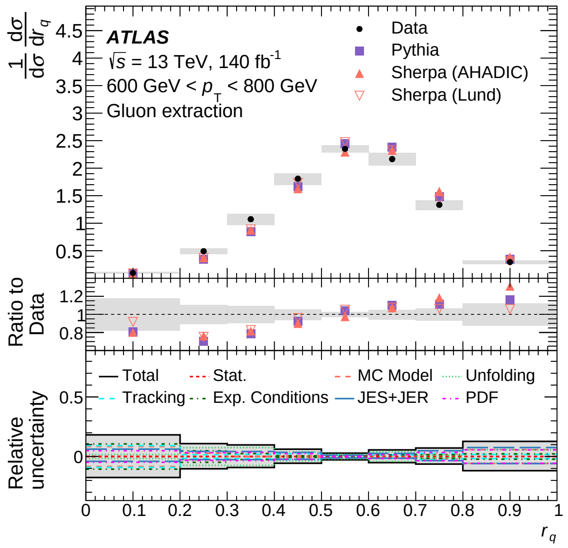
[2] The jet flavor is determined by the highest energy parton associated to the jet.



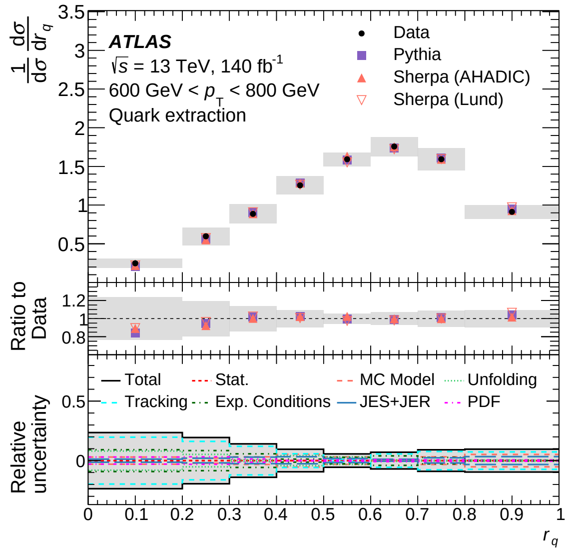
(a)



(b)



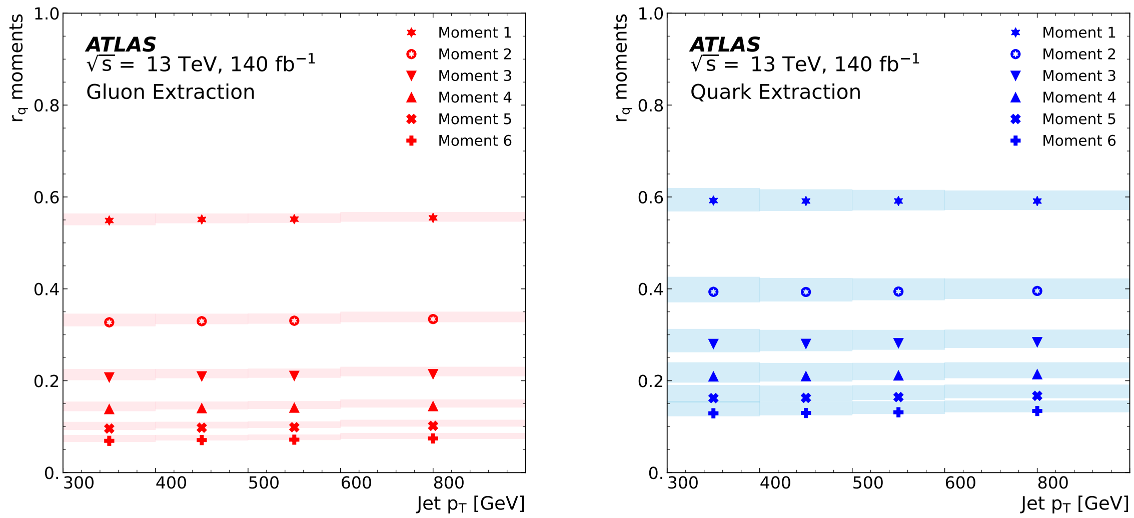
(c)



(d)

Figure 5: The demixed (a, c) gluon and (b, d) quark interpretation of the unfolded r_q cross-sections for (a, b) 300 GeV $< p_{\mathrm{T}} <$ 400 GeV, and (c, d) 600 GeV $< p_{\mathrm{T}} <$ 800 GeV for data compared to predictions from several MC generators. The grey uncertainty band shows the combined statistical and systematic uncertainties on the measurement. The bottom panel shows the breakdown of the uncertainties grouped by their sources. In particular, the 'Exp. Conditions' group includes uncertainties related to the overlaid pileup events and potential biases due to differences between disabled modules of the Tile calorimeter.

larger color factor, but the overall distributions are very similar. The central moments of the r_q distribution are shown in Figure 6 for the extracted quark and gluon cross-sections. All six moments extracted from the demixed r_q distributions are systematically higher for quark-initiated jets than for gluon-initiated jets.



(a) (b)

Figure 6: The first six moments of the demixed (a) gluon and (b) quark r_q distributions in jet p_{T} bins. The uncertainty bands show the combined statistical and systematic uncertainties on the measurement.

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