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2 **Shanghai Jiao Tong University for the degree of**
3 **Doctor of Philosophy in Physics**

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6 Search for new phenomena in dijet events with
7 quark/gluon tagger using the ATLAS detector

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在 ATLAS 双喷注末态中利用 夸克/胶子标定寻找新粒子

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摘要

59

60 这篇论文中所呈现的物理分析旨在寻找标准模型之外的新物理现象，使用由
61 ATLAS 探测器记录的质子-质子碰撞数据，其积分亮度为 140 fb^{-1} ，中心质心能量
62 为 13 TeV 。该分析在三个不同的谱中寻找超越标准模型的新共振态证据：未标
63 记双喷注不变质量、一个胶子标记和两个胶子标记信号道。为了增加寻找新共振
64 态的灵敏度，该分析采用了一种基于关联粒子轨迹数量的胶子标记方法，以更优
65 地寻找一个或多个胶子衰变的共振体迹象。由于来自夸克和胶子的喷注可以使用
66 夸克/胶子标记器进行识别，因此本研究开发了两种标记器：一种基于与喷注关联
67 的带电径迹数目，而另一种则采用增强决策树来结合各种喷注次级结构可观测量，
68 同时提供了标记效率的对撞数据与蒙特卡洛模拟之间的差异。在数据上运用矩阵
69 方法，从两个富含夸克/胶子地子样本中提取真实的夸克/胶子喷注比例，该样本由
70 喷注的赝快度定义。在分析中，利用了将量子色动力学本底估计为参数化双喷注
71 质量谱的统计框架。然后在 95% 的置信水平上，针对多种超出标准模型物理理论
72 的信号，设置了上限。

73

74 **关键词：**标准模型，ATLAS 探测器，喷注判定

ABSTRACT

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ABSTRACT

76

77 The physics analyses presented in this PhD dissertation search for new physics be-
78 yond the Standard Model (BSM) in the dijet mass distribution using an integrated lumi-
79 nosity of 140 fb^{-1} of proton-proton collisions with a centre-of-mass energy at 13 TeV
80 recorded by the ATLAS detector. This analysis aims at searching for the evidence of the
81 BSM resonances that decay into two jets. Jets originating from quarks and gluons can be
82 identified using quark/gluon tagger. Two taggers are investigated: one tagger based on
83 the number of charged tracks associated with the jets, while the other employs a boosted
84 decision tree to combine various jet substructure observables. Differences between data
85 and Monte Carlo simulation of tagging efficiency are provided. A matrix method is
86 performed on data to retrieve the quark/gluon fraction from quark/gluon-enriched sub-
87 samples, defined by the pseudorapidity of the jet. In the analysis, the quantum chromo-
88 dynamics (QCD) background is estimated by the statistical framework which parame-
89 terised the dijet mass spectrum. Upper limits then are set at the 95% confidence level on
90 a variety of signal models of BSM physics.

91

92 **KEY WORDS:** Standard Model, ATLAS, calibration, jet tagging

93 **Contents**

94	1 Introduction	1
95	2 The theory framework	3
96	2.1 The Standard Model	3
97	2.1.1 Quantum chromodynamics	5
98	2.2 Physics beyond the Standard Model	7
99	2.2.1 Kaluza-Klein Graviton	7
100	2.2.2 Quantum Black Hole	8
101	3 The ATLAS Experiment	9
102	3.1 The Large Hadron Collider	9
103	3.2 The ATLAS detector	11
104	3.2.1 Inner detector	11
105	3.2.2 Calorimeters	14
106	3.2.3 Muon spectrometer	18
107	3.2.4 Trigger and data acquisition	19
108	4 Jets in ATLAS	21
109	4.1 Jet reconstruction	21
110	4.2 Jet calibration and cleaning	24
111	4.2.1 Pile-up corrections	24
112	4.2.2 Jet energy scale and η calibration	25
113	4.2.3 Global sequential calibration	26
114	4.2.4 Residual <i>in situ</i> calibration	27
115	5 The calibration of quark/gluon jets taggers	28
116	5.1 Data and Monte Carlo samples	28
117	5.1.1 Data	28
118	5.1.2 Monte Carlo simulation	29
119	5.2 Object and Event selection	30
120	5.2.1 Physics object definition	31
121	5.2.2 Event Selection and definition of quark and gluon-enriched samples	32
122	5.3 Quark/gluon tagging variables	32
123	5.3.1 The BDT tagger	34

Contents

124	5.3.1.1	Feature selections	35
125	5.3.1.2	Training weights	36
126	5.3.1.3	Training Configuration	39
127	5.4	Matrix Method	42
128	5.5	MC non-closure	45
129	5.5.1	Closure test for BDT tagger	47
130	5.5.2	Summary for the MC Closure test	51
131	5.6	Scale factor	51
132	5.7	Systematic uncertainties	59
133	5.7.1	Parton shower modelling uncertainty	59
134	5.7.2	Hadronisation modelling uncertainty	60
135	5.7.3	Matrix element uncertainty	61
136	5.7.4	PDF uncertainty	61
137	5.7.5	Scale variation uncertainty	61
138	5.7.6	Splitting-Kernel variation uncertainty	62
139	5.7.7	Tracking uncertainty	62
140	5.7.8	JES /JER uncertainty	63
141	5.7.9	N_{trk} / BDT re-weighting	63
142	5.7.10	The MC non-closure	67
143	5.7.11	Statistical uncertainty	67
144	5.8	Results	68
145	6	Search for new phenomena in dijet events	86
146	6.1	Monte Carlo models	87
147	6.1.1	QCD background	87
148	6.1.2	Kaluza-Klein Graviton	87
149	6.1.3	Quantum Black Hole	87
150	6.1.4	Gaussian resonances	88
151	6.2	Events selections	90
152	6.2.1	Observables and Kinematic Variables	90
153	6.2.2	Baseline selection	91
154	6.3	Quark-Gluon Sample Selection	92
155	6.3.1	Selection Criteria	93
156	6.4	Signal Optimisation	99

Contents

157	6.4.1	y^* Cut Optimisation	99
158	6.4.2	Optimised Selection	102
159	6.4.3	Selected Kinematic Plots	102
160	6.5	Statistical Framework	105
161	6.5.1	Fitting Framework	105
162	6.5.2	Statistical Method	106
163	6.5.2.1	Parametric background models	106
164	6.5.2.2	Uncertainties	107
165	6.5.2.3	Likelihood function definition	107
166	6.5.2.4	Statistical Method	108
167	6.5.2.5	Test statistic and p-value definitions	109
168	6.5.2.6	Generation of pseudo-data	110
169	6.5.2.7	Definition of exclusion limit	110
170	6.5.2.8	Implementation	111
171	6.5.3	Background Estimation	111
172	6.5.4	Analysis Strategy	111
173	6.5.5	Spurious Signal Tests	112
174	6.5.6	Fit Stability Tests	116
175	6.6	Systematic uncertainties	118
176	6.7	Results	120
177	7	Conclusions	122
178	8	Acknowledgements	136

179

1 Introduction

180 Over the past seventy years, the theories and discoveries of thousands of physi-
181 cists have developed a notable insight into the fundamental structure of matters, called
182 fundamental particles, which are governed by four fundamental forces. One of the best
183 understandings of how these particles and three of the forces interact with each other
184 is encapsulated in the Standard Model (SM) [1, 2] of particle physics. Developed in the
185 early 1970s, it has been successfully proved by almost all experimental results. The huge
186 success of the discovery of Higgs Boson in 2012 predicted by the SM was awarded the
187 Nobel Prize in Physics in 2013. The SM has become established as a well-tested physics
188 theory.

189 Although the SM accurately describes the phenomena within its domain, there are
190 still theoretical flaws that prevent some fundamental physical phenomena from being
191 fully explained by the SM. First of all, the model contains many parameters that cannot
192 be derived from calculations alone but must be determined by experiment. In 1998, the
193 Japanese Super Kamioka neutrino detector published results on neutrino oscillations that
194 suggested the neutrinos have a non-zero rest mass, which did not match the prediction
195 made by the SM. Besides, the existence of gravity and dark matter has not yet been
196 described by the SM theory.

197 Many models of physics beyond the Standard Model (BSM) [3] predict the presence
198 of new particles that couple to quarks and/or gluons. Such particles could be produced
199 in proton-proton collisions at the Large Hadron Collider (LHC) [4] and then decay into
200 quarks and gluons, during this process two hadronic jets are created, which then can be
201 seen by the detector. The new energy regime ($\sqrt{s} = 13$ TeV) with an integrated luminosity
202 of 140 fb^{-1} provided by the LHC opens a window to search for BSM particles.

203 In the SM, these dijet events are generated mainly by quantum chromodynamic
204 (QCD) processes and appeared to be a smoothly decreasing invariant mass (m_{jj}) dis-
205 tribution, however, a new particle that decays into quarks or gluons could appear as a
206 resonance in the m_{jj} spectrum. If the resonant samples can be classified based on the
207 type of parton that initiated the jets, the sensitivity of the search for such resonances
208 could be largely increased. Hence, classifying jets as initiated from a quark or a gluon
209 can be effective for improving SM measurements and searches for BSM physics.

210 Recent developments [5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21]

Introduction

211 in quark/gluon (q/g) tagging have resulted from advances in the theoretical [22], phe-
212 nomenological [23, 24, 25, 26] and experimental understanding of q/g tagging as well
213 as the development of powerful machine learning techniques that can utilize the entire
214 jet internal radiation pattern. The calibration of q/g taggers is performed to account for
215 the systematics of searching results.

216 This thesis is structured as follows. Chapter 2. describes the theoretical framework
217 of the SM, its limitations and various potential extensions beyond it. An introduction
218 to the LHC and the ATLAS detector is given in Chapter 3. Jet reconstructions and cal-
219ibrations are briefly described in Chapter 4. The quark/gluon tagger definitions and the
220 selection criteria used to generate the various event samples employed in the discriminant
221 extraction, the method and the scale factor results are presented in Chapter 5. The details
222 of the search for new resonances in the dijet spectrum and the limit setting results are
223 shown in Chapter 6. In the end, the conclusion and outlook of the research are presented
224 in Chapter 7.

225

2 The theory framework

226 2.1 The Standard Model

227 The SM of particle physics, which describes the three fundamental interactions -
 228 strong, weak and electromagnetic interactions, alongside the elemental constituents that
 229 constitute all forms of matter, stands as the most triumphant theory within the realm of
 230 particle physics. The SM divides particles into two categories, fermions and bosons,
 231 based on the values of their spin: fermions are the particles that makeup matter, such as
 232 electrons in leptons, quarks and neutrinos, which have half-integer spin; bosons are the
 233 particles that transmit forces, such as photons and mesons that transmit electromagnetic
 234 forces, gluons that transmit strong nuclear forces, W and Z that transmit weak nuclear
 235 forces, have integer spin. Different properties shown in fermions and bosons are due to
 236 the difference in spin. According to the spin-statistics theorem, fermions obey the Pauli
 237 exclusion principle, whereas bosons do not, thus bosons do not have a theoretical limit
 238 on their spatial density. All particles and forces with their masses, charges and spines are
 239 summarised in Figure 2.1.

240 The SM serves as an exemplar of a quantum field theory, offering the mathematical
 241 underpinning for such a framework. The Lagrangian controlled the dynamics and kine-
 242 matics of the system satisfies the $SU(3) \times SU(2)_L \times U(1)_Y$ gauge symmetry, in which
 243 $U(1)_Y$ corresponds to a particle B with weak hypercharge Y . $SU(2)_L$ corresponds to
 244 particles W_α ($\alpha = 1, 2, 3$) with weak isospin T and only left-handed chiral particles.
 245 The electroweak force which unifies the electromagnetism and the weak interaction as a
 246 Yang-Mills field is represented by the group $SU(2)_L \times U(1)_Y$, mathematically. In SM,
 247 the Z^0 boson and the photon (γ) are given by:

$$\begin{pmatrix} \gamma \\ Z^0 \end{pmatrix} = \begin{pmatrix} \cos \theta_W & \sin \theta_W \\ -\sin \theta_W & \cos \theta_W \end{pmatrix} \begin{pmatrix} B \\ W_3 \end{pmatrix} \quad (2.1)$$

248 where θ_W is the weak mixing angle.

249 The charged massive bosons W^\pm are given by W_1 and W_2 :

$$W^\pm = \frac{1}{\sqrt{2}} (W_1 \mp iW_2) \quad (2.2)$$

250 $SU(3)$ corresponds to eight vector fields A^α ($\alpha = 1, 2, \dots, 8$) representing gluon fields,

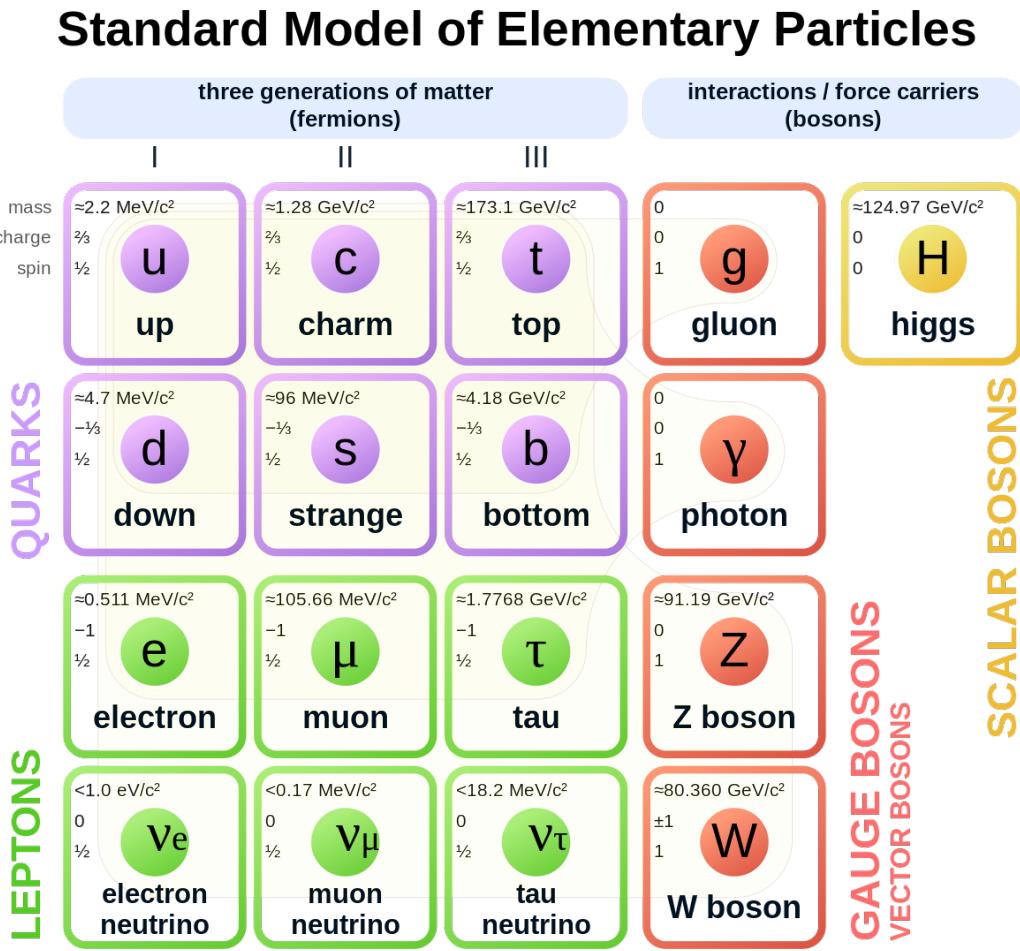


Figure 2.1 The Standard Model of particle physics

which are vector gauge bosons that carry the colour charge of the strong interaction and mediate between quarks in QCD. The Higgs boson, unlike all other known bosons such as the photon, is a scalar boson and has a non-zero average value in vacuum. It resulted from the process of spontaneous symmetry breaking. The Higgs mechanism explains the generation of the property "mass" for gauge bosons. At a critical temperature, the Higgs field introduces a vacuum expectation value that causes spontaneous symmetry breaking during interactions, leads the bosons it interacts with acquire masses. A Yukawa coupling is used in the SM to describe the interaction between the Higgs field and fundamental fermions, explain the generation of the masses of fermions.

This chapter therefore focuses on the present SM, various extensions and variants of the SM that have been proposed by theoretical physicists are explored in Section 2.2.

262 **2.1.1 Quantum chromodynamics**

263 QCD is the theory of the strong interaction between quarks and gluons, and it is a
 264 fundamental component of the SM of particle physics. Satisfying the $SU(3)$ symmetry
 265 group invariant, QCD is a non-abelian gauge theory, over the years, QCD has collected
 266 a huge body of experimental evidence, proved that it has been a successful application
 267 from a quantum field theory.

268 The Lagrangian of QCD can be expressed as:

$$\mathcal{L}_{\text{QCD}} = \bar{\psi}_i \left(i\gamma^\mu (D_\mu)_{ij} - m\delta_{ij} \right) \psi_j - \frac{1}{4} G_{\mu\nu}^a G_a^{\mu\nu} \quad (2.3)$$

269 where ψ_i is the quark field in the fundamental representation of the $SU(3)$ gauge group,
 270 indexed by i and j running from 1 to 3; m corresponds to the quark mass; the γ^μ are Dirac
 271 matrices relating the spinor representation to the vector representation of the Lorentz
 272 group.

273 D_μ is defined as the gauge covariant derivative:

$$(D_\mu)_{ij} = \partial_\mu \delta_{ij} - ig_s (T_a)_{ij} \mathcal{A}_\mu^a \quad (2.4)$$

274 which couples the quark field with a coupling strength g_s to the gluon fields via the
 275 infinitesimal $SU(3)$ generators T_a . By including the Gell-Mann matrices λ_a ($a=1\dots 8$), an
 276 explicit representation of T_a is defined by $T_a = \lambda_a/2$.

277 The gauge invariant gluon field strength tensor $G_{\mu\nu}^a$ is given by:

$$G_{\mu\nu}^a = \partial_\mu \mathcal{A}_\nu^a - \partial_\nu \mathcal{A}_\mu^a + g_s f^{abc} \mathcal{A}_\mu^b \mathcal{A}_\nu^c \quad (2.5)$$

278 where \mathcal{A}_μ^a are the gluon fields, indexed by a, b and c running from 1 to 8; f^{abc}
 279 are the structure constants of $SU(3)$. The coupling strength g_s can be referred to strong
 280 coupling constant α_s :

$$\alpha_s = \frac{g_s^2}{4\pi} \quad (2.6)$$

281 There are some salient properties that QCD exhibits:

282 **Colour confinement**

283 This is a consequence of the force between two colour-charged particles that can

284 not be isolated in a condition that below the Hagedorn temperature of approxi-
 285 mately 2 terakelvin. To separate two quarks in a hadron, extremely high energy
 286 is required, leading to the creation of a quark-antiquark pair that formed a pair of
 287 hadrons rather than a single hadron. In addition, glueballs which are formed only
 288 of gluons are colourless and also consistent with confinement, causing difficulty
 289 in identification in experiments.

290 **Asymptotic freedom and the running coupling**

291 This is a feature of QCD that demonstrates the strong interactions between quarks
 292 and gluons become asymptotically weaker as the energy scale of them increases
 293 and the corresponding length scale decreases. This is opposite to the behaviour of
 294 colour-charged particles at low energies where the confinement of quarks and glu-
 295 ons exhibits. At high energy, the coupling decreases logarithmically as a function
 296 of momentum transfer Q :

$$\alpha_s(Q^2) \stackrel{\text{def}}{=} \frac{g_s^2(Q^2)}{4\pi} \approx \frac{1}{\beta_0 \ln(Q^2/\Lambda^2)} \quad (2.7)$$

297 where β_0 is a one-loop beta function in QCD and has the dependence of the cou-
 298 pling parameter g_s . The quantity Λ is referred to QCD scale that is measured
 299 in processes where the strong coupling constant and other measurables vary with
 300 momentum transfer Q . However, this is only effective at leading order (LO). By
 301 including higher order terms, the calculation expanded in order of α_s resulted in
 302 more complexity and less significance as the scale of Q increases. On the other
 303 hand, as Q tends to be infinite large, the coupling strength becomes zero thus the
 304 behaviors of quarks are asymptotically free. These variation of coupling α_s under
 305 the different scales of energy in QCD is described as the running coupling.

306 The calculation of matrix element in QCD can be rather complex as more and more
 307 perturbative contributions are considered, which requires the application of complicated
 308 integrals over a large number of variables. A Feynman diagram is used as a representa-
 309 tion of the expressions of these integrals pictorially and an improvement of undertaking
 310 the critical calculations.

311 With more interactions points involved in, more complicated the calculations be-
 312 come. The effects of self-interactions between particles themselves can happen by pro-
 313 ducing a virtual particle which is restricted by the uncertainty principle, represented as a

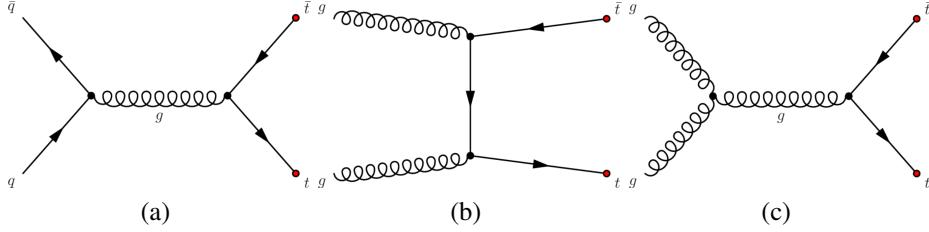


Figure 2.2 Feynman diagrams of strong interaction in top-antitop quarks production via (a) one gluon exchange in quark-antiquark annihilation, gluon-gluon fusion in (b) t-channel and (c) s-channel.

loop in a Feynman diagram. The accuracy of the calculation has dependency on the coupling α_s and is contributed to a fraction at each order. By including an infinite number of virtual particles, the calculations are led to divergent and infinite. A set of techniques named renormalization are employed in solving the infinities showed up in the calculations, by which the infinite self-interactions are parameterised by re-scaling them as finite values to compensate the effects. The ultraviolet divergence that occurs from integrating the contributions at extreme high energy is represented by renormalization scale μ_R , on the contrast, μ_F represents the condition of an integral diverges at infinitesimal energy.

2.2 Physics beyond the Standard Model

2.2.1 Kaluza-Klein Graviton

In particle physics, Kaluza–Klein theory (KK theory) [33] is a significant concept in physics. It's a classical unified field theory that attempts to unify gravitation and electromagnetism by introducing the notion of a fifth dimension beyond the four dimensions of space and time that we commonly encounter. This theory is regarded as an important precursor to more modern theories like string theory, which also incorporates the concept of extra dimensions. KK theory's exploration of additional dimensions has played a crucial role in advancing our understanding of fundamental forces and particles in the universe.

in the context of the KK theory, the Randall-Sundrum (RS) [34] model is distinguished by its introduction of an extra dimension, which is constrained within finite bounds by two distinct three-dimensional branes situated at either end. These branes essentially represent the four-dimensional spacetime familiar to us, while the additional

337 spatial dimension is localized and limited within this confined region. This theoretical
338 framework was formulated as a potential solution to the hierarchy problem of the SM,
339 and it offers a unique perspective on the behaviour of gravity and fundamental forces
340 within our universe. In this model, there exist KK towers of massive spin-2 gravitons
341 that can interact with the SM fields. The graviton sector within the RS1 model is fully
342 determined by two key parameters: m_{KK} and k/\bar{M}_{Pl} , where m_{KK} is the mass of KK gravi-
343 ton, k is a scale of order the Planck scale, M_{Pl} is effective four-dimensional (reduced)
344 Planck scale.

345 **2.2.2 Quantum Black Hole**

346 Quantum Black Hole (QBH), also called micro black holes, is regarded as hypothet-
347 ical mini (less than a solar mass unit) black hole that dominated by quantum mechanical
348 effects [35]. Some hypotheses predict that QBH could be produced at energies as low as
349 the TeV range, which can be generated in particle accelerators such as the LHC and can
350 be observed through the particles that are emitted by the process of Hawking radiation.
351 Theoretical calculations indicate that as black holes decrease in size, their rate of evap-
352 oration accelerates. This phenomenon leads to an abrupt release of particles, akin to a
353 sudden eruption, when a micro black hole approaches its final stages of evaporation.

354 In the simplest scenario, the decay of QBH via Hawking radiation [36] can be ap-
355 proximately described as isotropic decay to a many-particle final state. The threshold
356 of quantum-gravity energy scale M_D is set to be well below the the actual thermal black
357 hole production threshold for gravitational interactions so that two-body states in final
358 states are the dominant, a resonance-like result is expected in predominantly two-body
359 final states as jets near M_D . Such isotropic final states is aimed as probes of quantum
360 gravitational effects in this dijet analysis.

361

3 The ATLAS Experiment

362

3.1 The Large Hadron Collider

363

The LHC, built by European Organization for Nuclear Research (CERN) located in Geneva, Switzerland, is the largest circular particle accelerator in the world. The goal of it is to probe the various theoretical predictions made by physicists.

366

It consists superconducting magnets that construct a 27-kilometer ring lying in the tunnel under the ground. Inside the LHC, two beams made of protons or ions are accelerated to extreme high speed in opposite direction in individual vacuum pipes then made into collision by a strong magnetic field within the structures.

370

The LHC is the last section of the CERN accelerator complex where a series of machines accelerates the particles to increasingly higher and higher energies. The highest energies of beams are reached at the LHC.

373

Seven detectors are placed around four collision points in the collider. Different types of particles are accelerated according to the research, the main beams are protons, but the LHC also run beams of heavy ions as lead–lead collision or proton–lead collisions.

376

The energy of particles is increased by a series of processes before being injected into the main accelerator. For a proton-proton collision, negative hydrogen ions are generated by the linear particle accelerator Linac4 at 160 MeV then injected into the Proton Synchrotron Booster, where protons are obtained by stripping electrons away from the atom and accelerated to 2 GeV. After entered the Proton Synchrotron the energy of the protons is 26 GeV, and then their energies are increased in Super Proton Synchrotron to 450 GeV before they are finally injected into the main ring.

383

One of the characteristics that defines the power of an accelerator is the centre-of-mass energy, which represents the total momentum of the system and thus indicates the total mass of potential new particles as well as probes the internal structure of known particles under the law of energy invariant within the system. In 2010, the first collisions were made at an energy of 3.5 TeV each beam, later in 2018, an energy of 6.5 TeV per beam was achieved, resulted in the centre-of-mass energy of 13 TeV where the protons moved at a 99.9% speed of light. It took less than 90 μ s for photons to go through the whole LHC ring.

391

Other quantities such as luminosity, denoted as \mathcal{L} , also represents the performance

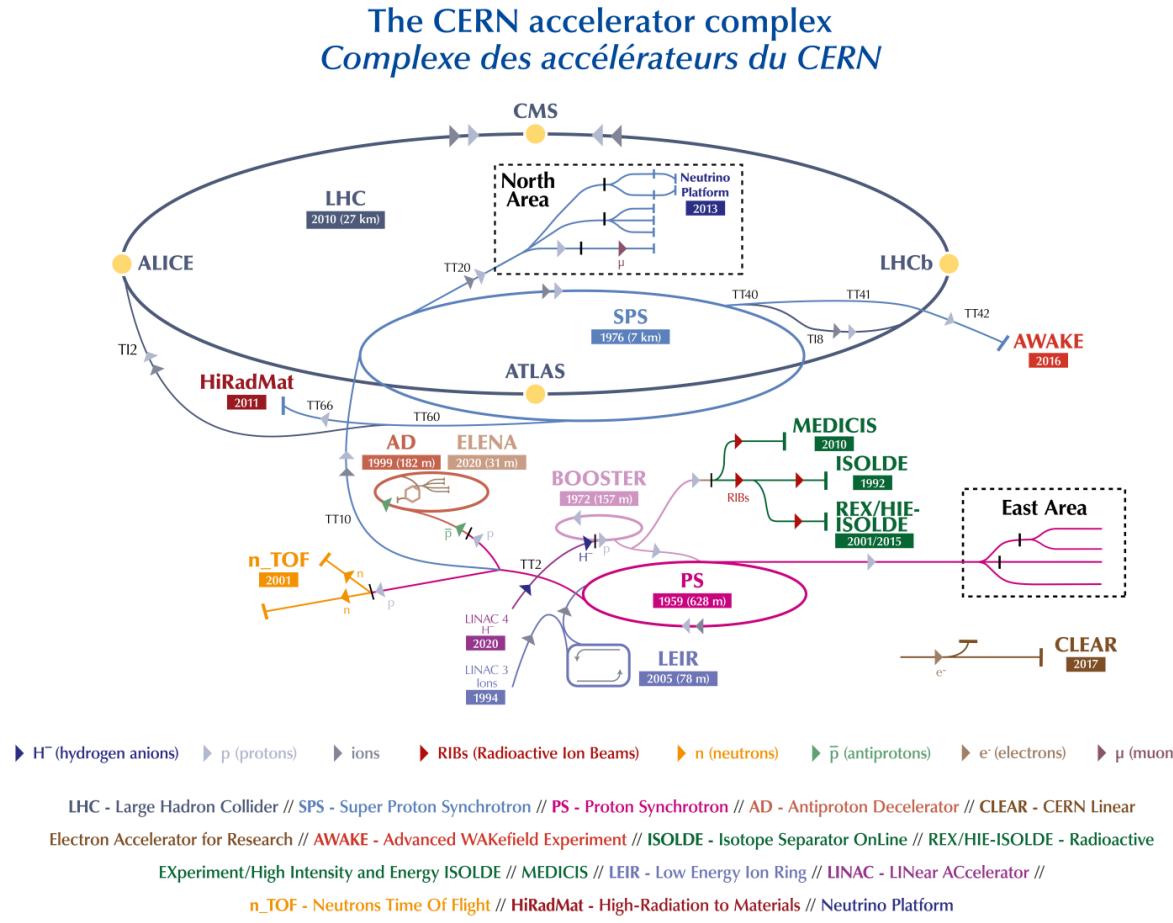


Figure 3.3 The CERN accelerator complex

392 of an accelerator. It is the rate of interactions during a certain period of time and can be
393 expressed as:

$$\mathcal{L} = \frac{N^2 f_{rev}}{4\pi\sigma_x\sigma_y} \quad (3.1)$$

394 where N is the number of particles in a bunch, in the case that a beam has Gaussian
395 distribution and has bunches crossing frequency f_{rev} . σ_x and σ_y denote as transverse
396 beam widths in the x- and y-plane. The luminosity takes the units of $\text{cm}^{-2} \cdot \text{s}^{-1}$.

397 The total number of physics events detected can be express as:

$$N_{\text{event}} = \sigma_{\text{event}} \cdot \int \mathcal{L} dt \equiv \sigma_{\text{event}} \cdot L \quad (3.2)$$

398 where L is the integrated luminosity with respect to time, σ_{event} is referred to the
 399 cross section of a specific physics process. The integrated luminosity takes the units of
 400 cm^{-2} which equals to the unit femtobarn (fb).

401 At the LHC, thousands of magnets around the accelerator are operated at a very
 402 low temperature of 271.3°C to maintain its superconducting state which allow them to
 403 conduct electricity without loss of energy. Hence, a system of liquid helium is used for
 404 cooling the accelerator and supply services.

405 Besides, superconducting radio frequency cavities which resonate electromagnetic
 406 fields are employed to accelerate the protons. Instead of having continuous beams, the
 407 protons are made into bunches, so that the collisions are taken place at discrete intervals
 408 between two beams with 115 billion protons per bunch at the frequency of 25 ns.

409 3.2 The ATLAS detector

410 The ATLAS detector [37] is the largest volume detector ever constructed for general-
 411 purpose particle research at the LHC. It has the shape of a cylinder with 44 meters long,
 412 7000 tonnes in weight and 25 meters in diameter, sitting in a cavern underground. It
 413 is designed to collect evidence of the properties of SM and search for new predictions
 414 made by particle physics beyond the SM.

415 To record the energy, momentum and trajectory of particles after collisions, the
 416 detector consisting of 6 different detecting subsystems placed in layers surrounding the
 417 interaction point to measure them individually and effectively.

418 An overall layout of the ATLAS detector is shown in Figure 3.4.

419 3.2.1 Inner detector

420 Charged particles above a certain p_{T} threshold are detected by the ATLAS Inner
 421 Detector (ID) which immersed in a 2 T solenoidal field, covered the pseudorapidity range
 422 $|\eta| < 2.5$. Appearing as tracks in the ID, an excellent momentum resolution as well as
 423 both primary and secondary vertex of them are provided by the ID. Within the range
 424 $|\eta| < 2.0$, electron identification is also provided.

425 The layout of the ID is shown in Figure 3.5 in cylindrical coordinate: $r = \sqrt{x^2 + y^2}$,
 426 where x -axis alongside the LHC ring and y -axis is perpendicular to the x -axis.

427 A cylindrical container around the ID has a length of 3512 mm each way and a
 428 radius of 1150 mm, tracks of 10 GeV traverse the sensors and structural elements in the

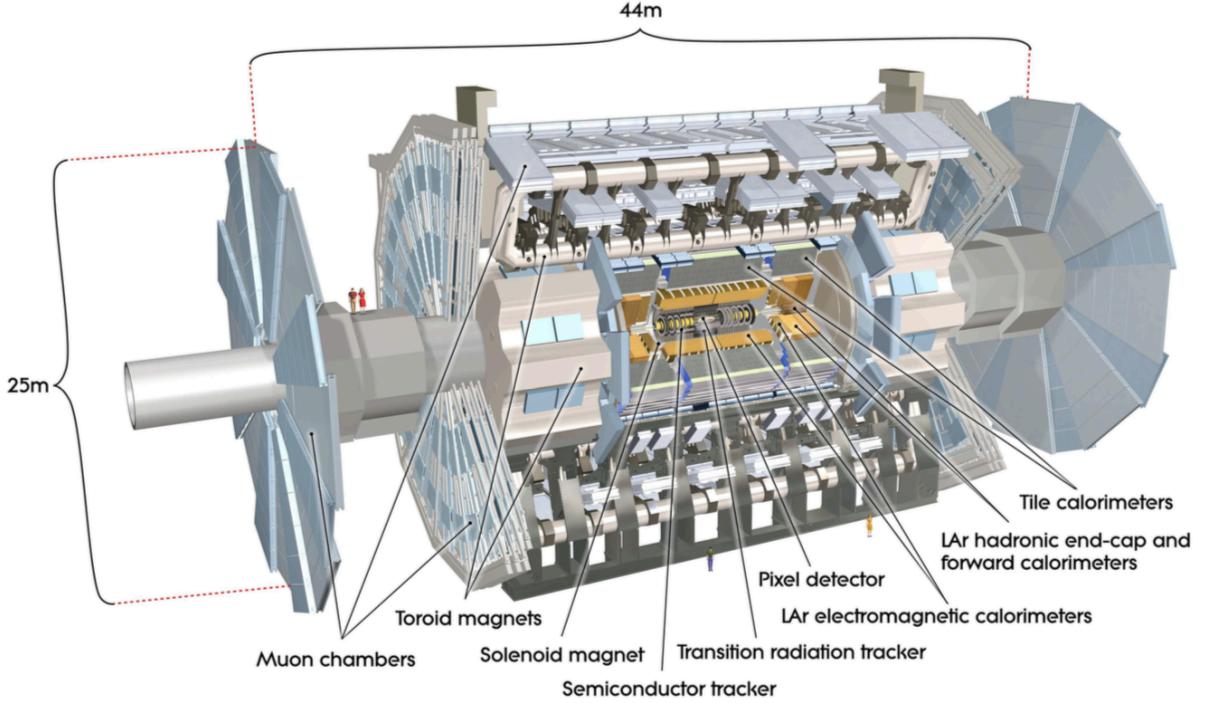


Figure 3.4 Cut-away view of the ATLAS detector

429 barrel and end-cap regions, respectively.

430 Within the inner region, a series of discrete space points provided by the silicon
 431 pixel detector and stereo pairs of silicon microstrip semiconductor tracking (SCT) lay-
 432 ers gives high-resolution pattern recognition abilities. By increasing radial distances,
 433 the transition radiation tracker (TRT) provides extra pattern recognition and momentum
 434 resolution capabilities.

435 The pixel detector

436 A series of high-granularity measurements is provided by the pixel detector [38]
 437 which is composed of the innermost sub-detector of the ID, it is designed as close
 438 to the interaction point as possible. Three sub-sections: two end-cap perpendicular
 439 to the beam axis and a barrel alongside the beam axis as a concentric cylinder with
 440 four layers (average radii of 33.25, 50.5, 88.5 and 122.5 mm, respectively) in it.

441 The innermost pixel layer (or B-layer, IBL) is essential to b-tagging performance
 442 and supersymmetry searches as it cover the full acceptance of short-lived parti-
 443 cles such as B hadrons and τ leptons from the beginning of Run-2 to enhance the
 444 measurement of the secondary vertex. Besides, a new readout sensor and chip

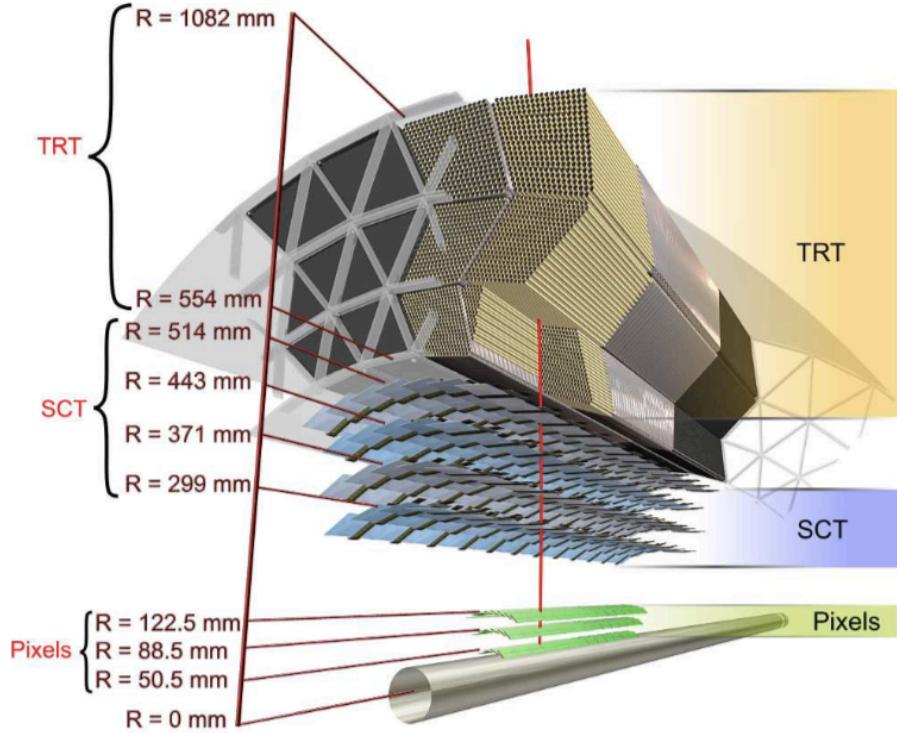


Figure 3.5 Cut-away view of the ATLAS ID. Sensors and structural elements traversed by a charged track of $10 \text{ GeV } p_T$ in the barrel inner detector along with their envelopes in r .

445 responsible for higher radiation damage and higher hit rate, respectively, is em-
 446 ployed in the IBL compared to the other three layers in the barrel region. A new
 447 n-in-n planar and 3D silicon sensors with hit efficiency of greater than 97% is de-
 448 veloped as well. The better impact parameter resolution is achieved by reducing
 449 the pixel size of the chip down to $50 \times 250 \mu\text{m}^2$. Around 80 million readout sec-
 450 tions counting them all provide the great hit resolution of $10 \mu\text{m}$ in radius plane
 451 and $115 \mu\text{m}$ alongside the z-axis in the pixel detector.

452 The semiconductor tracker

453 Surrounding the pixel detector is the SCT which encompasses silicon based semi-
 454 conductor sensing components in barrel and end-cap geometries. Four silicon mi-
 455 crostrip layers, located at radii of 300, 373, 447 and 520 mm, in the barrel region
 456 of the SCT provide high granularity points. The mean size of each strip pitch is
 457 $80 \mu\text{m}$ for the rectangular barrel sensors as daisy-chained with 6 cm-long. For
 458 the end-cap sensors, nine disks cover $|\eta| < 2.5$ are chosen. As a results, there are

459 thus 768 readout strips with $6.36 \times 6.40 \text{ cm}^2$ in size in total, with additional two
460 strips at the edge of the sensor. 6.1 m^2 of silicon detectors with 6.2 million readout
461 channels as a whole intergrated the SCT.

462 **The transition radiation tracker**

463 The outermost layer of the ID is the TRT which encompasses polyimide drift(straw)
464 tubes that designed to enable as much less wall thickness and material as possible
465 while maintaining the good experimental properties. With 4 mm in diameter and
466 150 cm in length, 73 layers of 144 cm alongside the beam with 50 thousands tubes
467 and 37 cm tubes consisting 160 tubes planes in the end-cap with 320 thousands
468 radial tubes.

469 The xenon-based gas filled up in a given tube provides the track hit of a particle as
470 it ionized as the emitting electrons drifting to the center wire of the tube volume.
471 An average of 36 hits per charged-particle track is given by the TRT, The result-
472 ing electrical signals are obtained by converting the drifting charge currents. In
473 total 420 thousands of electronics channels in which a good spatial resolution and
474 drift-time measurement are provided by the TRT, enhancing the precision mea-
475 surements of momentum in the ID.

476 **3.2.2 Calorimeters**

477 Outside of the ID lies the ATLAS calorimeters system which is designed to obtain
478 the energy lost of the particles that travel through the detector components. Multiple
479 layers of high-density material are placed to consume the energy of the incoming par-
480 ticles inside the materials and stop them from further moving. An “active” medium
481 is left inside the layers that allows experimental physicists measure the energy of those
482 particles.

483 Two types of calorimeters are employed in the ATLAS calorimeters system: the en-
484 ergy of electrons and photons are measured by the electromagnetic calorimeters as they
485 create reaction with matter. Hadronic showers that created by the interaction between
486 hadrons and atomic nuclei, are sampled by the hadronic calorimeters. Muons and neutrili-
487 nos can not be stopped by the calorimeters as they interact only weak force but the track
488 footprints could be seem in the calorimeters. The layout of the calorimeters is shown in
489 Figure 3.6.

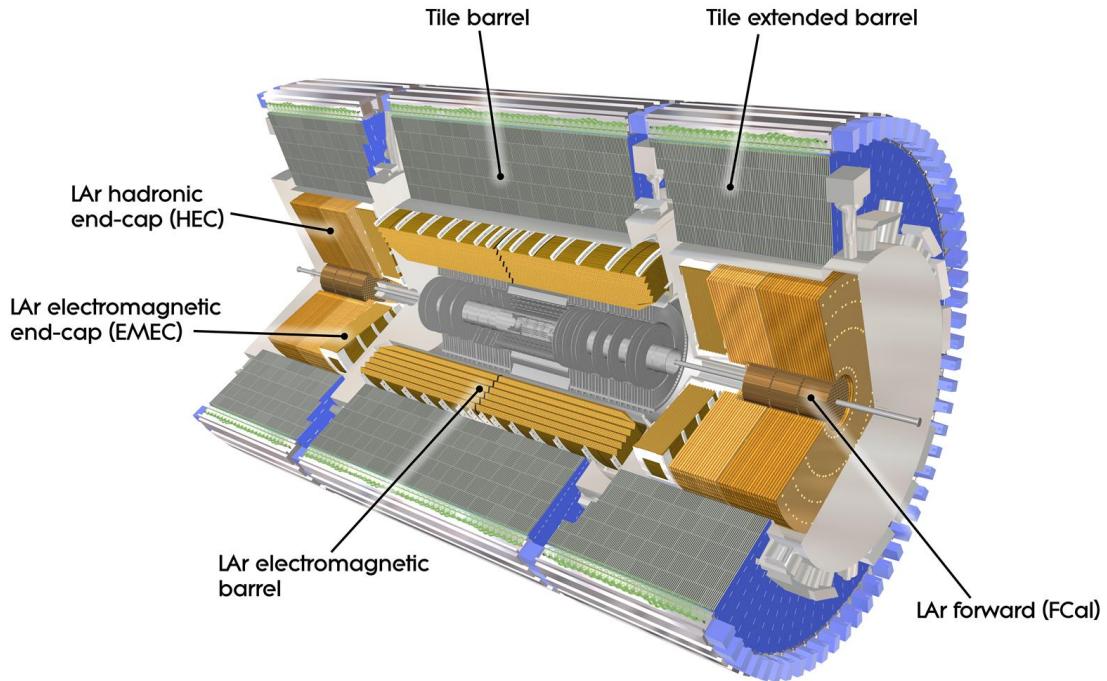


Figure 3.6 Outline of the ATLAS Run 2 trigger and data-acquisition system.

490 The electromagnetic (EM) calorimeter covers a range of $|\eta| < 3.2$ by combining
 491 the one barrel and two end-cap modules as cylindrical cryostat, with an outer radius of
 492 2.25 m, an end-cap thickness of 0.632 m and a length of 3.17 m. The hadronic calorime-
 493 ter covers the central barrel region of $|\eta| < 1.0$ and two extended barrels in a region of
 494 $0.8 < |\eta| < 1.7$, with a radius of 2.28 m at the inside and 4.25 m at the outside. Fig-
 495 ure 3.7 demonstrates the positions of the end-cap of the calorimeters including the EM
 496 and Hadronic calorimeters.

497 **The electromagnetic calorimeter**

498 The EM calorimeter that surrounds the ATLAS ID is designed for the high-
 499 granularity measurements of the energy of photons, electrons and hadrons with
 500 Liquid Argon (LAr) sandwiched between the multiple layers ionised. It converts
 501 the incoming particles into electric currents by absorbing the energy of these par-
 502 ticles as they interact with the metal with the bremsstrahlung phenomenon. A pair
 503 of electron-positron produced by an electron radiation in the EM calorimeter can
 504 initiate further electron-positron pairs (as showers) until the energy of the parti-
 505 cles fall below the certain threshold, the dominate process thus become ionisation

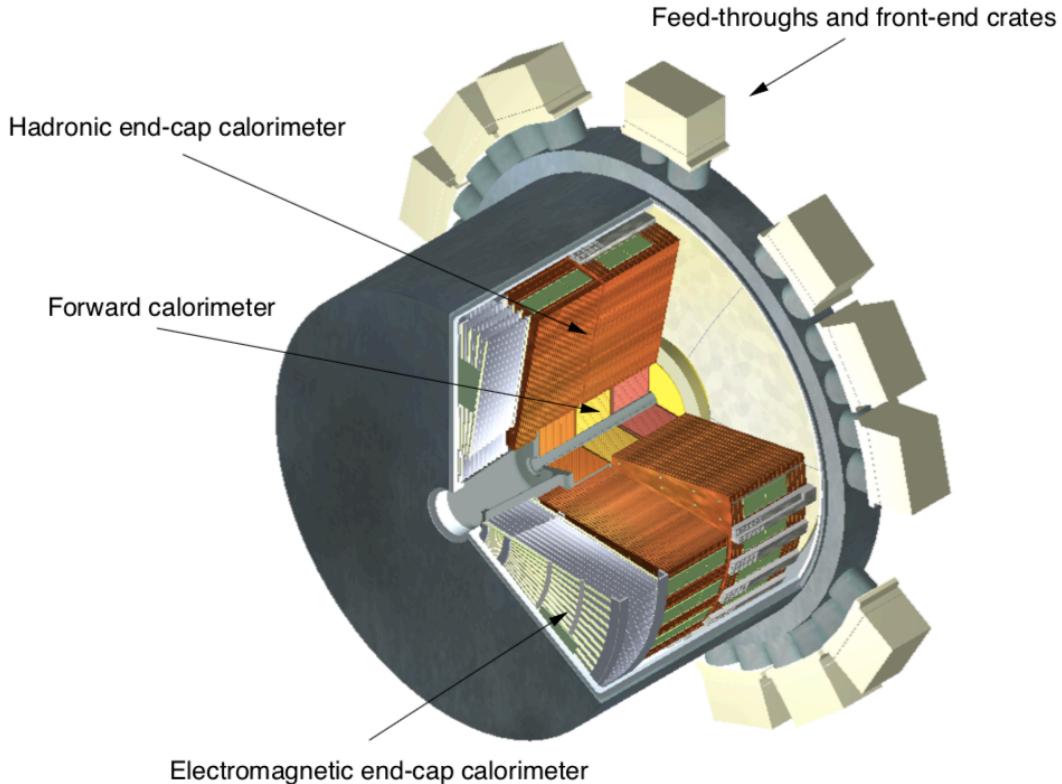


Figure 3.7 Cut-away view of an end-cap cryostat of the ATLAS calorimeter system.

506 in the LAr where drifting electrons are produced. Furthermore, the missing trans-
 507 verse energy can be obtained by subtracting the total energy of the known particles,
 508 which contributes to the analysis of neutrinos and new particles.

509 At -184 °C where the argon exists in liquid form, the calorimeter is kept as the
 510 cables that transverse electronic signals are sealed in vacuum and connected to the
 511 warmer area where located the readout system.

512 **The hadronic calorimeter**

513 Surrounded the EM calorimeter, lies the tile hadronic calorimeter where hadrons
 514 that contain strong force thus could not fully deposit their relatively large energy in
 515 the EM calorimeter are absorbed by the tile calorimeter. Steel and plastic scintillat-
 516 ing tiles are placed in layers in order to record the trajectories of incoming particles
 517 as hadronic showers are formed by the interactions of the particles with the ma-
 518 terials and emitting particles continue interacting with materials in the hadronic
 519 calorimeter and more particles are produced in steel layers. On the other hand,

520 photons are produced by the plastic scintillators where electric currents are gained
521 according to the energy of the particle.

522 By enveloping the EM calorimeter, a hadronic shower that contained EM showers
523 can be fully absorbed by the great thickness in the hadronic calorimeter. Around
524 420 thousands of plastic scintillator tiles are placed in sync, leading a weight of
525 2.9 thousands tonne in total.

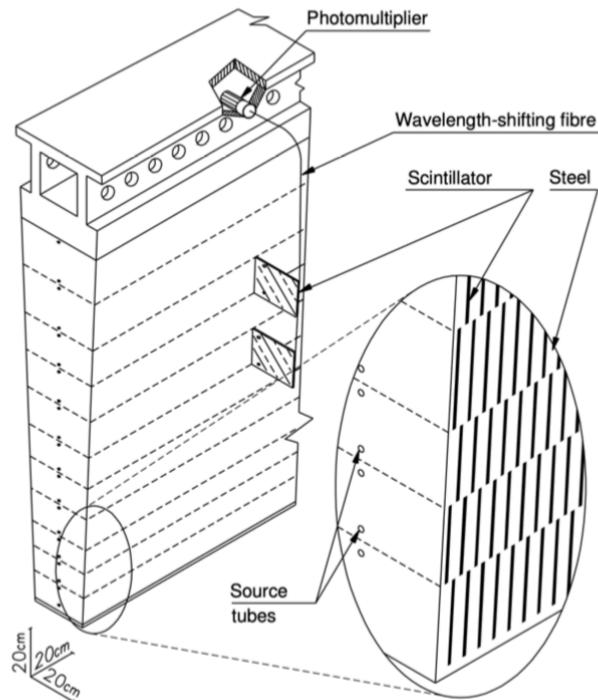


Figure 3.8 A schematic view of a tile calorimeter components of optical readout tiles and scintillating tiles.

526 As illustrated in Figure 3.8, photomultiplier tubes (PMT) are placed around the
527 outer radii of the tile calorimeter and connected with wavelength-shifting fibres
528 by which scintillation light is transferred. Projective geometry is designed for
529 the whole readout system as the energy of most hadronic showers is deposited in
530 the first or last two layers. Though the coarser granularity of the readout cells
531 of hadronic calorimeter has been compared to the EM calorimeter, the hadronic
532 calorimeter is qualified for the measurement of transverse momentum and jet re-
533 construction.

534 In the forward regions, the hadronic calorimeters are integrated with LAr calorime-
535 ters due to higher radiation exposition compared to the barrel regions. There are
536 two calorimeters that were developed to tackle such issue: the hadronic end-cap
537 calorimeter (HEC) that covers $1.5 < |\eta| < 3.2$ and the forward calorimeter (FCal)
538 that covers $3.1 < |\eta| < 4.9$.

539 The HEC located further beside the EM end-cap calorimeter has two wheels in
540 each end-cap. LAr is used for filling up 8.5 mm between copper layers in the HEC,
541 by which the active medium is provided. The readout electrodes are provided in
542 separate drift zones in order to secure the stability of the whole system. The FCal
543 has three wheels placed alongside the z-direction: one electromagnetic layer (FCal
544 1) and two hadronic layers (FCal 2 and FCal 3). LAr is also used as an active
545 medium in all of the layers. As for the absorber, copper is employed in FCal 1 as
546 it has heat removal properties. Tungsten is used in both FCal 2 and FCal 3 in order
547 to constrain the lateral spread of hadronic showers.

548 **3.2.3 Muon spectrometer**

549 The muon spectrometer (MS), specially designed for the muon detection is located
550 in the outermost section of the ATLAS in order to provide sufficient measurement of
551 high-momentum muons which are almost "invisible" to the ID and calorimeters due to
552 little energy deposit when traveled through the them. By deflecting the trajectories of
553 muons, the MS employs the magnetic field by a barrel toroid magnet system in $|\eta| < 1.4$
554 and end-cap toriod systems in $1.6 < |\eta| < 2.7$.

555 Four subsections of the MS: add up to 4000 separate muon chambers. Thin Gap
556 Chambers (TGC) and Resistive Plate Chambers (RPC) account for triggering and the
557 second coordinate measurement of muons. TGC is set at the end of the detector whereas
558 RPC which provides 5,000 V/mm electric field is placed in the central region. Monitored
559 Drift Tubes (MDT) is designed for the curve of muon tracks measurement with fine tube
560 resolution of 80 μm . Cathode Strip Chambers (CSC) accounts for measuring coordi-
561 nates precisely located at ends of detector with a fine resolution of 60 μm . Figure 3.9
562 demonstrates the MS with all four subsections. In total three separate points within the
563 muon trajectory are measured to reconstruct the momentum of the muon.

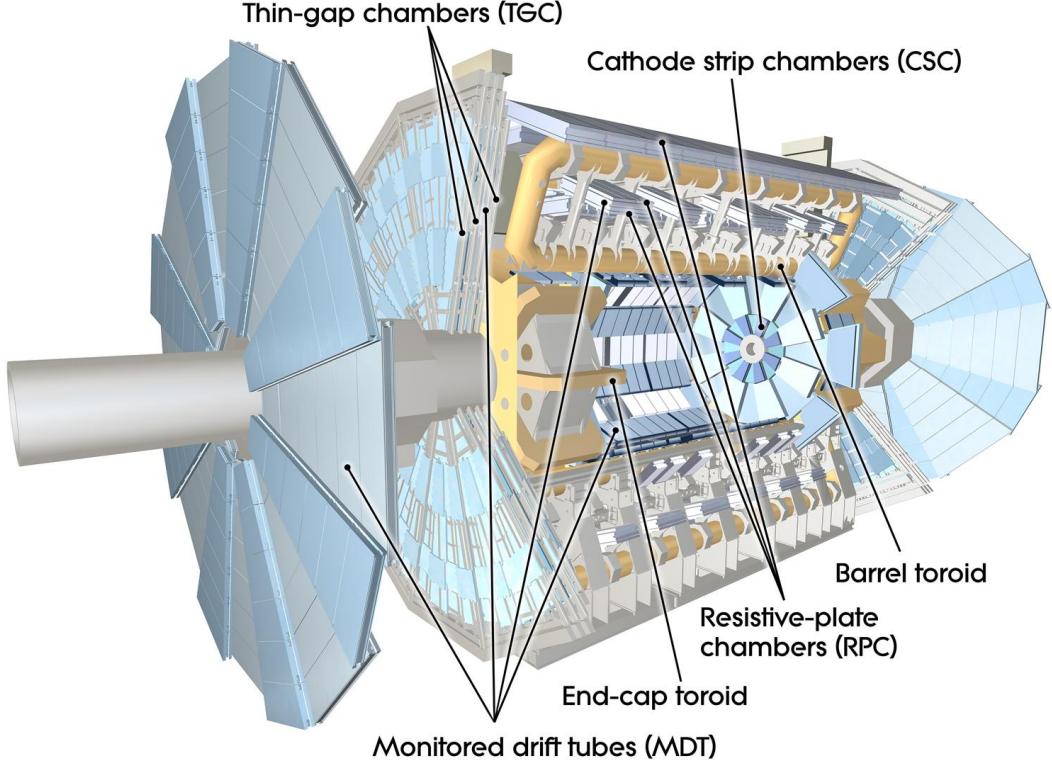


Figure 3.9 Cut-away view of the ATLAS Muons Spectrometer with subsections labeled.

564 3.2.4 Trigger and data acquisition

565 At the LHC, approximately 1.7 billion proton-proton collisions occur per second at
 566 an integrated luminosity of 140 fb^{-1} . However, many of these collisions are unlikely to
 567 produce characteristics of interest. As a result, large numbers of events can be discarded
 568 without affecting the search for new physics. The trigger and data acquisition systems
 569 are introduced to eliminate the irrelevant data so that only events of suitable quality and
 570 quantity are recorded.

571 During the year of 2015-2018, the trigger system in ATLAS selected significant
 572 events in a two staged process, as illustrated in Figure 3.10: The first-level (L1) trigger is
 573 implemented on hardware, and reduced event rates from 40 MHz to 100 kHz in less than
 574 $2.5 \mu\text{s}$ right after the data happened. Working with the electrical information provided
 575 by the calorimeters and the MS, the L1 trigger employs custom-made electronics to filter
 576 and store the events in the readout sections as buffers before passing them to the High-
 577 Level trigger (HLT) [39]. Certain physics objects such as photons, jets and leptons are
 578 identified in the L1 trigger, in which energy depositions of electrons and photons in the

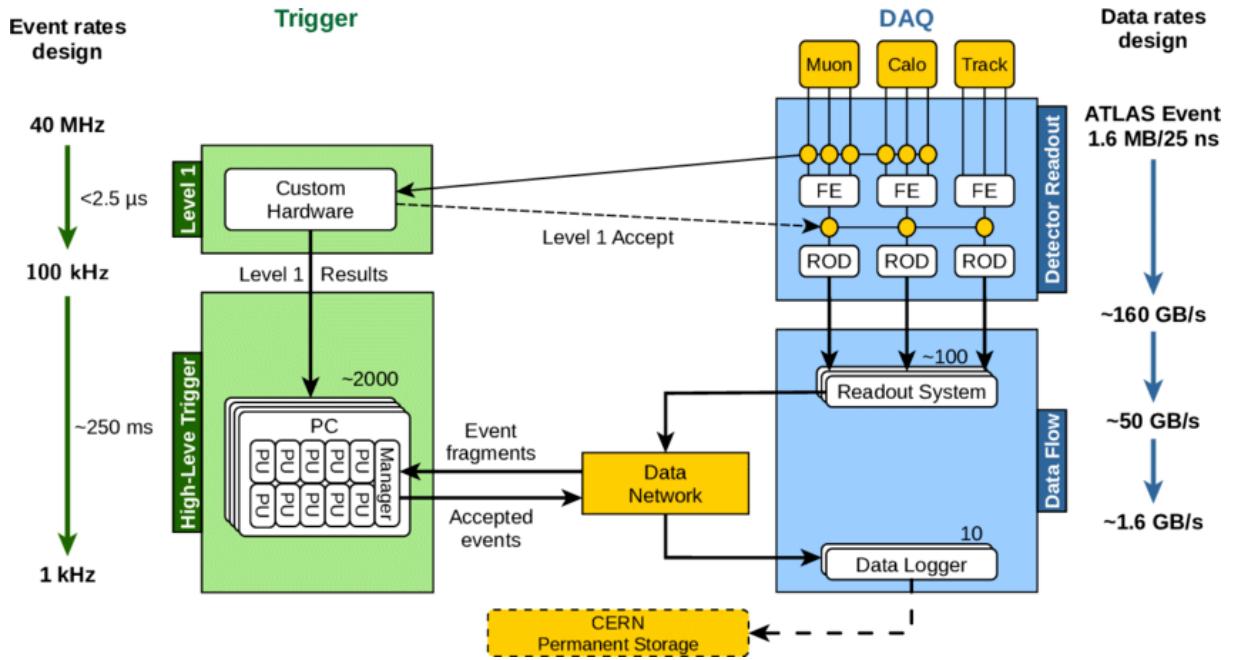


Figure 3.10 illustration of the ATLAS Run 2 trigger and data acquisition system.

579 EM calorimeter and jets in the hadronic calorimeter are provided. Information of tracks
 580 in high-momentum muons is recorded in the layers of the MS and forwarded to the L1
 581 trigger.

582 The events are further reduced from 100 kHz to 1 kHz in merely 250 microseconds
 583 by the second level trigger: HLT. Based on the offline software, the HLT utilize fast
 584 selection algorithms to analyse and reject events in the early stage, resulting in better
 585 precision and intense CPU usage of about 1.6 GB per second. The accepted data from
 586 the HLT will be passed to permanent storage at CERN via Data Logger [40].

587

4 Jets in ATLAS

588 In the LHC, a large number of quarks and gluons are produced during the inelastic
 589 proton-proton collisions, resulting in jets. These collimated outcome particles are hadro-
 590 nised because of colour confinement in the QCD process. As a result of this, only colour-
 591 neutral jets clustered by particles can be seen in the detector.

592 The information of jets is crucial to most of the analysis such as the measurements
 593 of the SM particles and searches for the BSM phenomena. Good qualities of jets, for
 594 example the high efficiency of jet reconstruction, jet energy calibration including energy
 595 scale and energy resolution, are thus important to the analysis.

596 **4.1 Jet reconstruction**

597 Jets are defined in two way: Monte Carlo (MC) simulated jets at particle level and
 598 detector level jets with the information from the ID and calorimeters. The production
 599 and hadronisation processes of jets are illustrated in Figure 4.11.

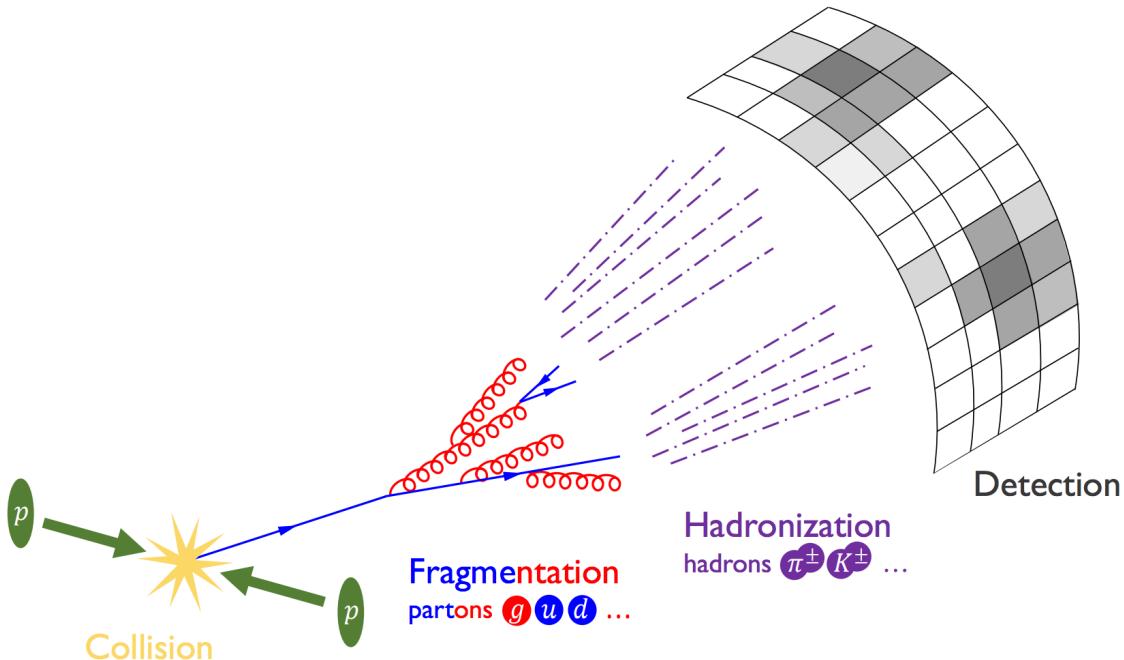


Figure 4.11 illustration of jets produced by pp collision and hadronised before seen by the detector.

600 Jets from the MC simulation are defined as truth-particle jets which have lifetimes

longer than 10 ps as stable particles. Truth-particles indicate the ideal measurement from a detector under perfect-condition and high resolution without defects or the effects from pile-up (background interactions per bunch-crossing in the LHC). Whereas track jets are constructed with the use of charged information in the ID, and calorimeter jets with the use of energy information in the calorimeters.

There are several types of jets aim for different analysis depended on the constituents and algorithm used for reconstructing the jets. ATLAS previously used topo-cluster jets, which is a group of topological related cells in calorimeter with significantly high energy deposits. A pile-up suppressed algorithm is applied to select certain cells with low noise. Cell above certain signal-to-noise (S/N) threshold (usually by four times its standard deviation) are used to seed the algorithm. By neighbouring the seed a topo-cluster is defined. In the hard-scatter process, jets of interest are expected to produced from the primary interaction point (known as vertex). The primary vertex is defined if there are at least two tracks with the highest sum of squared track momentum associated to it.

Jets are constructed from any set of four-vectors. EMTopo jets are the jets that use topo-cluster initially calibrated to electromagnetic (EM) scale in the calorimeters. A local cluster weighting (LCW) scale is also used for calibrating hadronic clusters by applying weights for low hadronic interaction response. Besides, particle flow (PFlow) [41] jets are built by combining the information from both the ID and the calorimeter, where the energy deposited from the calorimeter are removed by the momentum in the ID by a cell-based energy subtraction algorithm. The inputs to the particle flow algorithm are the separate topo-clusters with local energy maxima, respectively.

A recombination algorithm called anti- k_t algorithm is employed to build the jets with a radius parameter R in rapidity-azimuth ($y - \phi$) plane around a cluster. The algorithms are defined as follows:

$$d_{ij} = \min \left(k_{ti}^{2p}, k_{tj}^{2p} \right) \frac{\Delta_{ij}^2}{R^2} \quad (4.1)$$

$$\Delta_{ij}^2 = (y_i - y_j)^2 + (\phi_i - \phi_j)^2 \quad (4.2)$$

$$d_{iB} = k_{ti}^{2p} \quad (4.3)$$

where the distance d_{ij} between any pair of particles i and j is given by the minimum transverse momenta k_t of the two particles. The geometrical distance Δ_{ij} represents the separation of a pair of particles in $(y - \phi)$ plane. Radius parameter R indicates the size of the final jets. The distance d_{iB} between any detected particle i and the beam B is also given. Parameter p indicates the relative power of energy with respect to geometrical scales and is used to distinguish the different types of algorithms.

When p is set to 0, the Cambridge-Aachen (CA) algorithm is given as the distance d_{ij} and d_{iB} only based on spatial separation and are independent of the transverse momenta. This algorithm is usually used for large-radius jets and jet substructure performance study.

For the k_t algorithm, p is set to 1 so that the distance d_{ij} is dominated by the minimum k_t . This algorithm is preferred for clusters that are soft and collinear splits are merged first, resulted in irregular footprint with the most interesting splits.

The algorithm [42] on the other hand set $p = -1$, leaving the distance $d_{ij} \propto \min\left(\frac{1}{k_{ti}^2}, \frac{1}{k_{tj}^2}\right)$ shorten as the transverse momenta of two particles increase. This is widely used in the LHC for hard clustering as it is less vulnerable to the effects from the pile-up and resulted in circular footprint as shown in Figure 4.12 for $R = 1.0$.

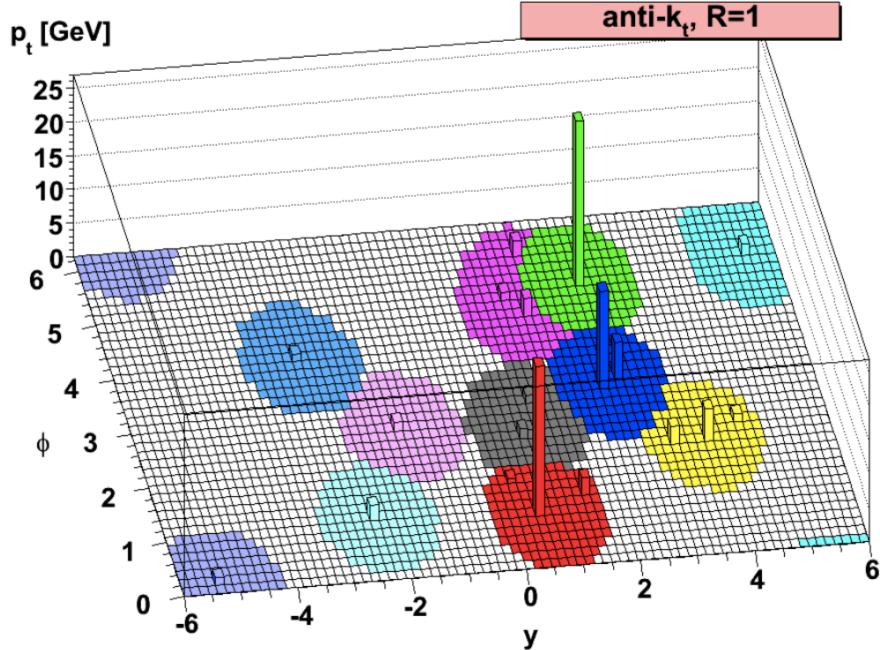


Figure 4.12 Plot of parton-level jets clustered using algorithms with radius parameter set to 1.

For most of ATLAS analysis, jets with $R = 0.4$ are used for quarks and gluons

analysis. Other ones such as $R = 1.0$ are also widely used to study energetic particles like W and Z bosons. $R = 0.2, 0.6, 1.2, 1.5$ and variable radii are also analysed.

The $R = 0.4$ PLow jets are used in the quark/gluon taggers calibration described in this thesis.

4.2 Jet calibration and cleaning

The motivation of jet calibration [43, 44] is to correct the translation from received signals to initial partons for several detector effects, including energy deposited in dead or beyond areas in the detectors, low response to hadronic reactions, pile-up, radiations that outside jet cone, etc. The calibration process is thus needed to account for the energy of jets to that of MC simulated jets at particle-level.

Calibration is performed to topological clusters at the EM scale where the sum of the energies in all constituent cell are taken, or at the LCW scale where low hadronic response in the ATLAS calorimeters is taken into account. The diagrams 4.13 shows the calibration scheme for small- R jets.

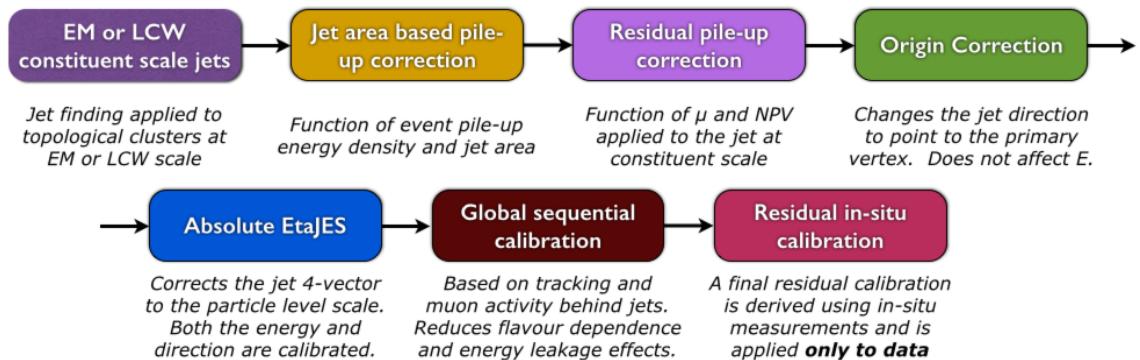


Figure 4.13 Overview scheme of jet calibration in the ATLAS.

4.2.1 Pile-up corrections

In order to eliminate a great amount of energy deposits from pile-up, a jet area-based subtraction of pile-up contribution to the p_T of each jet per event is applied as the start of the calibration chain.

After all pile-up corrections are applied, the jet p_T is given by:

$$p_T^{\text{corr}} = p_T^{\text{reco}} - \rho \times A - \alpha \times (N_{\text{PV}} - 1) - \beta \times \mu \quad (4.4)$$

where p_T^{reco} indicates the reconstructed jet p_T before any pile-up correction is applied. The jet area A is defined by certain number of ghost tracks associated with a jet after clustering thus can quantify the liability of a jet to pile-up. The pile-up p_T density ρ is used to evaluate the contribution from pile-up in the y - ϕ plane. To calculate the density ρ of each jet in the distribution p_T/A , a k_t algorithm with radius $R = 0.4$ is employed to reconstruct jet from positive-energy topo-clusters within the range of $|\eta| < 2$. The calculation of ρ performed in such η range for pile-up measurement is due to the fact that ρ tend to be zero beyond $|\eta| \approx 2$ as a result of lower occupancy in coarser segmentation in the forward region. Therefore, pile-up sensitivity in the forward region is not fully described after such correction.

An additional residual correction is thus applied from the MC simulation to account for the difference between the reconstructed jet p_T and truth jet p_T as a function of the number of reconstructed primary vertices in the event N_{PV} and the mean number of interactions per bunch crossing μ , which are sensitive to in-time and out-of-time pile-up, separately.

Both the initial values of α and β coefficients are derived in bins of truth jet p_T and geometric centre of the detector $|\eta_{\text{det}}|$. A logarithmic dependence on truth jet p_T is observed.

4.2.2 Jet energy scale and η calibration

Following the pile-up mitigation, the absolute jet energy scale and η calibration are introduced to correct the four-momentum of the reconstructed jet to the truth-particle jets, accounting for defecting calorimeter response, energy losses when particles passed through certain materials, boundary effects and biases in the reconstructed jet in different η due to the transition between the granularities and technologies changes in calorimeter.

Since the detector responses differ across the detector η range, the reconstructed jets are thus divided into small bins of η_{det} and the energy of the truth jet E^{truth} as the response distribution for fixed E^{truth} is Gaussian. The average jet energy response \mathcal{R} is defined as $E^{\text{reco}}/E^{\text{true}}$ using the mean of a Gaussian fit in η_{det} and E^{truth} bins, and is further parameterized as a function of E^{reco} . Such response for PFlow jets is higher than that for EMtopo jet at low energies as the tracking information is considered.

Besides Jet energy scale (JES) correction, the bias from the η of the reconstructed jet to that of the truth jet is taken into account. The bias is defined as a significant devi-

696 ation from zero in the signed difference between the reconstructed jet η^{reco} and truth jet
 697 η^{truth} , separately. Then a second correction is applied as such difference is parameterized
 698 as a function of η_{det} and E^{truth} .

699 The calibration is derived as a function of energy and η from the MC samples which
 700 do not have the effects from pile-up, and only correct the jet p_T and η instead of full four-
 701 momentum. The EMtopo and PFlow jets after full JES and η calibration are regarded as
 702 EM+JES scale and PFlow+JES scale, respectively. Small non-closures beyond $|\eta_{det}| \approx$
 703 3.2 in the calibration are seen due to approximate treatment of hadronic showers in the
 704 forward region, lead to an additional systematic uncertainty.

705 4.2.3 Global sequential calibration

706 The global sequential calibration (GSC), based the global jet observables such as
 707 the fraction of jet energy measured in the different layer of hadronic and the EM
 708 calorimeters, the tracking information associated with the jets, and the number of muon
 709 track segment. For each observable, a series of multiplicative corrections are applied on
 710 the four-momentum as a function of p_T^{truth} and $|\eta_{det}|$. Considered any observable x , the
 711 correction is derived from the inverted jet response \mathcal{R} :

$$C(x) = \frac{\mathcal{R}^{-1}}{\langle \mathcal{R}^{-1}(x) \rangle} \quad (4.5)$$

712 where $\langle \mathcal{R} \rangle$ is the average jet response.

713 As a result, the fluctuations in the jet particle composition are reduced and the jet
 714 resolution can be improved without changing the average jet energy response which
 715 depends on the flavour and the energy distribution of the constituent particles. The shape
 716 of a jet varies between quark- and gluon-initiated jets as hadrons are often included in a
 717 quark-initiated jet with higher fraction of the jet p_T with higher calorimeter response.

718 After applied GSC for PFlow jet, the average jet p_T response on each observable is
 719 reduced to lower than 2% with small deviations from correlations between observables.

720 The fractional jet resolution $\sigma_{\mathcal{R}}/\mathcal{R}$ is derived from the jet resolution $\sigma_{\mathcal{R}}$, which is
 721 defined by the standard deviation of a Gaussian fit to the distributionof jet p_T response.
 722 This fractional jet resolution is used to determine the size of the fluctuations in the jet
 723 energy reconstruction.

724 **4.2.4 Residual *in situ* calibration**

725 The final step of the jet calibration is performed only in data to account for the
726 differences of jet response measurement in data and the MC, the derived ratio of it is
727 used as a correction in data. The differences are introduced by the inadequate nature of
728 the detector materials and the imperfect simulation of the real physics processes. Such
729 differences can be quantified by weighting the p_T of a jet to other reference objects that
730 are well-measured. The correction factor can be denoted as follows:

$$c = \frac{\mathcal{R}_{\text{in situ}}^{\text{data}}}{\mathcal{R}_{\text{in situ}}^{\text{MC}}} \quad (4.6)$$

731 the response $\mathcal{R}_{\text{in situ}}$ represents the average ratio of the jet p_T to the reference object
732 p_T in bins of reference object p_T , where the average value is founded from peak value
733 of a Gaussian fit to the distribution. The double ratio is robust to secondary effects thus
734 more reliable in term of the measurement of jet energy.

735 Three stages are carried out in such *in situ* calibration. First, η -intercalibration is
736 performed on the energy scale of forward jets ($0.8 \leq |\eta_{\text{det}}| < 4.5$) to match the central jets
737 ($|\eta_{\text{det}}| < 0.8$) using the jet p_T in dijet events. Then Z +jet and γ +jet analyses balance the
738 measurement of p_T response of a well-calibrated Z boson or photon. Finally, a multijet
739 balance (MJB) analysis is employed to calibrate low- p_T jets to a very high- p_T jet. Both
740 MJB and Z/γ +jet analyses are used only for jets in the central region ($|\eta| < 1.2$). All
741 three *in situ* calibrations are done sequentially so that the systematic uncertainties can be
742 propagated from each to the next. The systematic uncertainties in each calibration pro-
743 cess come from three sources: the MC modelling of physics processes, the uncertainties
744 in the measurement and from topology obtained by different event selections.

745

5 The calibration of quark/gluon jets taggers

746 The classification of jets originated from a quark or a gluon is useful for improving the
747 SM measurements and searches for BSM physics at the LHC. According to the QCD,
748 gluons are in the adjoint representation of the $SU(3)$ gauge group thus carry both colour
749 and anti-colour quantum numbers, whereas quarks are in the fundamental representation
750 and have only a single colour number [45]. As a result, a gluon-initiated jet (gluon-jet)
751 tend to have more constituents and a broader radiation pattern than a quark-initiated jet
752 (quark-jets).

753 The manifestation of colour charges is intrinsic to quarks and gluons; however,
754 the confinement phenomenon inherent in QCD theory indicates that only colour neutral
755 hadrons can be observed in the detector. Such principle brings significant challenges
756 for the identification of quark- or gluon-jets in ATLAS. The identification method relies
757 on the number of charged tracks within the jets and the reconstruction algorithm for
758 it. The calibration described in this paper demonstrates the measurement of the tagging
759 efficiencies of the aforementioned jet taggers. The more advanced boosted decision tree
760 (BDT) algorithm is employed to constructed the jet tagging variable based on the charge
761 multiplicity inside jets. A matrix method is established with the use of quark/gluon
762 fraction in quark-/gluon-enriched subsamples, defined by the pseudorapidity of jets. The
763 scale factors extracted from the difference between data and simulation are provided
764 for tagger working points corresponding to 50%, 60%, 70% and 80% fixed quark-jet
765 efficiencies for both quark- and gluon-jets, respectively.

766 In addition to earlier investigations that concentrated on single-variable taggers
767 within a lower p_T range [46, 47], this research emphasizes the development of a novel
768 q/g tagger that incorporates multiple jet substructure parameters. Additionally, it aims
769 to expand the application of q/g tagging to a broader energy spectrum.

770 5.1 Data and Monte Carlo samples

771 5.1.1 Data

772 The data recorded in 2015-2018 with integrated luminosity of 140 fb^{-1} (full Run 2
773 data)[48] is used in this study. The data samples are processed through the un-skimmed
774 DAOD_JETM1 derivation scheme in order to obtain multi-jet events. The lowest un-

prescaled small- R single-jet trigger is employed for this analysis. The jet p_T threshold for the trigger in this analysis is 420 GeV, keeping the selection consistent across years, together with additional requirements that ensure events of good qualities are used [49].
 The additional selections are:

- Good Run List (GRL): Make sure a steady state of all relevant detectors so that physics processes recorded by them are good.
- LAr: Liquid Argon Calorimeter error rejected.
- Tile: Tile Calorimeter error rejected.
- SCT: SCT single event upsets rejected.
- Core: Incomplete event build rejected.
- Primary Vertex: the highest $\sum p_T^2(\text{trk})$ vertex has at least two tracks associated with it
- Trigger: Passes the lowest unprescaled single-jet trigger, HLT_j420

Additional kinematic selection criteria are discussed in Section 5.2.

5.1.2 Monte Carlo simulation

For this calibration, multi-jet events are generated and modelled with several MC simulations, processed through the same DAOD_JETM1 derivation scheme. For the nominal result, PYTHIA 8.230 [50] MC generator is used with leading-order (LO) matrix element (ME) for dijet production. Parton density functions (PDFs) are considered for systematic uncertainties evaluation as the PDF set [51] is used for PYTHIA 8.230 with the A14 tune [52]. Alternative samples with different choices of parton shower modelling, ME generation, and the simulation of the multi-parton interactions are included to estimate the systematic uncertainties.

Two set of MC samples generated using SHERPA 2.2.5 [53] are used with the same ME for the (2→2) process at LO, to provide the uncertainties of hadronisation modelling [54, 55]. The CT10 PDF [56] sets are included in both SHERPA samples where one based on the cluster hadronisation whereas the other used SHERPA interface to the Lund string fragmentation [57] model as PYTHIA 8.230.

803 Two set of MC samples generated using HERWIG 7.1.3 [58] are used for parton
 804 shower uncertainties as one uses angular ordering shower whereas the other one uses
 805 dipole shower. These samples are produced at next-to-leading order (NLO) with a PDF
 806 set of MMHT [59].
 807

807 Another set of multijet samples that produced with POWHEG [60, 61, 62] interfaced
 808 to PYTHIA at NLO accuracy is employed with NNPDF2.3 LO PDF [63] set, to estimate
 809 the effects from the ME uncertainty as different perturbative scales in the ME and parton
 810 distribution functions are included. The renormalization and factorisation scales are set
 811 to the p_T of the underlying Born configuration. These samples included different pertur-
 812 bative scales in the ME and parton distribution functions are used for the estimation of
 813 ME uncertainty.
 814

A list of the MC samples used is given in table 5.1.

PDF set	Generator	Cross-section	Parton shower	Hadronisation
NNPDF2.3	PYTHIA 8.230	LO	p_T -ordered	String
CT10	SHERPA 2.2.5	LO	p_T -ordered	Cluste
CT10	SHERPA 2.2.5	LO	p_T -ordered	String
MMHT	HERWIG 7.1.3	NLO	Dipole	Cluster
MMHT	HERWIG 7.1.3	NLO	Angular-ordered	Cluster
NNPDF2.3	Powheg+PYTHIA	NLO	p_T -ordered	String

Table 5.1 The MC simulation used for the multi-jet processes in this calibration. The PDF sets, generators for a hard process, the order in α_s of cross-section calculations and the simulator of parton showers, and hadronisation are shown.

815 5.2 Object and Event selection

816 In order to perform the calibration of the quark-/gluon-jet tagger, it is requisite to
 817 establish two distinct subsamples. One subsample should be predominantly composed of
 818 quark-jets, called quark-enriched sample, while the other should predominantly consist
 819 of gluon-jets, as gluon-enriched sample. These subsamples are gained from the dijet
 820 events. This section describes the reconstruction and selection of jet objects used in this
 821 calibration, as well as the approach to construct quark- and gluon-enriched subsamples.
 822

822 **5.2.1 Physics object definition**

823 The PFlow jets that are reconstructed with the algorithm with a radius parameter
 824 R set to 0.4. An overall jet energy calibration described in section 4.2 has been done
 825 to rectify residual detector effects and pile-up. In order to ensure a good quality jet, an
 826 event-based jet cleaning with standard loose cut is applied to reject events with flawed
 827 leading or subleading jet.

828 Tracks that reconstructed [64] from the ID are required to have $p_T > 500$ MeV, and
 829 within the ID range $|\eta| < 2.5$. Additional criteria such as primary vertex are required to
 830 ensure selected tracks originating from the collision and prevent the mis-reconstructed
 831 tracks from pile-up hits in the detector. The alignment of tracks with calorimeter-based
 832 jets is executed through the application of the ghost-association technique. This entails
 833 a repetition of the jet clustering procedure augmented by the inclusion of 'ghost' repre-
 834 sentations of registered tracks [65]. These ghost tracks share the same direction as their
 835 actual counterparts but possess an infinitesimally small p_T , thereby ensuring that they do
 836 not induce any alterations to the intrinsic characteristics of the calorimeter-based jets. A
 837 criterion for track-jet correspondence is established: a given track is associated to a jet if
 838 its corresponding ghost track is contained in the jet after reclustering.

839 Jet reconstructed from the simulated MC is known as "truth jets" [43], with the
 840 same $R = 0.4$ algorithm as PFlow jets. Geometric correspondence between truth jets
 841 and PFlow jets is established via angular proximity, adhering to the criterion $\Delta R < 0.4$.
 842 Each truth jet is bestowed with a flavour label, referred to as a truth label [46, 47]. The
 843 truth flavour label attributed to a jet is defined by the flavour of the highest-energy parton
 844 situated within a cone of size $\Delta R < 0.4$ around the jet's axis, prior to the process of hadro-
 845 nisation in the parton shower. Following this definition, jets arising from the splintering
 846 of gluons into b - or c -quark pairs are labelled as heavy flavour jets. These heavy flavour
 847 jets are often identifiable by the long-lived or leptonically decaying hadrons. Therefore,
 848 no distinct discriminant tailored for heavy-flavour quarks is investigated within the cur-
 849 rent framework [66, 67]. Jets will be unlabelled if there is no corresponding truth parton
 850 with $p_T > 1$ GeV is found within the cone surrounding the truth jet. These instances of
 851 unlabelled jets commonly emerge as a consequence of pile-up effects, and less than 1%
 852 of the dataset used. They are thus ignored [68].

5.2.2 Event Selection and definition of quark and gluon-enriched samples

Events are chosen by the single-jet trigger, HLT_j420. The jet p_T is required to be greater than 500 GeV, as more quark-jets and better resolution on the jet constituents are given. Only the leading two jets with the highest p_T are used, as dijet events, and are required to be $|\eta| < 2.5$ so that their charged constituents are collected within the coverage of the ID. To maintain the equilibrium in p_T and suppress non-isolated jets, a criterion demands that the ratio of the p_T of the leading jet to that of the sub-leading jet remains within 1.5. The two leading p_T jets serve as the cornerstone for the formulation of quark-enriched and gluon-enriched subsamples.

The quark-enriched sample is derived from the jet with higher $|\eta|$ among the leading two jets, while the gluon-enriched sample is extracted from the jet with lower $|\eta|$. This selection strategy capitalizes on the intrinsic behaviour of PDFs at higher proton momentum fraction range, where there exists a higher likelihood of encompassing valence quark-jets. Consequently, jets situated in more forward regions (higher $|\eta|$) have a higher probability of being quark-jets, while jets positioned closer to the central region (lower $|\eta|$) manifest an increased likelihood of corresponding to gluon-jets [69].

Selection	Multi-jet sample
Trigger	HLT_j420
Number of jets	≥ 2
$p_T(j_1)$	> 500
$p_T(j_2)$	> 500
$p_T(j_1)/p_T(j_2)$	< 1.5
$ \eta(j_1) $	< 2.1
$ \eta(j_2) $	< 2.1
Target parton	Quark(Higher $ \eta $) or Gluon (Lower $ \eta $)

Table 5.2 The selections to retrieve quark/gluon-enriched samples. " j_i " represents the i -th jet in p_T -ordering.

The distribution of leading and subleading jets p_T in dijet event after selections is shown in Figure 5.14 for both MC and data.

5.3 Quark/gluon tagging variables

According to QCD, the colour factor of gluons is larger than that of quarks by factor 9/4 ("Casimir ratio") [45], which makes gluons emit more particles in the hadronisation

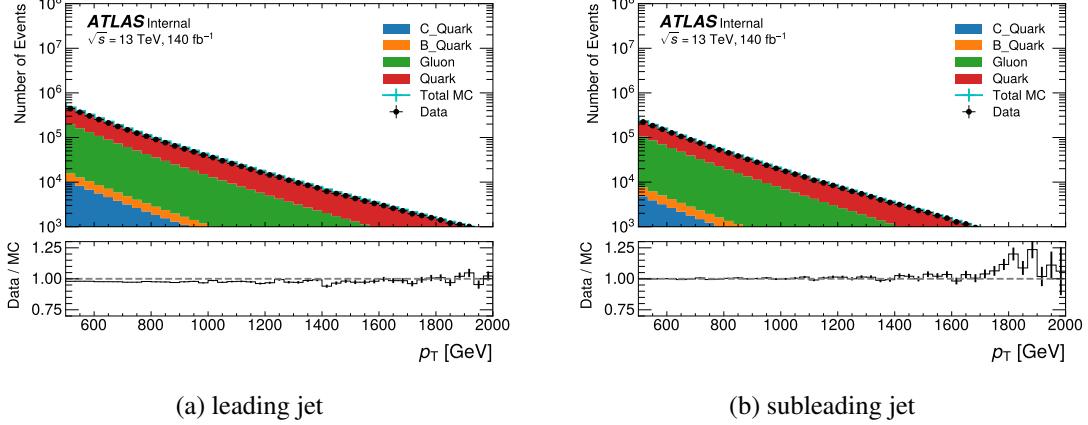


Figure 5.14 The p_T distribution of the leading jets and sub-leading jets with PYTHIA samples for dijet event.

than quarks. As a result, a gluon-initiated jet has more charged multiplicity associated and its width is larger than that of a quark-initiated jet. Therefore, the information of the track multiplicity inside a jet is crucial to distinguish quarks from gluons.

The q/g tagging variables used in this study are based on the track multiplicity and are specified as : number of tracks (N_{trk}), jet width (W_{trk}) [46, 70], and two point energy correlation function ($C_1^{\beta=0.2}$) [71, 72] computed from the associated tracks. The expressions are defined as follows:

$$N_{\text{trk}}$$

N_{trk} is a number of tracks associated with the jet.

$$N_{\text{trk}} = \sum_{\text{trk} \in \text{jet}} \quad (5.1)$$

$$W_{\text{trk}}$$

W_{trk} is a track- p_T -weighted width of the jet divided by the scalar sum of track transverse momenta. It is defined as

$$W_{\text{trk}} = \frac{\sum_{\text{trk} \in \text{jet}} p_{T,\text{trk}} \Delta R_{\text{trk},\text{jet}}}{\sum_{\text{trk} \in \text{jet}} p_{T,\text{trk}}}, \quad (5.2)$$

where $p_{T,\text{trk}}$ is a p_T of a charged track reconstructed by the ID and $\Delta R_{\text{trk},\text{jet}}$ is a distance in the $\eta - \phi$ plane between the track and the jet axis.

$$C_1^{\beta=0.2}$$

Two point energy correlation function is defined as

$$C_1^{\beta=0.2} = \frac{\sum_{i,j \in jet}^{i \neq j} p_{T,i} p_{T,j} (\Delta R_{i,j})^{\beta=0.2}}{\left(\sum_{trk \in jet} p_{T,trk} \right)^2}, \quad (5.3)$$

where i and j denote tracks associated with the jet and the sum runs over all the combination of two tracks. The β is fixed to 0.2, which is known to be suitable for q/g tagging.

5.3.1 The BDT tagger

Multivariate Analysis (MVA) is a technique introduced to discriminate signal from background, one type of classification algorithm in MVA is the BDT. A tree structure is built to classify datasets through a sequence of branching binary decisions. Data with desirable features is kept by discriminating algorithm whereas others are rejected. Each decision point made construct a node at each level of the decision tree, and a score is assigned to every classifier that goes into the boosting process based on its error rate. One decision node can have two or more branches to split the datasets. Such procedure is iterated from top to down so that a termination condition such as the minimum number of samples in a node or a maximum depth in a tree depth is met. A diagram of a single decision tree is shown in Figure 5.15. After all series of cuts are applied, the BDT is defined. Therefore, a cut based on the BDT score can be employed as the most correct classification of datasets.

The BDT tagger is constructed by the combination of tracking-related observables: N_{trk} , W_{trk} , $C_1^{\beta=0.2}$ and p_T of a jet are included as the distribution of the track multiplicity is affected by them. In this study, the BDT score is used to classify quark- or gluon-jets from the multi jet samples, with the truth-labelled information from MC to train until a quark signal efficiency larger than 90% is reached.

The BDT tagger is trained using the LGBMClassifier from lightGBM [73] framework, and hyper-parameter tuning is performed with Optuna [74]. The MC PYTHIA samples are employed.

An individual score is allocated to each BDT within the boosting procedure, factoring in its error rate. This BDT score serves as the criterion for classifying a given jet as either a quark-jet or a gluon-jet.

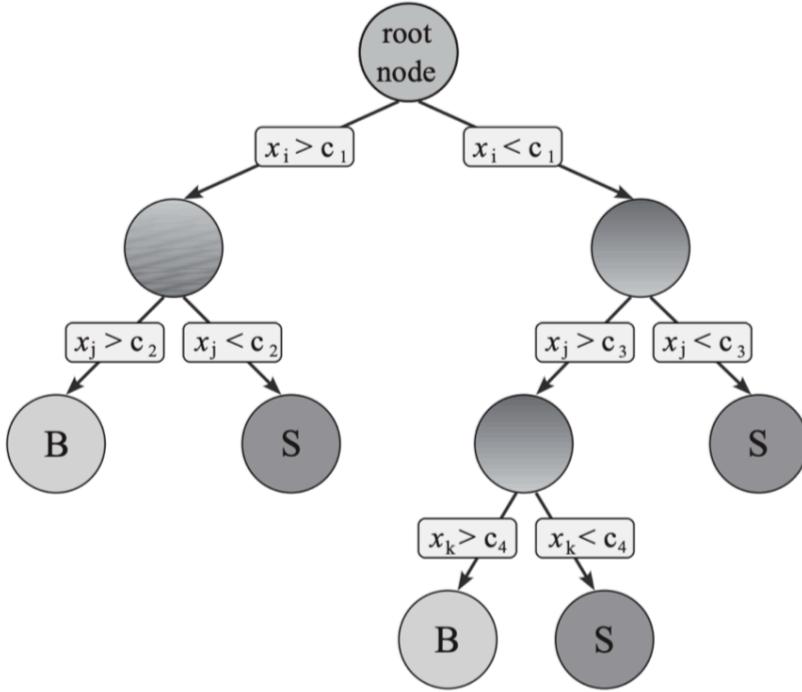


Figure 5.15 A scheme of a single decision tree with a depth of three

5.3.1.1 Feature selections

Drawing upon the features employed during the training process, an exploration of the correlation matrix is undertaken to assess the interdependence among jet attributes, including p_T , $|\eta|$, and jet substructure variables N_{trk} , W_{trk} , $C_1^{\beta=0.2}$, and the BDT. Figure 5.16 shows N_{trk} , W_{trk} and $C_1^{\beta=0.2}$ exhibit notable interrelationships among themselves, displaying relatively robust correlations. In contrast, p_T and η display a diminished level of correlation. The distributions of all single jet substructure variables and BDT score with systematic uncertainty in forward and central regions are shown in Figure 5.17. The distributions of all single jet substructure variables and BDT score with systematic uncertainty of quark- and gluon-jets in different p_T ranges from the MC simulation are shown in Figure 5.18.

Rather than employing multiple BDTs for different p_T ranges, an universal BDT can be trained using events in all p_T ranges. Given the intrinsic correlation between N_{trk} and the jet p_T , a natural way to choose features is including p_T in addition to three q/g tagging variables. Concerning the remaining variable, η , two comparative scenarios are juxtaposed: one involves its inclusion, and the other pertains to its exclusion. This comparison facilitates an assessment of whether or not to incorporate $|\eta|$.

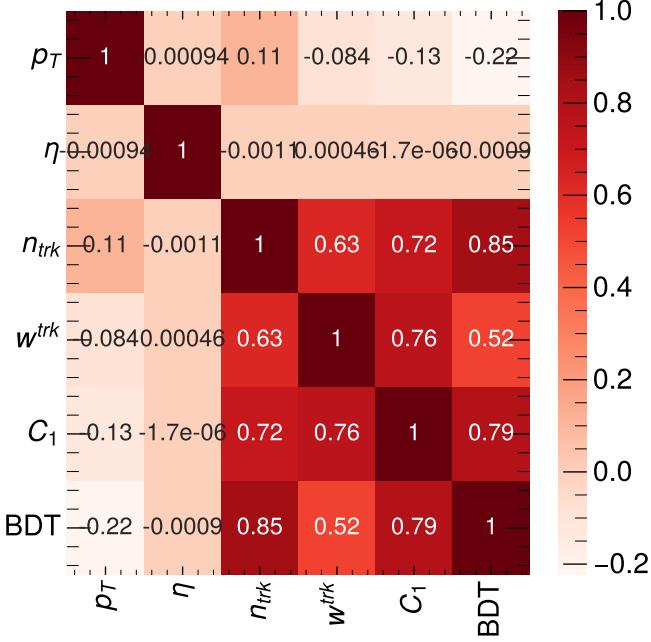


Figure 5.16 correlation matrix of jet variables.

- 934 1. p_T , N_{trk} , W_{trk} and $C_1^{\beta=0.2}$
 935 2. p_T , $|\eta|$, N_{trk} , W_{trk} and $C_1^{\beta=0.2}$

936 The result depicted in Figure 5.19 shows a distinct discrepancy when $|\eta|$ is encom-
 937 passed within the training. This violates the assumptions that the partons distribution in
 938 more forward and more central regions should not change. Specifically, the distribution
 939 of BDT scores for forward quarks substantially diverges from that of central quarks, a
 940 trend that is similarly observed for gluons. Moreover, adopting the BDT tagger that in-
 941 corporates $|\eta|$ would result in inadequate performance for jets situated within the central
 942 region when this tagger is applied to a pure sample of quark-jets (e.g., $Z+jet$ samples).
 943 In the present analysis, the BDT is endowed with the spectra of p_T , N_{trk} , W_{trk} , and $C_1^{\beta=0.2}$,
 944 as exemplified in scenario 1. At detector-level, however, the observed radiation pattern
 945 within jets no longer remains unaffected by $|\eta|$, owing to variances in the detector ma-
 946 terial and technology. To counteract this effect, a subsequent re-weighting procedure is
 947 implemented, described in Section 5.5.

948 **5.3.1.2 Training weights**

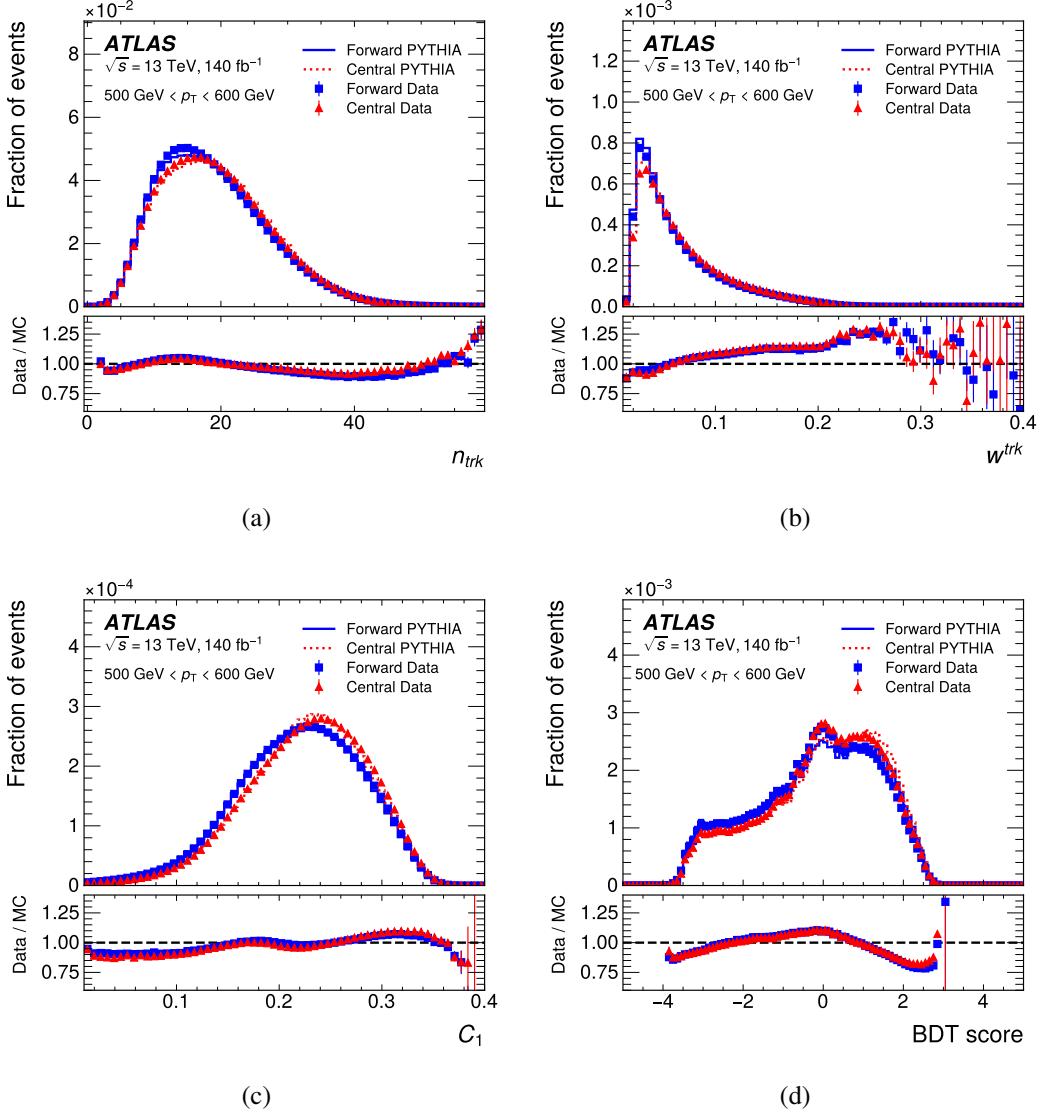


Figure 5.17 The distributions of N_{trk} (a), W_{trk} (b), C_1 (c) and BDT score (d) in the forward and central regions in data (closed symbols) and the PYTHIA MC (lines) are shown in the upper panels. The bottom panels show the ratio of the data and the MC. The distributions shown are for jet p_T in the range between 500 GeV and 600 GeV. The vertical error bars show the statistical uncertainty.

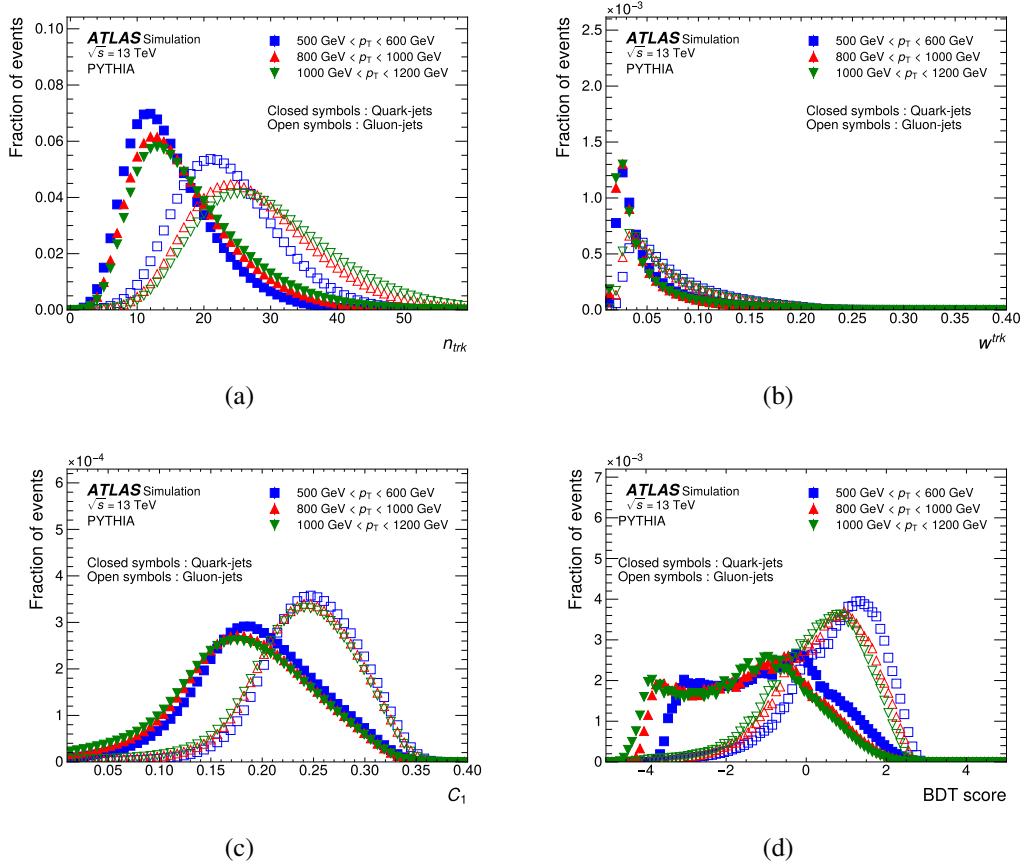


Figure 5.18 The distributions of N_{trk} (a), W_{trk} (b), C_1 (c) and BDT score (d) in the quark-jets (closed symbols) and gluon-jets (open symbols) in given p_T regions using the PYTHIA MC samples.

The calibration of quark/gluon jets taggers

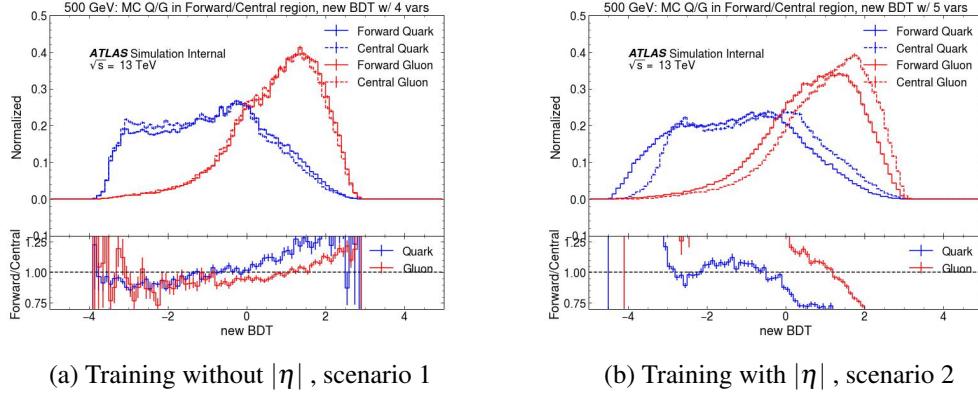


Figure 5.19 The comparison of BDT distribution for different scenarios in the jet p_T range from 500 to 600 GeV.

An additional data processing step is conducted to modify the event weights, such that a flat distribution of the p_T spectrum is given. This adjustment is motivated by the observation that higher p_T jets have less probability to occur, so the training on the higher p_T jets need to be emphasise. This newly introduced weight, referred to as the "flat p_T -weight" within this context, is exclusively employed during the training process. Conversely, for other scenarios, such as assessing tagger performance on validation datasets and subsequent calibration endeavours, the original event weights based on physical considerations remain employed.

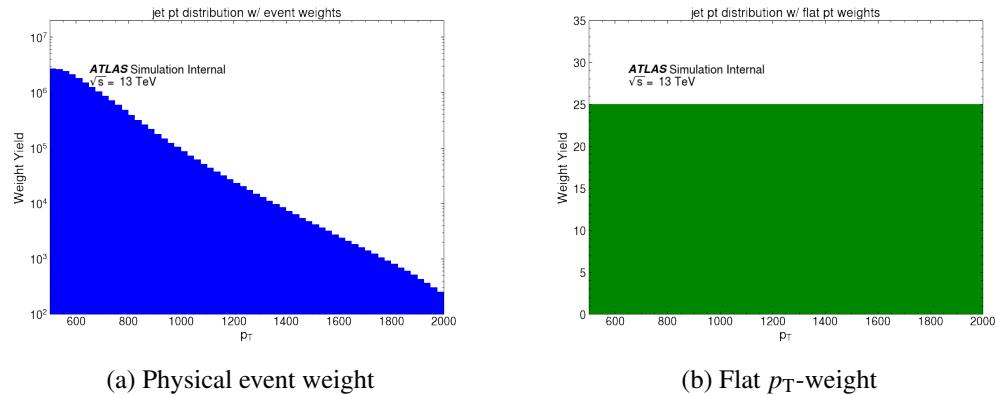


Figure 5.20 The comparison of jet p_T distributions with different weights.

957 5.3.1.3 Training Configuration

958 Approximately 30% of the data from each period of the MC PYTHIA 8 A, D, E is
 959 randomly allocated for the training investigation, constituting an aggregate of roughly 60
 960 million jets. The dataset division for training, validation, and testing is structured in a
 961 ratio of 80% for training, 10% for validation, and 10% for testing.

962 Optuna is employed to conduct a search for optimal hyperparameters. Following the
 963 hyperparameter tuning process, the most optimal model is achieved after 100 iterations
 964 of such procedure. The optimised parameters are listed:

- 965 • bagging_fraction 0.9176347488279626
- 966 • bagging_freq 2
- 967 • feature_fraction 0.9084973008559477
- 968 • lambda_11 0.0016400096502256838
- 969 • lambda_10 0.006327330258011633
- 970 • min_child_samples 13
- 971 • num_leaves 224

972 The performance of a classification model at all classification criteria can be illus-
 973 trated using a receiver operating characteristic (ROC) curve. The idea is to compare
 974 the true positive rate (TPR, also known as sensitivity, recall or probability of detection)
 975 against the false positive rate (FPR, also known as the probability of false alarm) at dif-
 976 ferent criteria given. Consider a binary classification case, where the outputs are either
 977 labelled as positive (p) or negative (n), in total there are four possible outputs from a two-
 978 class prediction problem. A true positive (TP) is given if the output from a prediction is
 979 p and the actual value is also p, otherwise a false positive (FP) is assigned if the actual
 980 value is n. Conversely, a true negative (TN) is given if both the prediction outcome and
 981 the actual value are n, whereas a false negative (FN) is assigned if the actual value is p.
 982 TPR as a synonym for recall is defined as:

$$TPR = TP / (TP + FN) \quad (5.4)$$

983 while the FPR is defined as:

$$FPR = FP / (FP + TN) \quad (5.5)$$

In this analysis, the prediction true is defined by higher $|\eta|$ jet and prediction negative is defined by lower $|\eta|$ jet. The actual truth value is given by the quark jet from the MC truth information, whereas the actual negative value is given by the gluon truth information. Thus the quark efficiency is the TPR and the gluon rejection is FPR. An Area Under the ROC Curve (AUC) is used to evaluate the performance of a classifier, the better performance is indicated by higher AUC values.

Several ROC plots are made to compare different features and the BDT in different p_T ranges. To check whether the BDT tagger is overtrained, the shape comparison is shown in Figure 5.21, between training dataset and validation dataset. No overtraining is observed as the distribution of training dataset is very similar to that of testing dataset.

Figure 5.22 shows the ROC curve for all single jet variables and the BDT-tagger in given p_T ranges in forward and central regions. Figure 5.23 shows the AUC of both N_{trk} -only tagger and the BDT-tagger as a function of jet p_T .

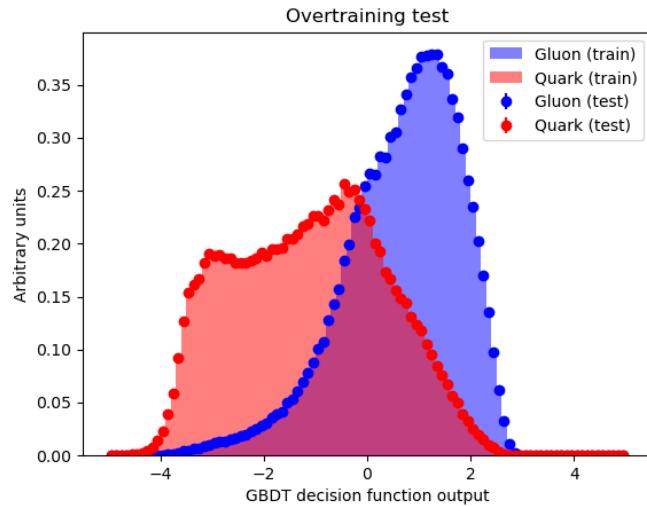
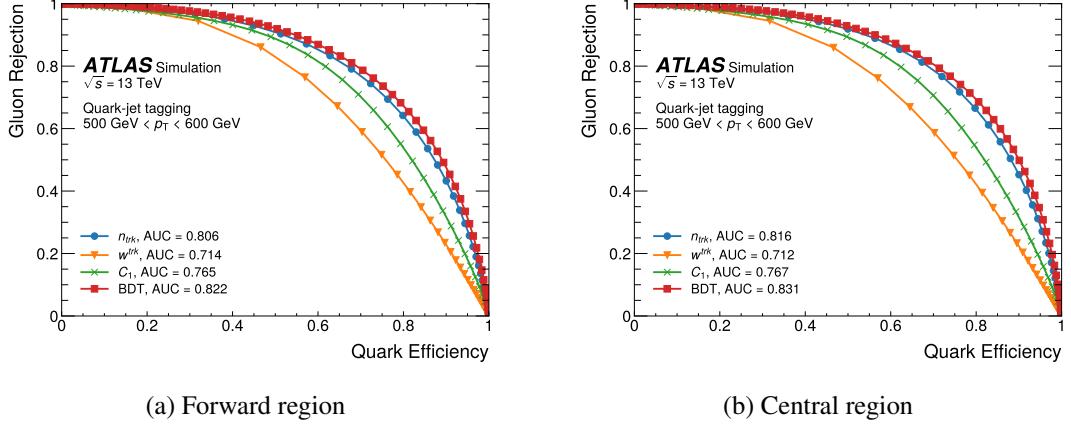
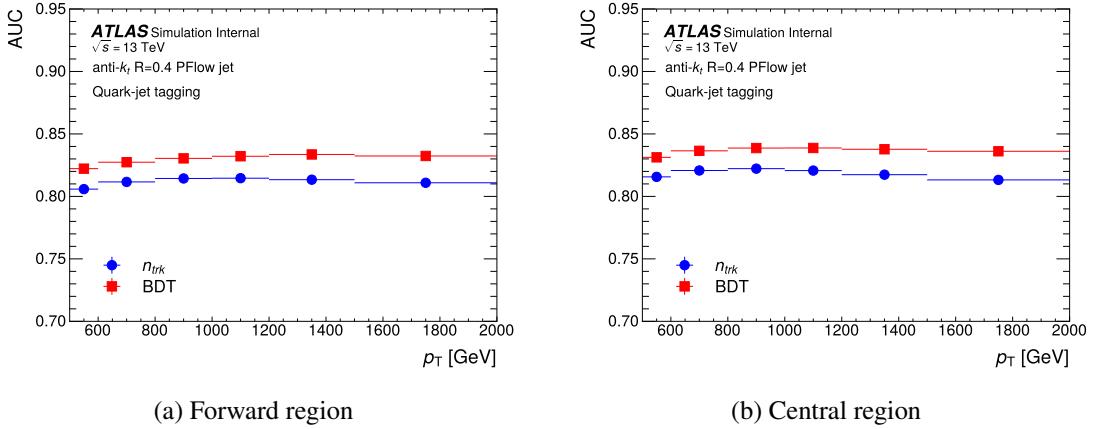


Figure 5.21 Overtraining validation

The N_{trk} -only tagger is found to be the most sensitive observable than other individual jet substructure variables for q/g tagging, W_{trk} and $C_1^{\beta=0.2}$ are less sensitive to the number of tracks inefficiencies because they are defined as ratios, the BDT-tagger which include the W_{trk} and $C_1^{\beta=0.2}$ has better AUC than N_{trk} -only tagger across all jet p_T ranges. This indicates that the BDT-based tagging mechanism has a heightened capacity to discriminate against gluon-jets at the same level of efficiency in identifying quark-jets with N_{trk} -only tagger . Both taggers are calibrated in this paper, more details are presented in


 Figure 5.22 The ROC Curve for different taggers in the given jet p_T .

 Figure 5.23 The AUC for different taggers across jet p_T .

the next section.

5.4 Matrix Method

The distribution of q/g tagging variables depend strongly on jet p_T . Thus a matrix method [47] approach used to extract the shape of the q/g tagging variables is performed on each p_T bin defined in Table 5.3 for quark- and gluon-jets, separately.

To measure the performance of the q/g taggers under study, samples exclusively composed of either quark-jets or gluon-jets are needed. In order to deduce the distribution shapes of the q/g tagging variables pertaining to quark- and gluon-jets within the empirical data, a methodology that capitalizes on samples possessing varying q/g ratios is

p_T bin boundary [GeV]					
500-600	600-800	800-1000	1000-1200	1200-1500	1500-2000
Forward & Central $ \eta $ jet samples in multi-jet					

Table 5.3 The p_T range division for the calibration of the q/g tagging variables and samples used in extraction of pure quark and gluon jets.

1013 employed. This approach, known as the matrix method [47], facilitates the extraction of
 1014 the distinct distributions of q/g tagging variables for the aforementioned jet categories.

1015 Pure quark- or gluon-jets can be extracted from forward and central jet samples
 1016 following the matrix:

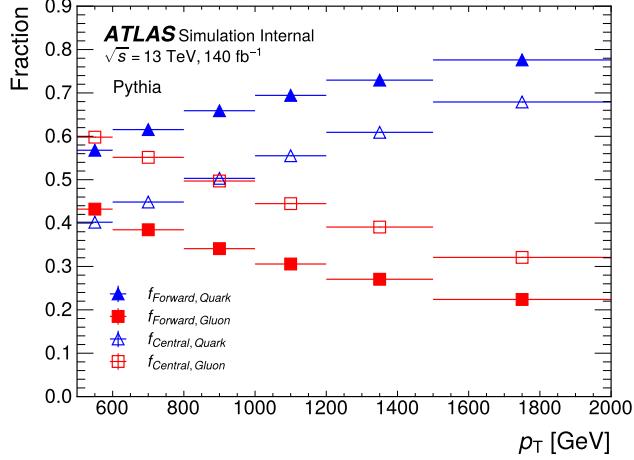
$$\begin{pmatrix} p_F(x) \\ p_C(x) \end{pmatrix} = \underbrace{\begin{pmatrix} f_{F,Q} & f_{F,G} \\ f_{C,Q} & f_{C,G} \end{pmatrix}}_{\equiv F} \begin{pmatrix} p_Q(x) \\ p_G(x) \end{pmatrix} \quad (5.6)$$

$$\begin{pmatrix} p_Q(x) \\ p_G(x) \end{pmatrix} = F^{-1} \begin{pmatrix} p_F(x) \\ p_C(x) \end{pmatrix}. \quad (5.7)$$

1017 where $p_{Q,G}(x)$ represents the distributions of the q/g tagging variable x in pure
 1018 quark- and gluon-enriched jet samples, $p_F(x)$ and $p_C(x)$ show the distributions of jet
 1019 variables in forward and central regions, respectively, $f_{F/C,Q/G}$ are the fractions of quarks
 1020 and gluons in a forward or central region. The inverse matrix of F is thus constructed
 1021 and used to extract pure quark/gluon $p_{Q,G}$. Data is used to obtain the distributions of
 1022 the quark- and gluon-enriched samples, MC is used to calculate the fraction of quarks
 1023 and gluons in them as shown in Figure 5.24, as well as the distributions of q/g tagging
 1024 variables. The matrix is calculated in each x bin and each jet p_T range.

1025 Figure ?? illustrates the fraction of light and heavy quark- and gluon-jets in the
 1026 PYTHIA 8 dijet sample. These fractions are depicted in a stacked format, summing up to
 1027 a cumulative value of 1. It should be noted that the involvement of heavy flavour quarks
 1028 constitutes a minor fraction, amounting to a few percent, and is deemed negligible for
 1029 the later study. Previous investigations [ref21] have established that any discrepancies
 1030 among the fractions derived from various MC event generators remain minimal. Fur-
 1031 thermore, the shapes of distributions obtained from the MC simulations generally exhibit
 1032 congruence with those observed within the data. The distributions of N_{trk} and BDT score
 1033 in higher and lower jet regions are shown in Figure 5.25 and Figure 5.26 in jet p_T range

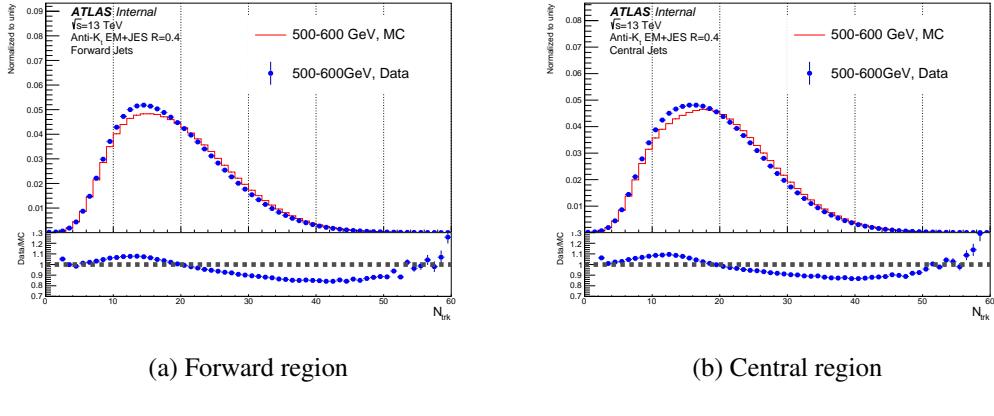
The calibration of quark/gluon jets taggers



(a)

Figure 5.24 Fractions of quark-jets and gluon-jets in forward jet and central jet regions from PYTHIA dijet process. These values are used as elements in F matrix in Equation 5.6.

1034 500 GeV - 600 GeV. The shapes of distributions obtained from the MC simulations is
 1035 generally consistent with that from data.



(a) Forward region

(b) Central region

Figure 5.25 The N_{trk} distribution of the leading two jets with PYTHIA 8 in the MC and data.

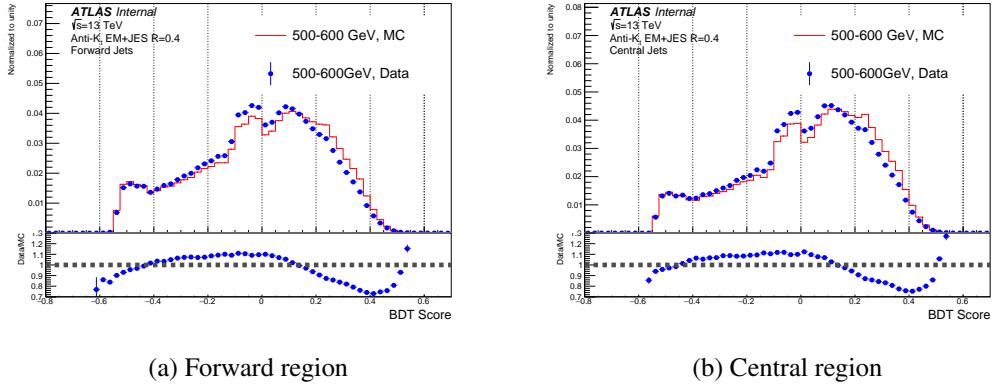


Figure 5.26 The BDT score distribution of the leading two jets with PYTHIA 8 in the MC and data.

5.5 MC non-closure

The matrix method is valid under the assumption that the shapes of $p_Q(x)$ and $p_G(x)$ remain consistent, regardless of whether the jets are situated in the central or forward regions. Jet fragmentation at a pp collider is expected to be predominantly influenced by the jet p_T and is generally considered independent of η , considering the underlying parton type. Consequently, an approach aimed at extracting distributions associated with the radiation patterns of quark-jets and gluon-jets should be valid at the particle level. At the detector level, however, the measured radiation pattern within jets no longer retains its η -independence. This is due to variations arising from differences in detector materials and technologies, leading to distinctions between the central and forward regions in terms of response. As a consequence of these effects, the matrix method experiences deviations from closure, indicating a disparity between the expected and actual outcomes.

The distributions of N_{trk} have been seen to have systematic difference for the truth-labelled quark/gluon jets in the quark-enriched and gluon-enriched regions in each p_T bin. To rectify this discrepancy and ensure alignment in the distribution of jet tagging variables between the central and forward regions, a re-weighting procedure is implemented. This procedure involves applying adjustments to account for the observed differences. For each event, the central jet is weighted by a re-weighting factor :

$$w_{Q/G}(x; p_{T,j}) = \frac{p_{Q/G, \text{forward}}(x; p_{T,j})}{p_{Q/G, \text{central}}(x; p_{T,j})} \quad (5.8)$$

1054 where q/g tagging variable x is calculated in each jet p_T bin for quark and gluon jets,
 1055 respectively. By default the re-weighting factor derived from truth-labelled quark-jets is
 1056 implemented for both types of jets, whereas the re-weighting factor derived from truth-
 1057 labelled gluon-jets is used as an alternative to evaluate the systematic uncertainty from
 1058 the re-weighting procedure, known as MC non-closure systematic uncertainty for the
 1059 calibration.

1060 The distributions of N_{trk} in extracted pure quark- and gluon-jets and truth-labelled
 1061 MC before re-weighting as shown in Figure 5.27. After the re-weighting the distributions
 1062 of N_{trk} are shown in Figure 5.28. The non-closure is at few percent level and is taken
 1063 as MC non-closure systematic uncertainty.

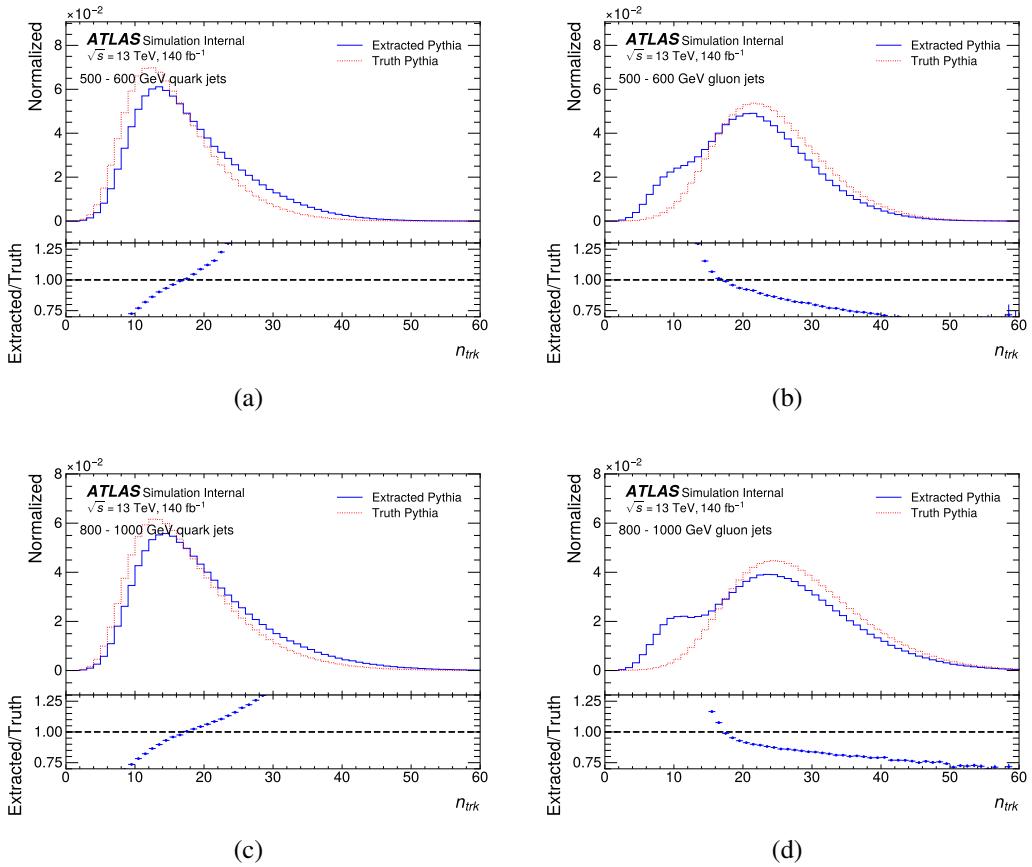


Figure 5.27 Before re-weighting: the N_{trk} distributions of quark-jet (a) (c) and gluon-jet in (b) (d) from PYTHIA 8 sample. Dashed and solid-line show the N_{trk} distributions in the truth MC and extracted MC, respectively. Bottom panels show the ratio of the extracted MC to the truth MC.

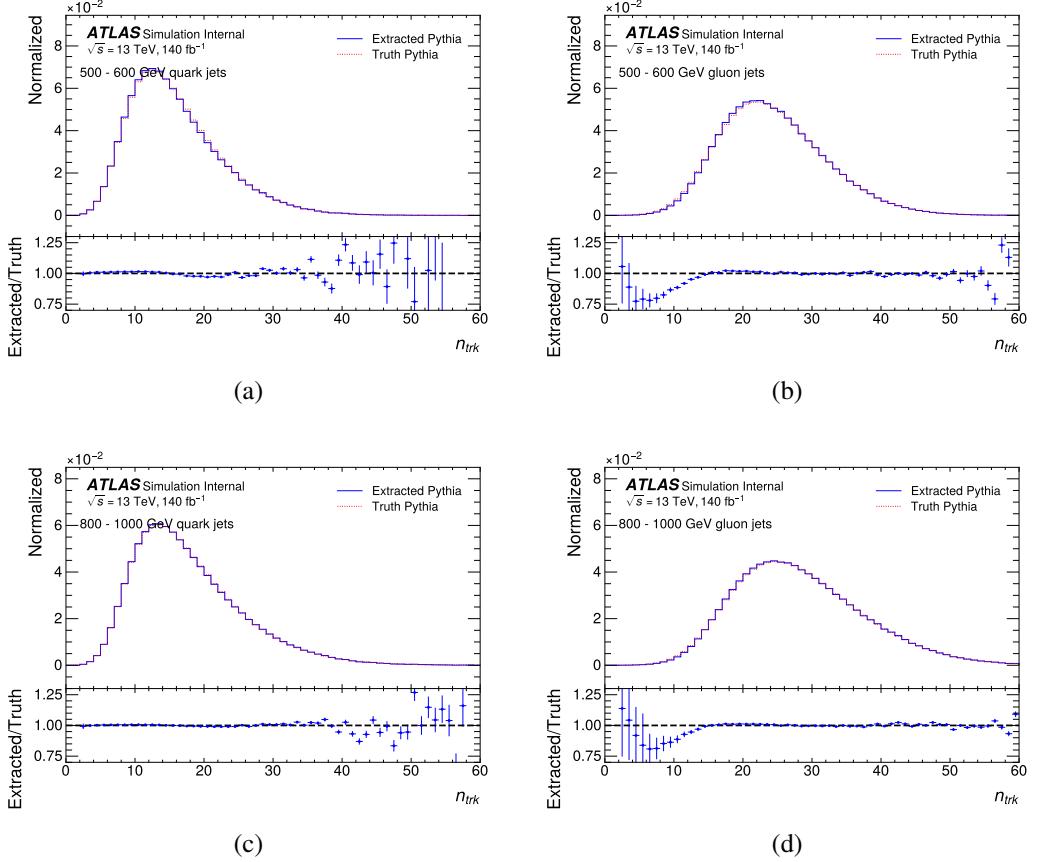


Figure 5.28 After re-weighting with quark factor: the N_{trk} distributions of quark-jet (a) (c) and gluon-jet in (b) (d) from PYTHIA 8 sample. Dashed and solid-line show the N_{trk} distributions in the truth MC and extracted MC, respectively. Bottom panels show the ratio of the extracted MC to the truth MC.

1064 5.5.1 Closure test for BDT tagger

1065 Similar to the distribution of N_{trk} , the distributions of BDT score for truth labelled-
 1066 jets exhibit systematic disparities in forward and central regions. Therefore, the same
 1067 re-weighting procedure as described is performed for BDT tagger as well. The MC non-
 1068 closure test is thus conducted by comparing the distributions of BDT score for extracted
 1069 and truth quark- and gluon-jets, separately, as shown in Figure 5.29. The distributions
 1070 of BDT before and after re-weighting are shown in Figure 5.30 and Figure 5.31. The
 1071 non-closure is about few percent level and taken as one systematic uncertainty.

The calibration of quark/gluon jets taggers

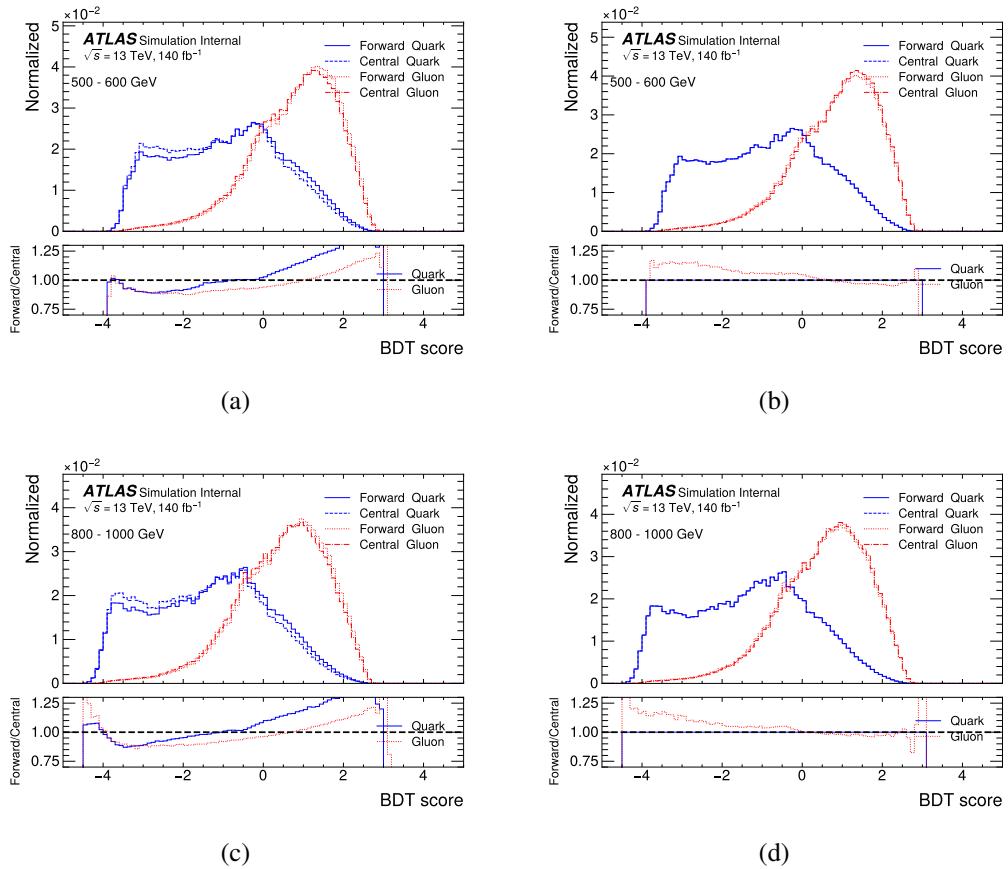


Figure 5.29 The distribution of BDT score for jets before (a) (c) and after (b) (d) re-weighting.

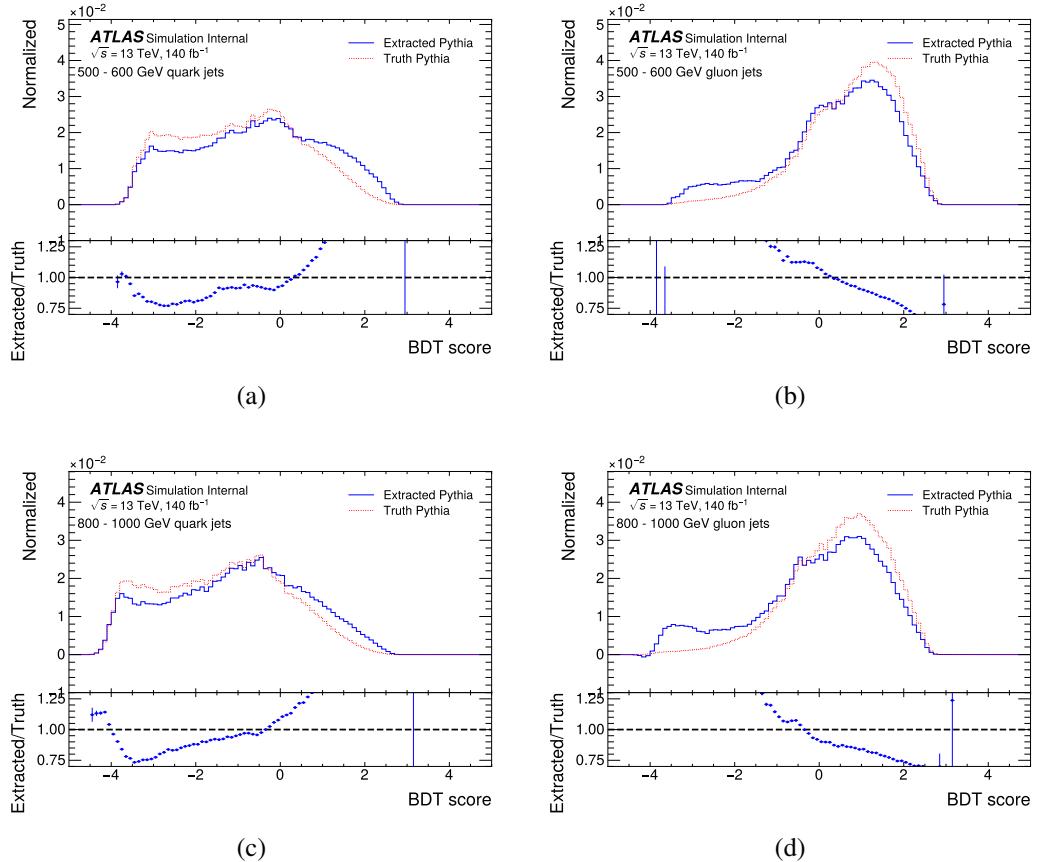


Figure 5.30 Before re-weighting: the MC-closure for quark-jet in (a) (c) and for gluon-jet in (b) (d) in BDT distributions from PYTHIA 8 sample. Dashed and solid-line histograms show the BDT distributions in the truth MC and extracted MC, respectively. Bottom panels show the ratio of the extracted MC to the truth MC.

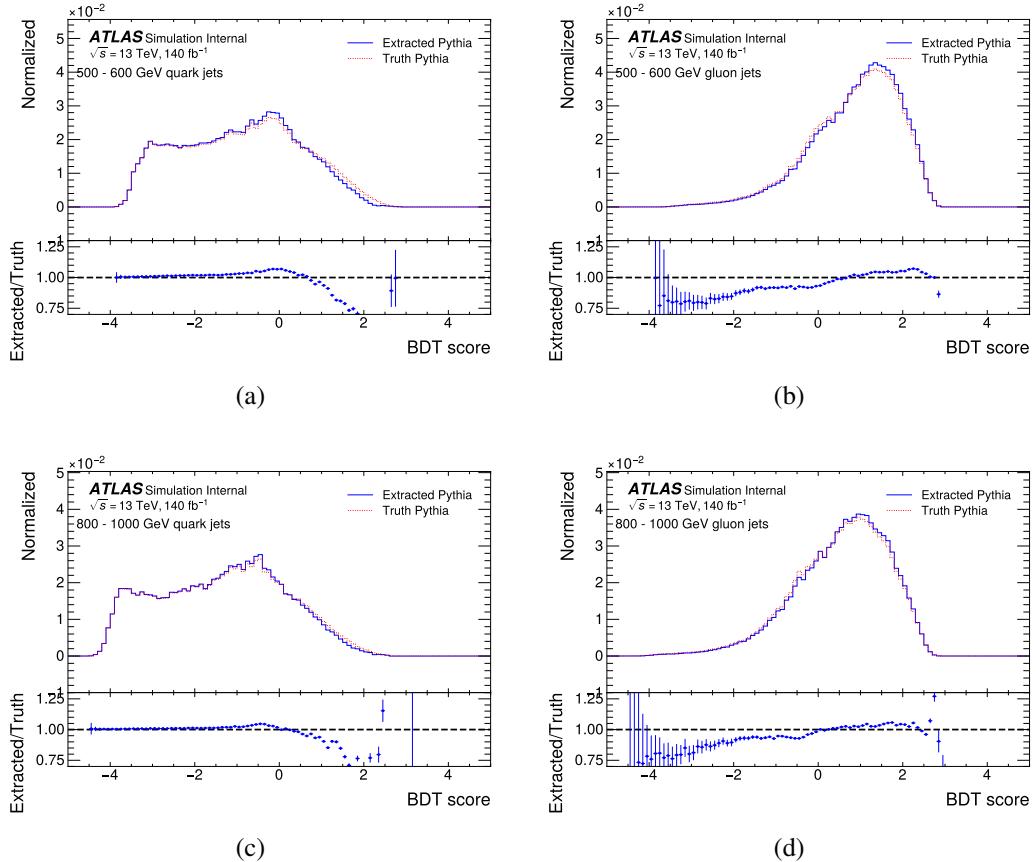


Figure 5.31 After re-weighting: the MC-closure for quark-jet in (a) (c) and for gluon-jet in (b) (d) in BDT distributions from PYTHIA 8 sample. Dashed and solid-line histograms show the BDT distributions in the truth MC and extracted MC, respectively. Bottom panels show the ratio of the extracted MC to the truth MC.

1072 **5.5.2 Summary for the MC Closure test**

1073 After applied the re-weighting factor to the jet tagging variables N_{trk} and BDT, the
 1074 distributions of extracted quark-and gluon-jets converge with those of truth jets. The
 1075 residual discrepancy, which has only few percent level to the total events is taken into
 1076 account as MC non-closure systematic uncertainty. No obvious dependency on jet η is
 1077 observed from the distributions of jet tagging variables.

1078 **5.6 Scale factor**

1079 The calibration of the q/g tagging variables is performed by applying binned scale
 1080 factor (SF) in the simulation for each quark- and gluon-jet, respectively. The scale factor
 1081 is obtained from distributions of the variables in quark- and gluon-jets from MC in order
 1082 to match the shape of the simulation to that of the data.

1083 The tagger working points (WP) are established for fixed quark-jets efficiency in
 1084 the nominal MC sample, for both taggers. At a given working point, the efficiencies for
 1085 quark- and gluon-jets are defined as follows:

$$\varepsilon_{Q/G}(x^{WP}) = \int_{x < x^{WP}} p_{Q/G}(x) dx. \quad (5.9)$$

1086 Rejection factors corresponding to quark- and gluon-jets can also be given as:

$$\xi_{Q/G}(x^{WP}) = 1 / \int_{x > x^{WP}} p_{Q/G}(x) dx = 1 / (1 - \varepsilon_{Q/G}(x^{WP})). \quad (5.10)$$

1087 Discrepancies observed between the quark-jet tagging efficiencies and gluon-jet re-
 1088 jections obtained from data and the corresponding values anticipated from the MC sim-
 1089 ulations are quantified using data-to-MC scale factors (SF). These factors are computed
 1090 separately for each q/g tagger in various p_T bins, at a fixed WP. The SF is defined using
 1091 Equation 5.9 and 5.10 for quark- and gluon-jets, respectively :

$$\text{SF}_Q(x^{WP}) = \frac{\varepsilon_Q^{\text{Data}}(x^{WP})}{\varepsilon_Q^{\text{MC}}(x^{WP})}. \quad (5.11)$$

$$\text{SF}_G(x^{WP}) = \frac{\xi_G^{\text{Data}}(x^{WP})}{\xi_G^{\text{MC}}(x^{WP})}. \quad (5.12)$$

1092 where $\varepsilon_{Q/G}^{\text{Data}}(x^{WP})$ and $\varepsilon_{Q/G}^{\text{MC}}(x^{WP})$ are $\varepsilon_{Q/G}(x^{WP})$ in data and MC, respectively. Same defi-
1093 nitions apply to $\xi_{Q/G}(x^{WP})$. The WPs corresponding to fixed quark-jets tagging efficien-
1094 cies of 50%, 60%, 70%, and 80% have been examined, revealing analogous trends in the
1095 characteristics of SFs.

1096 Figure 5.32 to 5.35 show the distribution of all jet tagging variables in quark- and
1097 gluon-jets after matrix method extraction in all different MC samples and data in given
1098 p_T range.

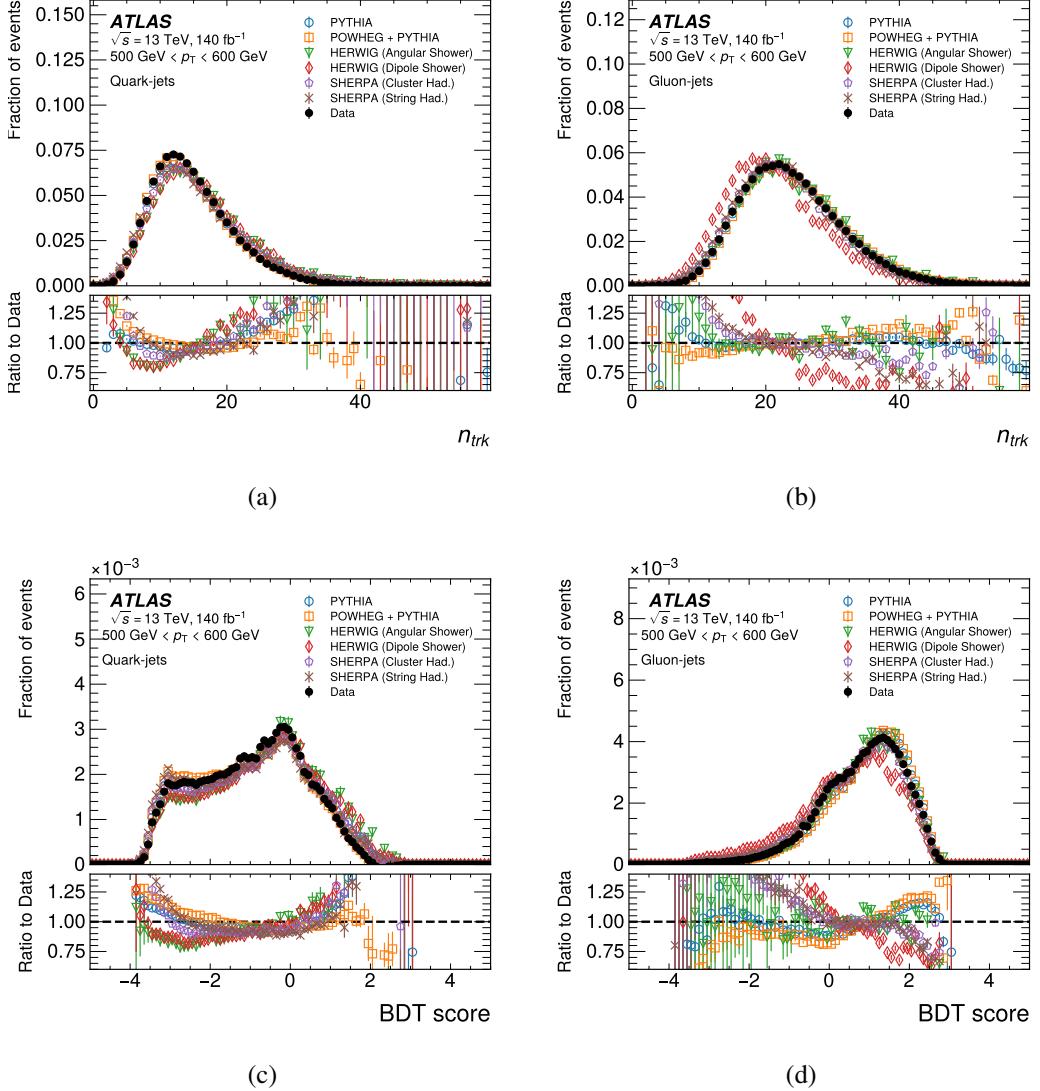


Figure 5.32 The distributions of N_{trk} (a,b) and BDT score (c,d) for quark-jets (left) and gluon-jets (right) using different generators (open symbols) and data (closed symbol) are shown in the upper panels. The lower panels show the ratio of each MC distribution and the data. The vertical error bars show the statistical uncertainty.

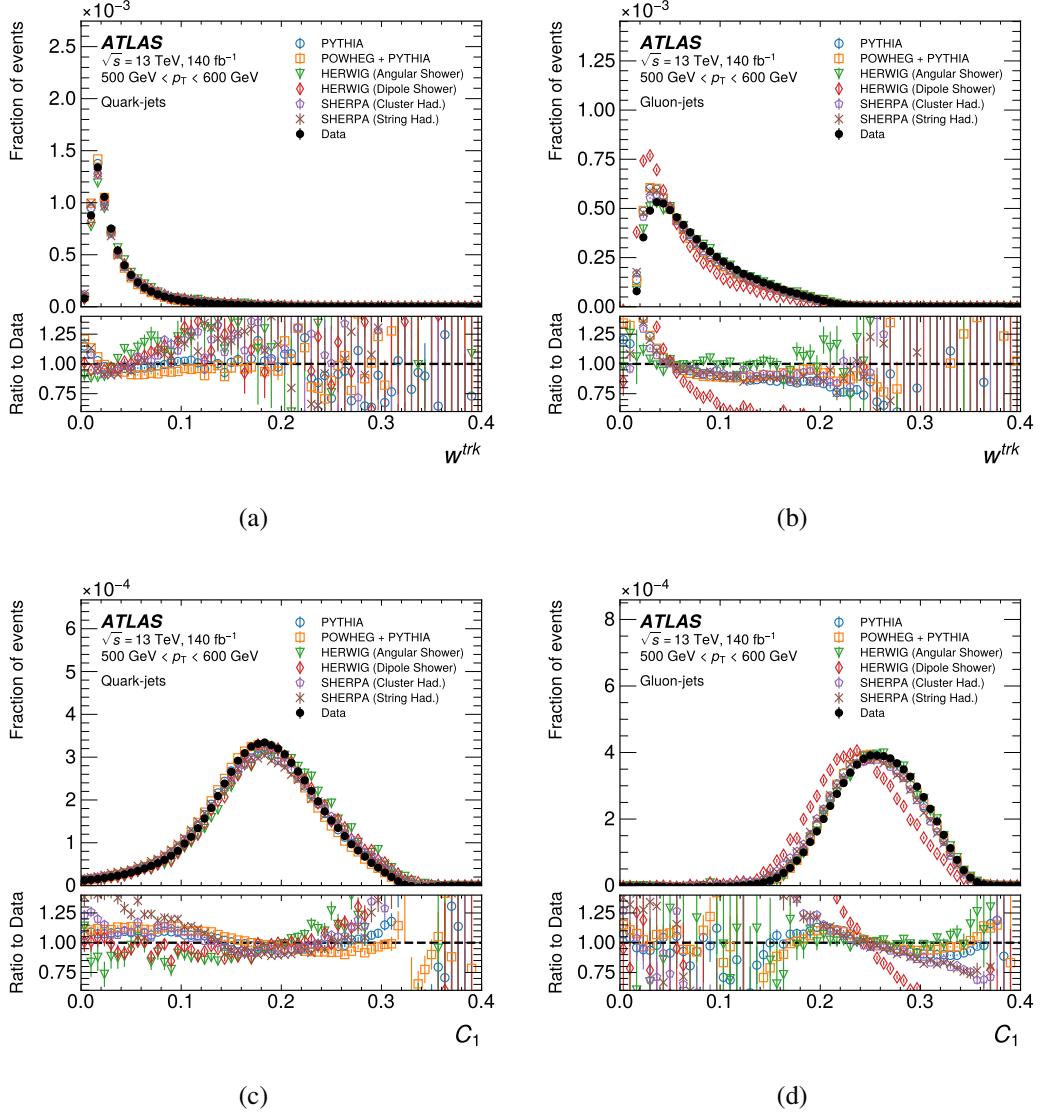


Figure 5.33 The distributions of W_{trk} (a,b) and C_1 (c,d) for quark-jets (left) and gluon-jets (right) using different generators (open symbols) and data (closed symbol) are shown in the upper panels. The lower panels show the ratio of each MC distribution and the data. The vertical error bars show the statistical uncertainty.

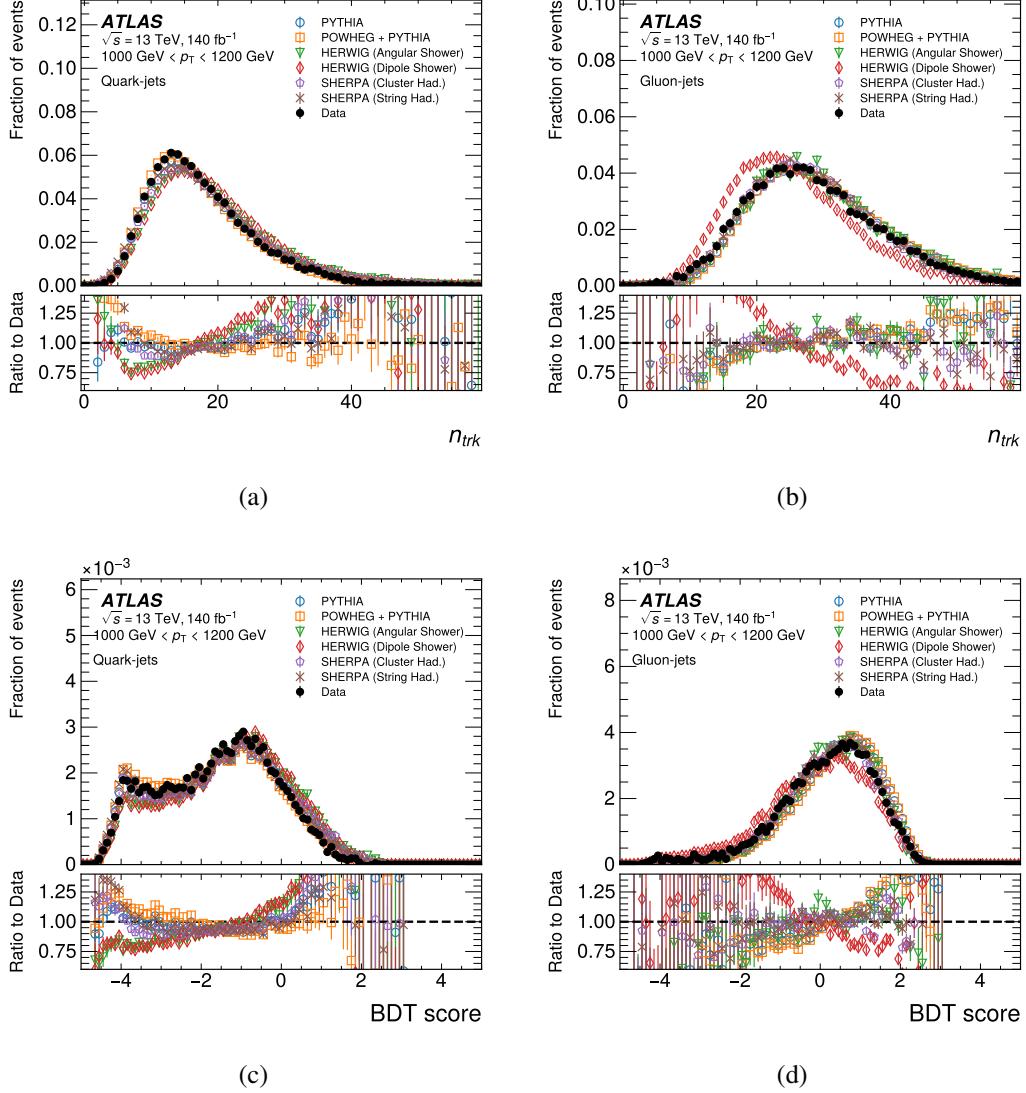


Figure 5.34 The distributions of N_{trk} (a,b) and BDT score (c,d) for quark-jets (left) and gluon-jets (right) using different generators (open symbols) and data (closed symbol) are shown in the upper panels. The lower panels show the ratio of each MC distribution and the data. The vertical error bars show the statistical uncertainty.

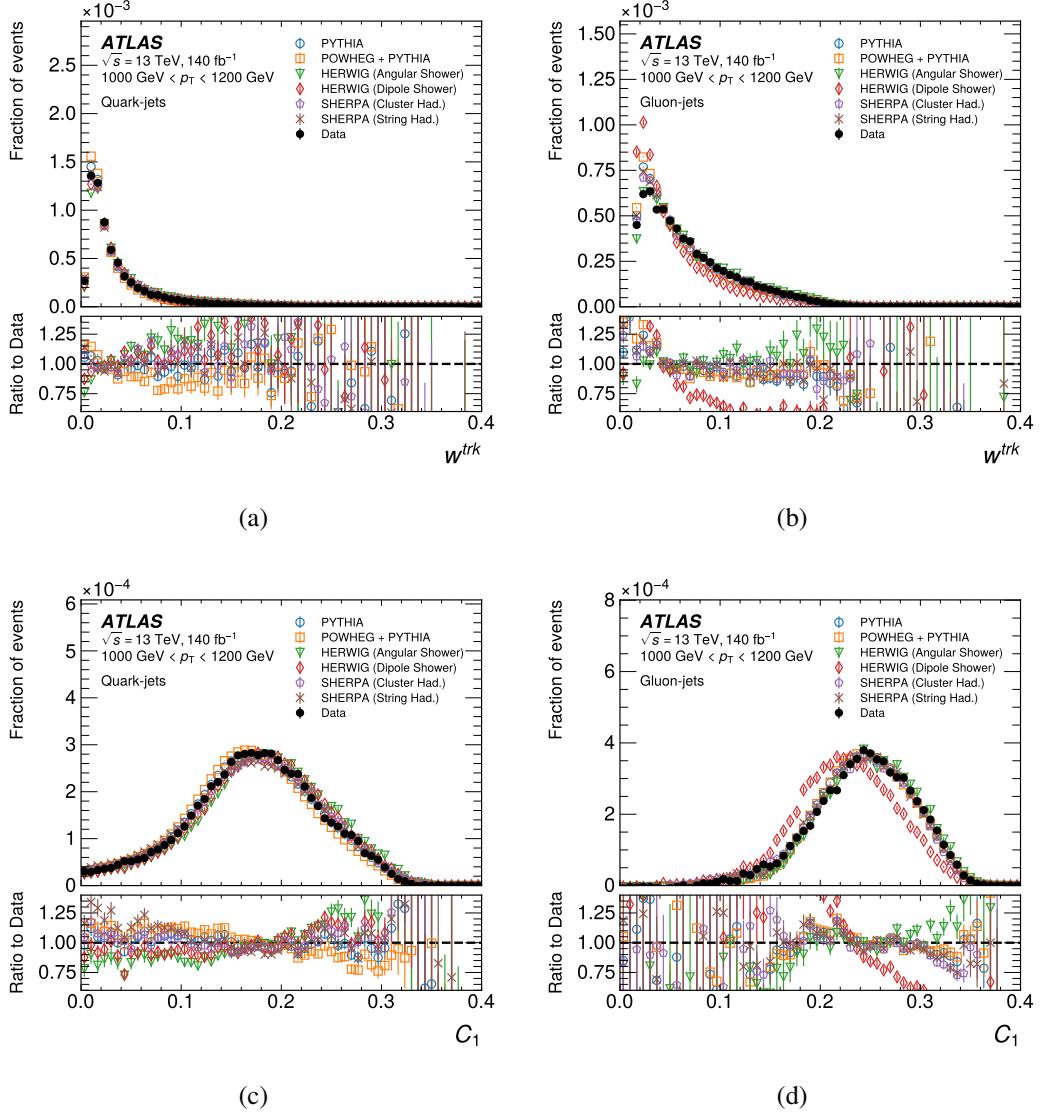


Figure 5.35 The distributions of W_{trk} (a,b) and C_1 (c,d) for quark-jets (left) and gluon-jets (right) using different generators (open symbols) and data (closed symbol) are shown in the upper panels. The lower panels show the ratio of each MC distribution and the data. The vertical error bars show the statistical uncertainty.

1099 Cut values corresponding to the 50% WP are summarised in Table 5.4 for the N_{trk} -
 1100 only tagger and Table 5.5 for the BDT-tagger. Figure 5.36 shows the gluon-jets efficiency
 1101 of both N_{trk} -only tagger and the BDT-tagger as a function of jet p_{T} , for the MC and data,
 1102 at four WPs.

1103 Both the N_{trk} -only and BDT-taggers demonstrate commendable performance on
 1104 data, with high quark signal efficiency across all p_{T} range. Notably, at the 50% work-
 1105 ing point, the N_{trk} -only tagger achieves approximately 90% rejection of gluon-jets, while
 1106 the BDT tagger surpasses this performance by rejecting around 93% of gluon-jets. The
 1107 BDT-tagger outperforms the N_{trk} -only tagger by exhibiting superior gluon-jets rejection
 1108 rates at the identical WP. This disparity in performance arises from the inclusion of a
 1109 more comprehensive set of jet substructure variables in the BDT approach. The discrep-
 1110 acy between the level of gluon-jet rejection observed in data and that predicted by the
 1111 MC samples increases as the jet p_{T} increases. This phenomenon is closely tied to the
 1112 dissimilarity between the modelling of gluons and their actual behaviour in data.

p_{T} [GeV]	500 - 600	600 - 800	800 - 1000	1000 - 1200	1200 - 1500	1500 - 2000
WP						
0.5	15.0	16.0	17.0	18.0	18.0	19.0
0.6	17.0	18.0	19.0	20.0	20.0	21.0
0.7	19.0	20.0	21.0	22.0	23.0	24.0
0.8	22.0	23.0	24.0	26.0	27.0	28.0

Table 5.4 Cut values of N_{trk} at different working point in each of jet p_{T} range

p_{T} [GeV]	500 - 600	600 - 800	800 - 1000	1000 - 1200	1200 - 1500	1500 - 2000
WP						
0.5	-0.8	-1.0	-1.2	-1.4	-1.6	-1.8
0.6	-0.4	-0.6	-0.8	-1.0	-1.2	-1.4
0.7	0.0	-0.2	-0.4	-0.6	-0.8	-1.0
0.8	0.4	0.2	0.0	-0.2	-0.3	-0.6

Table 5.5 Cut values of BDT at different working point in each of jet p_{T} range

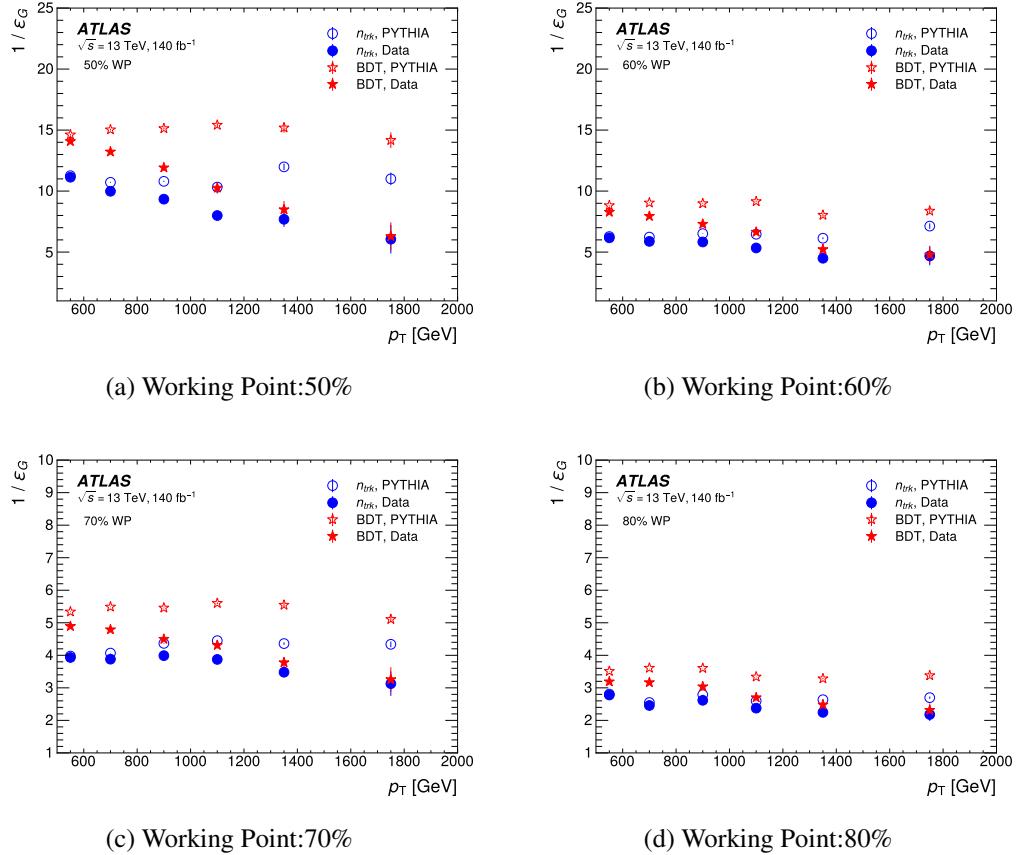


Figure 5.36 Inverse of the gluon-jet efficiency of N_{trk} (circles) and BDT (stars) as a function of jet p_T at the each WP in data (closed symbols) and the PYTHIA (open symbols) MC. The vertical error bars show the statistical uncertainty.

1113 **5.7 Systematic uncertainties**

1114 In this study, different types of systematic uncertainty are taken into account. The
1115 distribution of N_{trk} and BDT for truth-labelled quark-/gluon-jets are given by the MC
1116 simulation samples, therefore, theoretical uncertainties originate from aspects encom-
1117 passing the modelling of the MC simulation, such as choices involving parton showering,
1118 hadronisation, matrix element, PDFs, scale variations, and Splitting-Kernel effects. Fur-
1119 thermore, experimental uncertainties such as JES and JER, tracking reconstruction effi-
1120 ciencies are meticulously incorporated. The potential impact of methodological choices,
1121 including N_{trk} or BDT re-weighting, as well as the non-closure behaviour of MC simula-
1122 tions, is propagated to the resultant SFs.

1123 The nominal result in this analysis is provided using PYTHIA 8 MC samples, all
1124 other MC samples are considered as alternative samples to study corresponding system-
1125 atic uncertainty.

1126 **5.7.1 Parton shower modelling uncertainty**

1127 The different chose of algorithmic or parametric in the modelling of the parton
1128 shower could result in different SF result. This systematic uncertainty is estimated by
1129 comparing the SFs extracted from two MC samples with the same ME and hadronisation
1130 but different types of showers: HERWIG Angular-ordered and HERWIG Dipole samples.
1131 The corresponding fractions of quarks and gluons present in these two MC samples, are
1132 presented in Figure 5.37. The difference of extracted SFs between these two samples is
1133 less than 10% for quark signal efficiency and around 20% for gluon rejection efficiency.
1134 While the influence on quark scale factors is negligible, it takes on a dominant role in the
1135 context of gluon scale factors.

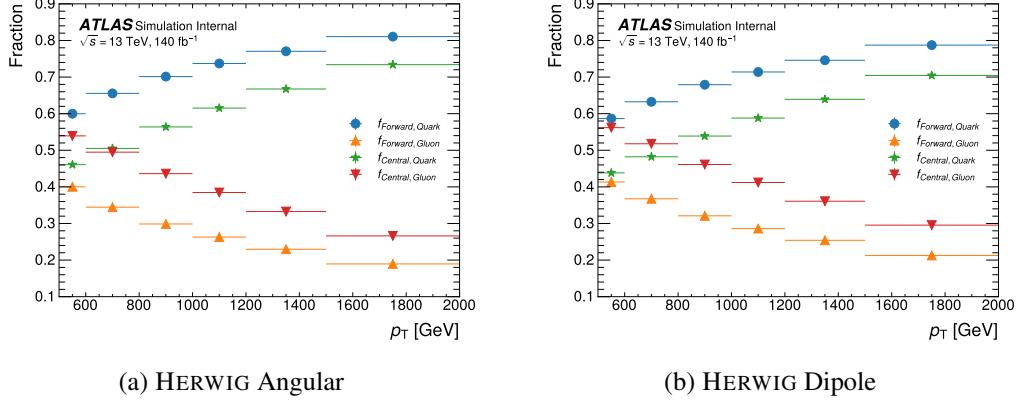


Figure 5.37 Fractions of quark- gluon-jets of HERWIG angular (a) and HERWIG dipole (b) samples.

1136 5.7.2 Hadronisation modelling uncertainty

1137 The uncertainty from hadronisation modelling is given by the difference between
 1138 the extracted SFs from the SHERPA MC samples with cluster-based hadronisation mod-
 1139 elling and string-based hadronisation modelling, separately. The corresponding fractions
 1140 of quarks and gluons present in these two MC samples are presented in Figure 5.38. The
 1141 uncertainty on the SFs range from 1% to 8% for both jet types.

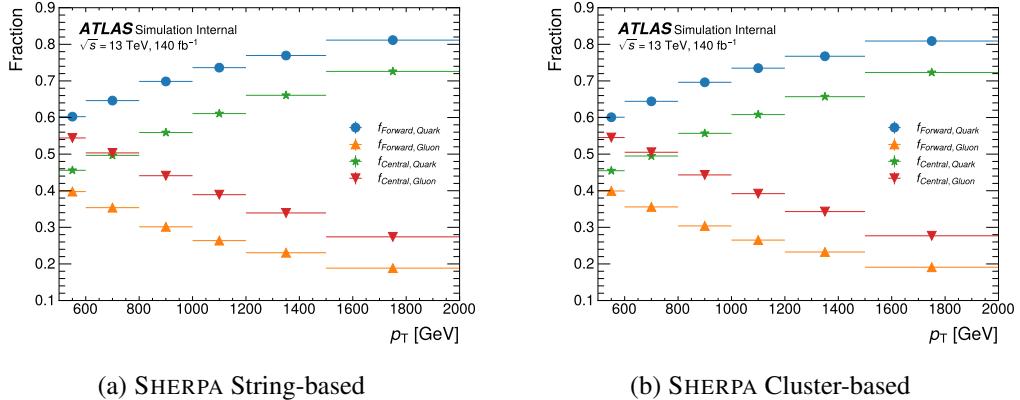


Figure 5.38 Fractions of quark- and gluon-jets in each SHERPA sample.

5.7.3 Matrix element uncertainty

The uncertainty introduced by different types of ME in the MC samples is taken from the differences in the extracted SFs in two MC samples with different ME : POWHEG and PYTHIA . The corresponding fractions of quarks and gluons present in the POWHEG samples are presented in Figure 5.39.

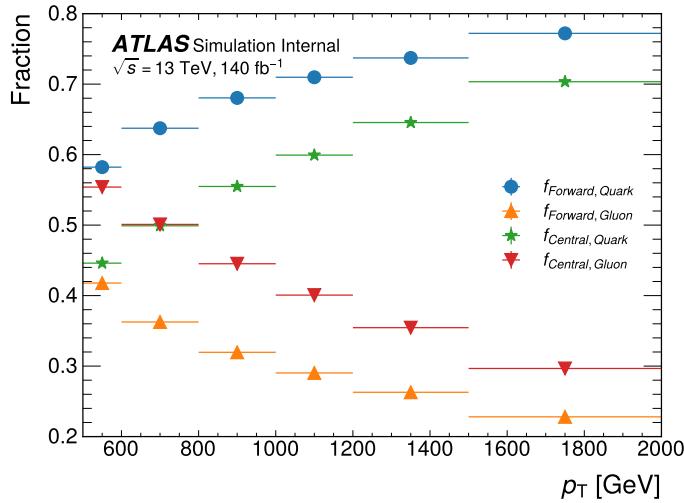


Figure 5.39 Fractions of quark jets and gluon jets in POWHEG samples.

5.7.4 PDF uncertainty

The uncertainty from the PDF set is evaluated using LHAPDF [75] package which provides the PDF internal variations for each PDF set, a NNPDF2.3 set is chosen to evaluate the various weights which depend on the momentum fraction. The PDF uncertainty is given by changing the nominal PDF weight to the systematic variation, then compare the SFs extracted from each of variations. The PDF uncertainty is around 5% - 7% level and almost negligible compared to others.

5.7.5 Scale variation uncertainty

The variation of the renormalisation (μ_R) and factorisation (μ_F) scales in QCD is used to evaluate the uncertainty caused by missing higher order corrections. The nominal PYTHIA sample is used for such estimation. In total there are 7 scale variations (μ_R, μ_F) in (2,2), (2,1), (1,1), (1,2), (1,0.5), (0.5,1), (0.5,0.5) studied in this analysis. The scale

1159 uncertainty is given by taking the maximum shift of the envelope with respect to the
1160 nominal one at each working points. The total scale uncertainty is around 4% - 7%.

1161 **5.7.6 Splitting-Kernel variation uncertainty**

1162 All formulations of shower processes are constructed on the fundamental founda-
1163 tion of the universal behaviour exhibited by singular infrared (soft and/or collinear) lim-
1164 its within QCD. Nonetheless, when one ventures beyond these limits into the physical
1165 phase space where these kernels are employed as approximations, there are in principle
1166 infinitely many different radiation functions to choose from, sharing the same singular
1167 terms but having different non-singular ones. The Splitting-Kernel variations [76] are
1168 variations of the non singular part of the splitting functions, for initial-state radiation and
1169 final-state radiation. Such uncertainty is less than 1%.

1170 **5.7.7 Tracking uncertainty**

1171 he number of associated tracks is the most important input for both taggers, with
1172 tracking-related systematics exerting an impact on the measurement of SFs. he uncer-
1173 tainty associated with reconstructed tracks is partitioned into two components: the un-
1174 certainty pertaining to track reconstruction efficiency and the MC fake rate [64]. Both
1175 sources of uncertainty are factored in to recalibrate the count of tracks associated with
1176 jets.

1177 The track reconstruction efficiency uncertainty originates from material-related un-
1178 certainties, which constitutes the prevailing source, as well as from considerations related
1179 to the physics model. These uncertainties are estimated through a comparison of track
1180 efficiency across samples that encompass diverse detector modelling configurations. On
1181 the other hand, the MC fake rate is determined by contrasting the trends in a specific
1182 aspect of track multiplicity as a function of the average number of interactions per bunch
1183 crossing between empirical data and the MC simulation. The disparity in final SFs be-
1184 tween the nominal value and the outcome of the systematic variation contributes to the
1185 tracking systematic uncertainty. This uncertainty spans a range of approximately 1% to
1186 8%.

1187 **5.7.8 JES /JER uncertainty**

1188 The uncertainties associated with JES stem from the process of calibrating the trans-
1189 verse momentum balance between jets located in the central and forward regions, while
1190 also accommodating uncertainties linked to single-particle and test beam measurements.
1191 The JER uncertainties encompass the disparities between data and the MC. For each
1192 JES/JER variation, a corresponding SF is derived, and the difference between the nom-
1193 inal value and the variation is computed to determine the systematic uncertainty. The
1194 cumulative JES/JER uncertainty amounts to approximately 0.2%.

1195 **5.7.9 N_{trk} / BDT re-weighting**

1196 The quark-enriched and gluon-enriched regions are defined by comparing the η of
1197 leading and subleading jets, introduces to an η dependency from track reconstruction
1198 process. A re-weighting factor defined by Equation 5.8 is applied on N_{trk} and BDT
1199 taggers for each event to reduce the impact from different track multiplicity in different
1200 η range. The re-weighting factors acquired from truth-labelled gluon jets are regarded
1201 as an alternative source of contribution to the systematic uncertainty. It's worth noting
1202 that the differences arising from the re-weighting procedure remain comparatively minor
1203 (about 0.1% - 0.5%) in comparison to other sources of uncertainty.

1204 The distributions of N_{trk} and BDT for extracted quark and gluon-jets after re-weighting
1205 with quark factor have been shown in the previous chapter. The truth distribution of
1206 quark/gluon in forward/central jets using gluon factors are shown in Figure 5.40 for
1207 N_{trk} and Figure 5.41 for BDT, respectively. Figure 5.42, Figure 5.43 shows the distribu-
1208 tions of extracted quark and gluon-jets after reweighting with gluon factor.

The calibration of quark/gluon jets taggers

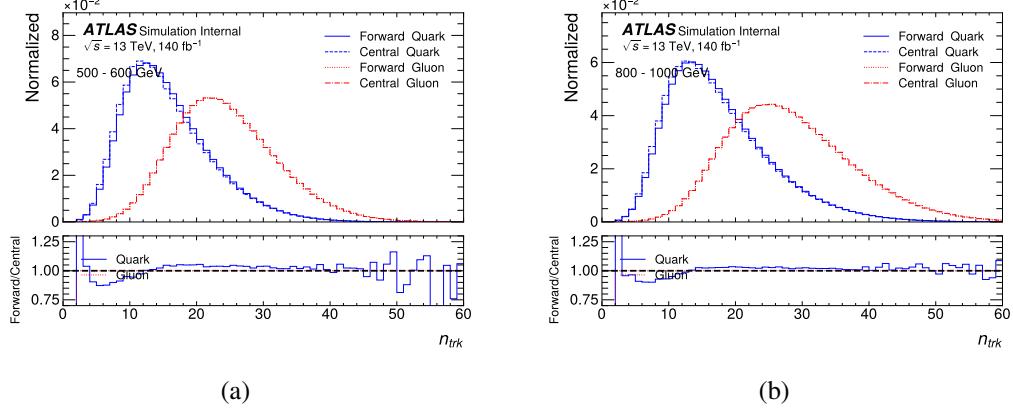


Figure 5.40 The distribution of N_{trk} for jets between 500-600 GeV (a) and 800-1000 GeV (b) after N_{trk} re-weighting using gluon factor.

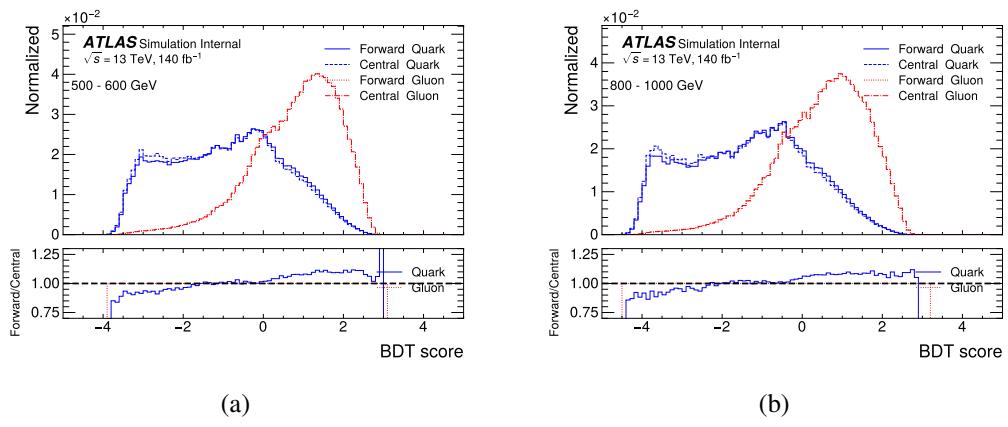


Figure 5.41 The distribution of BDT for jets between 500-600 GeV (a) and 800-1000 GeV (b) after re-weighting using gluon factor.

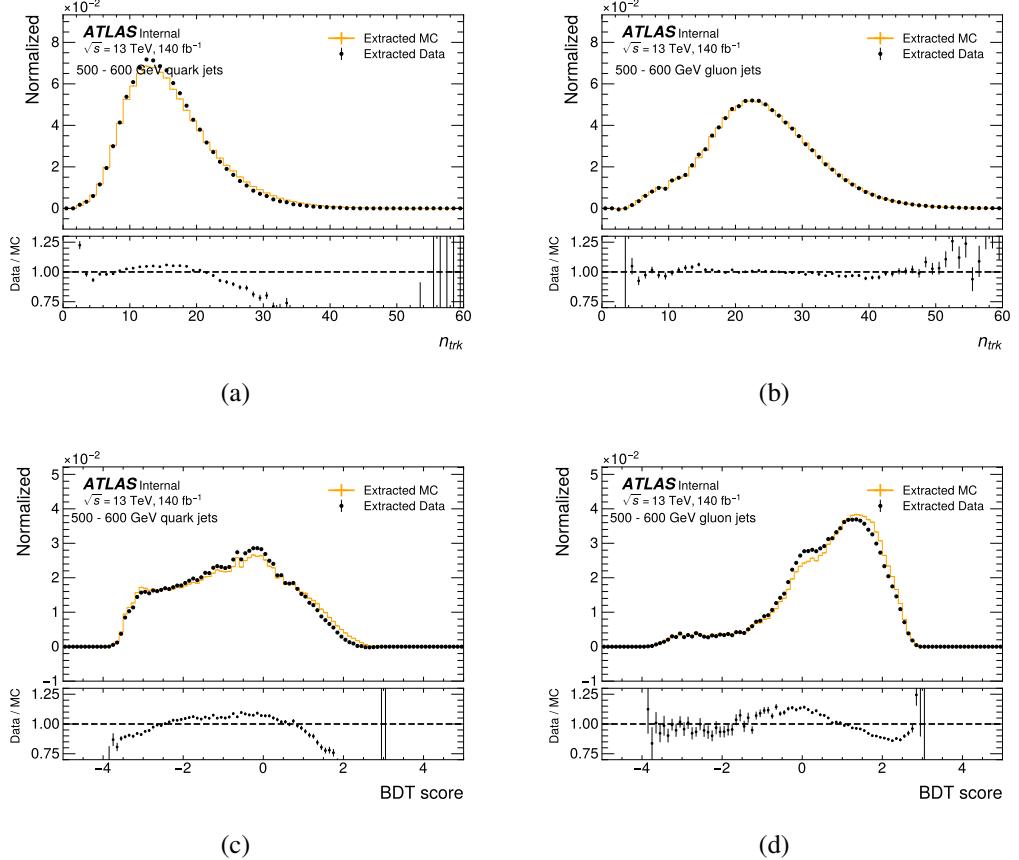


Figure 5.42 The N_{trk} (top) and BDT (bottom) distributions extracted by the matrix method from the data and MC of pure quark-jets (a) (c) and gluon-jets (b) (d) by PYTHIA 8. extracted by the matrix method from the data and MC. The gluon factor is applied. Solid-line histograms show the distributions of quark or gluon-jets defined by the jet parton flavour label in the MC. A bottom panel in each figure shows the ratio of the extracted data to the extracted MC by the matrix method.

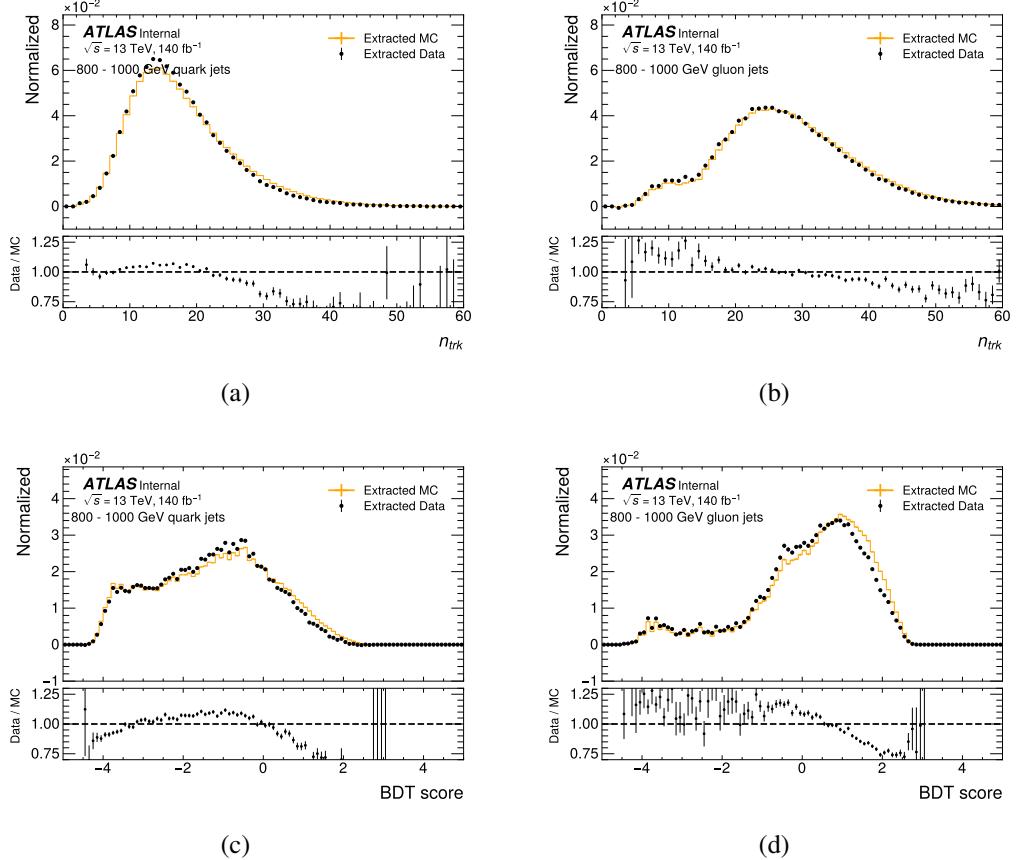


Figure 5.43 The N_{trk} (top) and BDT (bottom) distributions extracted by the matrix method from the data and MC of pure quark-jets (a) (c) and gluon-jets (b) (d) by PYTHIA 8. extracted by the matrix method from the data and MC. The gluon factor is applied. Solid-line histograms show the distributions of quark or gluon-jets defined by the jet parton flavour label in the MC. A bottom panel in each figure shows the ratio of the extracted data to the extracted MC by the matrix method.

5.7.10 The MC non-closure

As described in Section 5.5, the MC closure test is conducted using MC samples wherein each jet is assigned a truth label. After re-weighting, the distributions of N_{trk} and BDT obtained through the matrix method exhibit consistency with the truth-labelled ones for quark- and gluon-jets, respectively. The remaining difference for both taggers is only 1% level.

5.7.11 Statistical uncertainty

The estimation of statistical uncertainty involves a stepwise process. It commences by varying the input data/MC distributions bin-by-bin, using Poisson/Gaussian distributions wherein the number of data events within each bin serves as the central value. These variations of the input histograms yield templates, subsequently employed as inputs for the template variations technique. This procedure is iterated 5000 times, with the standard deviation of these uncertainties of all toys taken is used to derive the statistical uncertainty of the SFs. This uncertainty is around 0.1%.

The distributions of SFs are shown in 5.44 for N_{trk} and 5.45 for the BDT.

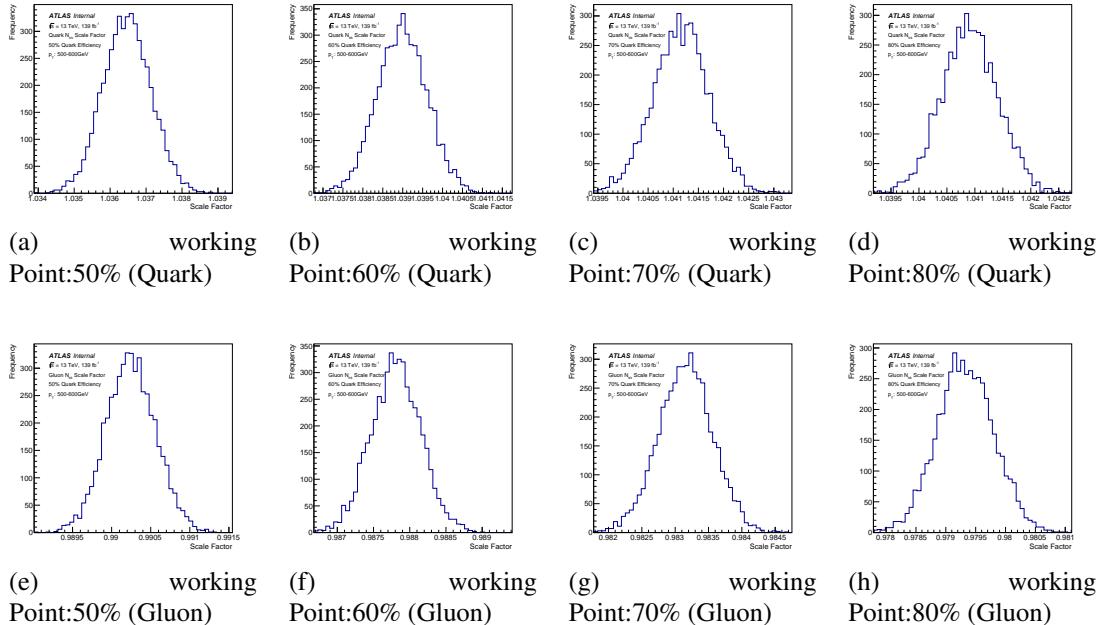


Figure 5.44 The distribution of SF by varying the input data distributions bin-by-bin using a Poisson distribution with the number of data events in each bin as the central value for 5000 times for working point of N_{trk} in jet p_T range 500-600 GeV.

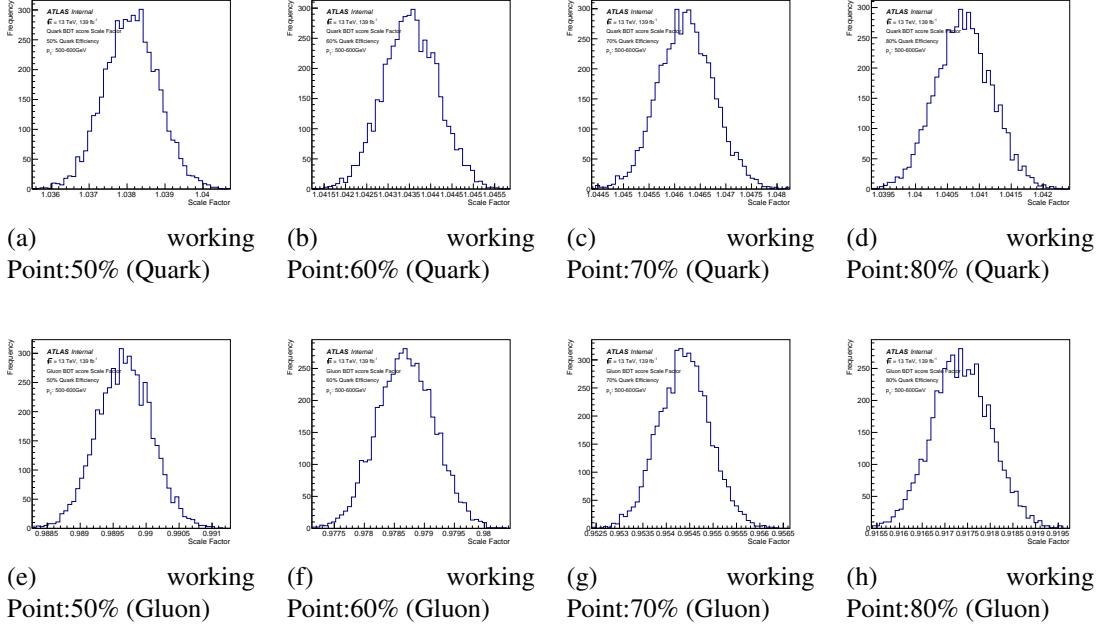


Figure 5.45 The distribution of SF by varying the input data distributions bin-by-bin using a Poisson distribution with the number of data events in each bin as the central value for 5000 times for working point of BDT in jet p_T range 500-600 GeV.

1223 5.8 Results

1224 Overall, both the N_{trk} -only tagger and the BDT-tagger exhibit commendable performance,
 1225 and can effectively distinguish quark-jet from gluon-jet with high efficiency. The
 1226 SFs for both quark- and gluon-jet fall within the range of approximately 0.9 to 1, indicating
 1227 a reasonable agreement. The systematic uncertainty for quark-jet SFs hovers around
 1228 10%, while for gluon-jet SFs it's approximately 20%. Detailed of each uncertainty are
 1229 shown in Section 5.7. The BDT-tagger showcases a slightly superior performance compared
 1230 to the N_{trk} only tagger, i.e. higher gluon-jet rejection at the same WP.

1231 The uncertainties of SF for each source of WP are estimated in each jet p_T range
 1232 are given from Table 5.6 to Table 5.13 for quark-jets. Table 5.14 to Table 5.21 show the
 1233 uncertainties of SF at each WP for gluon-jets. All systematics are ordered from largest to
 1234 smallest in p_T range 500 - 600 GeV. the systematic uncertainties associated with quark-
 1235 jet scale factors tend to be smaller than those linked to gluon-jet scale factors. Notably,

¹²³⁶ for both quark- and gluon-jets, these uncertainties are primarily governed by the source
¹²³⁷ of uncertainty stemming from parton showering.

Table 5.6 The quark scale factor (nominal) and the difference between the nominal and systematic variation results for 50% quark tag efficiency from $N_{\text{trk}}\text{tagger}$

	500-600	600-800	800-1000	1000-1200	1200-1500	1500-2000
nominal	1.02	1.04	1.04	1.03	1.02	1.01
scale variation	0.09	0.1	0.12	0.11	0.13	0.12
pdf weight	0.09	0.11	0.12	0.13	0.13	0.11
hadronization	0.09	0.07	0.06	0.05	0.04	0.04
tracking	0.08	0.07	0.06	0.05	0.05	0.04
matrix element	0.05	0.06	0.06	0.05	0.05	0.04
parton shower	0.02	0.03	0.05	0.06	0.07	0.08
MC nonclosure	0.02	0.04	0.04	0.03	0.02	0.01
splitting kernel	0.01	0.01	0.01	0.01	0.01	0.01
JES/JER	0.01	0.01	0.01	0.01	0.01	0.01
gluon reweight	0.01	0.01	0.01	0.01	0.01	0.01
Statistical	0.01	0.01	0.01	0.01	0.01	0.02
Total Uncertainty	0.19	0.19	0.21	0.21	0.22	0.19

Table 5.7 The quark scale factor (nominal) and the difference between the nominal and systematic variation results for 60% quark tag efficiency from $N_{\text{trk}}\text{tagger}$

	500-600	600-800	800-1000	1000-1200	1200-1500	1500-2000
nominal	1.03	1.04	1.04	1.03	1.01	1.01
pdf weight	0.09	0.1	0.12	0.12	0.12	0.1
tracking	0.08	0.07	0.06	0.05	0.05	0.04
scale variation	0.07	0.08	0.1	0.09	0.1	0.09
hadronization	0.06	0.05	0.04	0.04	0.03	0.03
matrix element	0.05	0.05	0.05	0.05	0.05	0.04
MC nonclosure	0.02	0.04	0.04	0.03	0.02	0.02
parton shower	0.02	0.03	0.03	0.04	0.06	0.08
splitting kernel	0.01	0.01	0.01	0.02	0.01	0.01
JES/JER	0.01	0.01	0.01	0.01	0.01	0.01
gluon reweight	0.01	0.01	0.01	0.01	0.01	0.01
Statistical	0.01	0.01	0.01	0.01	0.01	0.01
Total Uncertainty	0.16	0.17	0.18	0.18	0.18	0.17

The calibration of quark/gluon jets taggers

Table 5.8 The quark scale factor (nominal) and the difference between the nominal and systematic variation results for 70% quark tag efficiency from N_{trk} tagger

	500-600	600-800	800-1000	1000-1200	1200-1500	1500-2000
nominal	1.03	1.04	1.04	1.03	1.02	1.0
pdf weight	0.08	0.09	0.11	0.11	0.11	0.08
tracking	0.07	0.06	0.05	0.05	0.04	0.03
scale variation	0.06	0.06	0.07	0.07	0.07	0.06
hadronization	0.05	0.04	0.04	0.03	0.03	0.02
matrix element	0.04	0.05	0.04	0.04	0.04	0.03
MC nonclosure	0.03	0.04	0.04	0.04	0.02	0.01
parton shower	0.02	0.02	0.02	0.03	0.04	0.05
splitting kernel	0.01	0.01	0.01	0.02	0.02	0.01
JES/JER	0.01	0.01	0.01	0.01	0.01	0.01
gluon reweight	0.01	0.01	0.01	0.01	0.01	0.01
Statistical	0.01	0.01	0.01	0.01	0.01	0.01
Total Uncertainty	0.14	0.14	0.16	0.16	0.15	0.13

Table 5.9 The quark scale factor (nominal) and the difference between the nominal and systematic variation results for 80% quark tag efficiency from N_{trk} tagger

	500-600	600-800	800-1000	1000-1200	1200-1500	1500-2000
nominal	1.03	1.03	1.03	1.02	1.01	1.0
tracking	0.06	0.05	0.05	0.04	0.03	0.02
pdf weight	0.06	0.07	0.09	0.09	0.08	0.06
scale variation	0.03	0.04	0.05	0.04	0.04	0.05
MC nonclosure	0.03	0.04	0.04	0.03	0.02	0.01
hadronization	0.03	0.02	0.02	0.02	0.02	0.02
matrix element	0.03	0.04	0.03	0.03	0.03	0.02
parton shower	0.01	0.01	0.02	0.01	0.02	0.03
splitting kernel	0.01	0.01	0.01	0.02	0.02	0.01
JES/JER	0.01	0.01	0.01	0.01	0.01	0.01
gluon reweight	0.01	0.01	0.01	0.01	0.01	0.01
Statistical	0.01	0.01	0.01	0.01	0.01	0.01
Total Uncertainty	0.11	0.11	0.13	0.12	0.11	0.1

The calibration of quark/gluon jets taggers

Table 5.10 The quark scale factor (nominal) and the difference between the nominal and systematic variation results for 50% quark tag efficiency from BDT tagger

	500-600	600-800	800-1000	1000-1200	1200-1500	1500-2000
nominal	1.01	1.02	1.03	1.02	1.01	1.0
pdf weight	0.09	0.1	0.12	0.13	0.12	0.1
scale variation	0.09	0.1	0.12	0.12	0.13	0.1
hadronization	0.07	0.06	0.06	0.06	0.04	0.04
matrix element	0.05	0.06	0.06	0.05	0.05	0.04
tracking	0.05	0.05	0.05	0.04	0.04	0.04
MC nonclosure	0.01	0.01	0.02	0.01	0.01	0.01
parton shower	0.01	0.01	0.03	0.04	0.05	0.07
splitting kernel	0.01	0.01	0.01	0.01	0.02	0.01
gluon reweight	0.01	0.01	0.01	0.01	0.01	0.01
JES/JER	0.01	0.01	0.01	0.01	0.01	0.01
Statistical	0.01	0.01	0.01	0.01	0.01	0.02
Total Uncertainty	0.17	0.18	0.2	0.2	0.2	0.18

Table 5.11 The quark scale factor (nominal) and the difference between the nominal and systematic variation results for 60% quark tag efficiency from BDT tagger

	500-600	600-800	800-1000	1000-1200	1200-1500	1500-2000
nominal	1.02	1.03	1.04	1.03	1.02	1.01
pdf weight	0.09	0.1	0.11	0.12	0.12	0.1
scale variation	0.07	0.08	0.1	0.1	0.11	0.08
hadronization	0.06	0.05	0.05	0.05	0.03	0.04
tracking	0.05	0.05	0.05	0.04	0.04	0.04
matrix element	0.05	0.05	0.05	0.05	0.04	0.03
splitting kernel	0.01	0.01	0.01	0.01	0.02	0.01
gluon reweight	0.01	0.01	0.01	0.01	0.01	0.01
MC nonclosure	0.01	0.02	0.02	0.02	0.01	0.01
JES/JER	0.01	0.01	0.01	0.01	0.01	0.01
Statistical	0.01	0.01	0.01	0.01	0.01	0.01
parton shower	0.01	0.01	0.03	0.03	0.05	0.06
Total Uncertainty	0.15	0.16	0.18	0.18	0.18	0.15

The calibration of quark/gluon jets taggers

Table 5.12 The quark scale factor (nominal) and the difference between the nominal and systematic variation results for 70% quark tag efficiency from BDT tagger

	500-600	600-800	800-1000	1000-1200	1200-1500	1500-2000
nominal	1.03	1.04	1.04	1.03	1.02	1.02
pdf weight	0.08	0.09	0.1	0.11	0.1	0.08
scale variation	0.06	0.06	0.08	0.08	0.08	0.06
tracking	0.06	0.05	0.05	0.05	0.04	0.04
hadronization	0.05	0.04	0.04	0.04	0.03	0.03
matrix element	0.04	0.04	0.04	0.04	0.03	0.02
splitting kernel	0.01	0.01	0.01	0.02	0.01	0.01
parton shower	0.01	0.01	0.02	0.03	0.04	0.04
gluon reweight	0.01	0.01	0.01	0.01	0.01	0.01
JES/JER	0.01	0.01	0.01	0.01	0.01	0.01
MC nonclosure	0.01	0.02	0.03	0.02	0.01	0.01
Statistical	0.01	0.01	0.01	0.01	0.01	0.01
Total Uncertainty	0.13	0.13	0.15	0.15	0.15	0.12

Table 5.13 The quark scale factor (nominal) and the difference between the nominal and systematic variation results for 80% quark tag efficiency from BDT tagger

	500-600	600-800	800-1000	1000-1200	1200-1500	1500-2000
nominal	1.03	1.04	1.04	1.03	1.02	1.01
pdf weight	0.07	0.07	0.08	0.09	0.08	0.06
tracking	0.06	0.05	0.05	0.04	0.03	0.03
scale variation	0.04	0.05	0.06	0.06	0.05	0.05
hadronization	0.04	0.03	0.03	0.02	0.02	0.02
matrix element	0.03	0.04	0.03	0.03	0.02	0.02
splitting kernel	0.01	0.01	0.02	0.02	0.02	0.01
parton shower	0.01	0.01	0.02	0.02	0.02	0.03
gluon reweight	0.01	0.01	0.01	0.01	0.01	0.01
JES/JER	0.01	0.01	0.01	0.01	0.01	0.01
MC nonclosure	0.01	0.01	0.02	0.02	0.01	0.01
Statistical	0.01	0.01	0.01	0.01	0.01	0.01
Total Uncertainty	0.11	0.11	0.12	0.12	0.11	0.1

The calibration of quark/gluon jets taggers

Table 5.14 The gluon scale factor (nominal) and the difference between the nominal and systematic variation results for 50% gluon tag efficiency from N_{trk} tagger

	500-600	600-800	800-1000	1000-1200	1200-1500	1500-2000
nominal	0.99	0.98	0.98	0.96	0.94	0.92
parton shower	0.1	0.11	0.12	0.13	0.11	0.14
pdf weight	0.04	0.05	0.05	0.06	0.06	0.05
splitting kernel	0.02	0.01	0.01	0.01	0.01	0.01
tracking	0.01	0.02	0.02	0.02	0.02	0.01
hadronization	0.01	0.01	0.01	0.01	0.01	0.01
scale variation	0.01	0.01	0.01	0.01	0.01	0.01
MC nonclosure	0.01	0.01	0.02	0.04	0.06	0.07
matrix element	0.01	0.01	0.02	0.03	0.04	0.07
JES/JER	0.01	0.01	0.01	0.01	0.01	0.01
Statistical	0.01	0.01	0.01	0.01	0.01	0.02
gluon reweight	0.01	0.01	0.01	0.01	0.01	0.01
Total Uncertainty	0.11	0.12	0.13	0.15	0.15	0.18

Table 5.15 The gluon scale factor (nominal) and the difference between the nominal and systematic variation results for 60% gluon tag efficiency from N_{trk} tagger

	500-600	600-800	800-1000	1000-1200	1200-1500	1500-2000
nominal	0.99	0.98	0.97	0.95	0.92	0.91
parton shower	0.15	0.17	0.17	0.17	0.17	0.21
pdf weight	0.05	0.06	0.06	0.07	0.07	0.06
splitting kernel	0.03	0.01	0.01	0.01	0.01	0.02
scale variation	0.02	0.03	0.02	0.02	0.02	0.03
tracking	0.02	0.02	0.02	0.02	0.02	0.01
hadronization	0.01	0.01	0.01	0.01	0.01	0.01
MC nonclosure	0.01	0.02	0.02	0.04	0.07	0.08
matrix element	0.01	0.01	0.02	0.03	0.05	0.08
JES/JER	0.01	0.01	0.01	0.01	0.01	0.01
Statistical	0.01	0.01	0.01	0.01	0.01	0.03
gluon reweight	0.01	0.01	0.01	0.01	0.01	0.01
Total Uncertainty	0.17	0.18	0.18	0.2	0.2	0.25

The calibration of quark/gluon jets taggers

Table 5.16 The gluon scale factor (nominal) and the difference between the nominal and systematic variation results for 70% gluon tag efficiency from N_{trk} tagger

	500-600	600-800	800-1000	1000-1200	1200-1500	1500-2000
nominal	0.99	0.97	0.96	0.94	0.91	0.87
parton shower	0.21	0.22	0.23	0.24	0.25	0.31
pdf weight	0.06	0.06	0.07	0.08	0.08	0.07
splitting kernel	0.04	0.01	0.01	0.01	0.01	0.01
scale variation	0.04	0.04	0.03	0.04	0.03	0.04
tracking	0.02	0.02	0.02	0.02	0.01	0.01
hadronization	0.01	0.01	0.01	0.01	0.01	0.01
MC nonclosure	0.01	0.02	0.03	0.05	0.08	0.12
matrix element	0.01	0.01	0.02	0.03	0.06	0.09
JES/JER	0.01	0.01	0.01	0.01	0.01	0.01
gluon reweight	0.01	0.01	0.01	0.01	0.01	0.01
Statistical	0.01	0.01	0.01	0.01	0.01	0.03
Total Uncertainty	0.23	0.24	0.24	0.26	0.28	0.35

Table 5.17 The gluon scale factor (nominal) and the difference between the nominal and systematic variation results for 80% gluon tag efficiency from N_{trk} tagger

	500-600	600-800	800-1000	1000-1200	1200-1500	1500-2000
nominal	0.98	0.97	0.95	0.93	0.89	0.85
parton shower	0.32	0.31	0.33	0.37	0.37	0.45
scale variation	0.07	0.07	0.05	0.07	0.07	0.05
splitting kernel	0.07	0.02	0.02	0.03	0.01	0.02
pdf weight	0.06	0.07	0.07	0.09	0.09	0.08
tracking	0.01	0.01	0.01	0.01	0.01	0.01
MC nonclosure	0.01	0.03	0.04	0.06	0.1	0.15
matrix element	0.01	0.01	0.02	0.04	0.07	0.11
hadronization	0.01	0.01	0.01	0.01	0.01	0.01
JES/JER	0.01	0.01	0.01	0.01	0.01	0.01
gluon reweight	0.01	0.01	0.01	0.01	0.01	0.01
Statistical	0.01	0.01	0.01	0.01	0.01	0.03
Total Uncertainty	0.34	0.33	0.34	0.39	0.41	0.49

The calibration of quark/gluon jets taggers

Table 5.18 The gluon scale factor (nominal) and the difference between the nominal and systematic variation results for 50% gluon tag efficiency from BDT tagger

	500-600	600-800	800-1000	1000-1200	1200-1500	1500-2000
nominal	1.0	0.99	0.98	0.96	0.94	0.92
parton shower	0.09	0.08	0.1	0.1	0.1	0.13
pdf weight	0.04	0.04	0.05	0.05	0.06	0.04
splitting kernel	0.03	0.02	0.02	0.02	0.01	0.02
scale variation	0.01	0.01	0.01	0.01	0.01	0.03
MC nonclosure	0.01	0.02	0.03	0.05	0.06	0.09
hadronization	0.01	0.01	0.01	0.01	0.01	0.01
tracking	0.01	0.01	0.01	0.01	0.01	0.01
matrix element	0.01	0.01	0.02	0.02	0.04	0.07
gluon reweight	0.01	0.01	0.01	0.01	0.01	0.01
JES/JER	0.01	0.01	0.01	0.01	0.01	0.01
Statistical	0.01	0.01	0.01	0.01	0.01	0.02
Total Uncertainty	0.11	0.1	0.11	0.13	0.14	0.18

Table 5.19 The gluon scale factor (nominal) and the difference between the nominal and systematic variation results for 60% gluon tag efficiency from BDT tagger

	500-600	600-800	800-1000	1000-1200	1200-1500	1500-2000
nominal	0.99	0.98	0.97	0.95	0.93	0.91
parton shower	0.11	0.12	0.13	0.13	0.14	0.17
pdf weight	0.05	0.05	0.05	0.06	0.06	0.06
splitting kernel	0.05	0.03	0.03	0.03	0.01	0.04
MC nonclosure	0.02	0.03	0.04	0.06	0.08	0.1
scale variation	0.02	0.02	0.02	0.02	0.02	0.05
hadronization	0.01	0.01	0.01	0.01	0.02	0.01
tracking	0.01	0.01	0.01	0.01	0.01	0.01
matrix element	0.01	0.01	0.02	0.03	0.04	0.08
gluon reweight	0.01	0.01	0.01	0.01	0.01	0.01
JES/JER	0.01	0.01	0.01	0.01	0.01	0.01
Statistical	0.01	0.01	0.01	0.01	0.01	0.02
Total Uncertainty	0.13	0.14	0.15	0.16	0.18	0.23

The calibration of quark/gluon jets taggers

Table 5.20 The gluon scale factor (nominal) and the difference between the nominal and systematic variation results for 70% gluon tag efficiency from BDT tagger

	500-600	600-800	800-1000	1000-1200	1200-1500	1500-2000
nominal	0.98	0.97	0.95	0.93	0.89	0.86
parton shower	0.15	0.15	0.17	0.17	0.17	0.21
splitting kernel	0.07	0.05	0.05	0.04	0.03	0.05
pdf weight	0.05	0.06	0.06	0.07	0.07	0.06
MC nonclosure	0.05	0.05	0.07	0.09	0.12	0.15
scale variation	0.03	0.04	0.03	0.04	0.04	0.07
hadronization	0.02	0.01	0.01	0.01	0.01	0.01
tracking	0.01	0.01	0.01	0.01	0.01	0.01
matrix element	0.01	0.01	0.02	0.03	0.05	0.08
JES/JER	0.01	0.01	0.01	0.01	0.01	0.01
gluon reweight	0.01	0.01	0.01	0.01	0.01	0.01
Statistical	0.01	0.01	0.01	0.01	0.01	0.02
Total Uncertainty	0.18	0.18	0.2	0.21	0.23	0.29

Table 5.21 The gluon scale factor (nominal) and the difference between the nominal and systematic variation results for 80% gluon tag efficiency from BDT tagger

	500-600	600-800	800-1000	1000-1200	1200-1500	1500-2000
nominal	0.96	0.95	0.93	0.9	0.85	0.81
parton shower	0.19	0.18	0.21	0.2	0.22	0.28
splitting kernel	0.09	0.07	0.06	0.06	0.05	0.07
MC nonclosure	0.08	0.09	0.1	0.12	0.17	0.21
pdf weight	0.06	0.06	0.07	0.08	0.08	0.06
scale variation	0.05	0.05	0.05	0.05	0.07	0.08
hadronization	0.02	0.01	0.01	0.01	0.01	0.01
tracking	0.01	0.01	0.01	0.01	0.01	0.01
matrix element	0.01	0.01	0.02	0.03	0.06	0.09
JES/JER	0.01	0.01	0.01	0.01	0.01	0.01
Statistical	0.01	0.01	0.01	0.01	0.01	0.03
gluon reweight	0.01	0.01	0.01	0.01	0.01	0.02
Total Uncertainty	0.23	0.23	0.25	0.26	0.31	0.38

1238 Figure 5.46 to Figure 5.49 show the leading uncertainties with SFs for both tagger.
1239 The SFs for quark-jets and gluon-jets corresponding to the 50% quark-jets efficiency
1240 working point (WP) fall within the range of 0.92 to 1.02, while being subject to an ag-
1241 gregate systematic uncertainty of approximately 20%. Among the various sources of
1242 systematic uncertainty, theoretical modelling emerges as the dominant factor contribut-
1243 ing to the total uncertainty.

1244 To ascertain the robustness of the findings, tests are conducted to assess the stabili-
1245 ty of results across different regions of jet $|\eta|$. The SF measurements are recomputed
1246 through the normalization of jet $|\eta|$ in the quark-/gluon-enriched subsamples. The al-
1247 ternate results obtained in this manner are determined to be consistent with the nominal
1248 outcome, falling within the full range of reported uncertainties.

1249 Given the variations in the usage of different MC samples, a MC-to-MC SF is com-
1250 puted. This involves employing each alternative MC sample while treating the PYTHIA MC
1251 samples as pseudodata. This approach accommodates discrepancies arising from mod-
1252 elling difference between the PYTHIA and alternative MC samples. The MC-to-MC SFs
1253 for both jet taggers at each WP are shown in Figure 5.50 to Figure 5.53. Notably, there
1254 exists a large difference in gluon modelling between the HERWIG Dipole parton shower
1255 MC and the PYTHIA MC. This discrepancy is reflected in the relatively significant MC-
1256 to-MC SF, indicating substantial differences between these models.

The calibration of quark/gluon jets taggers

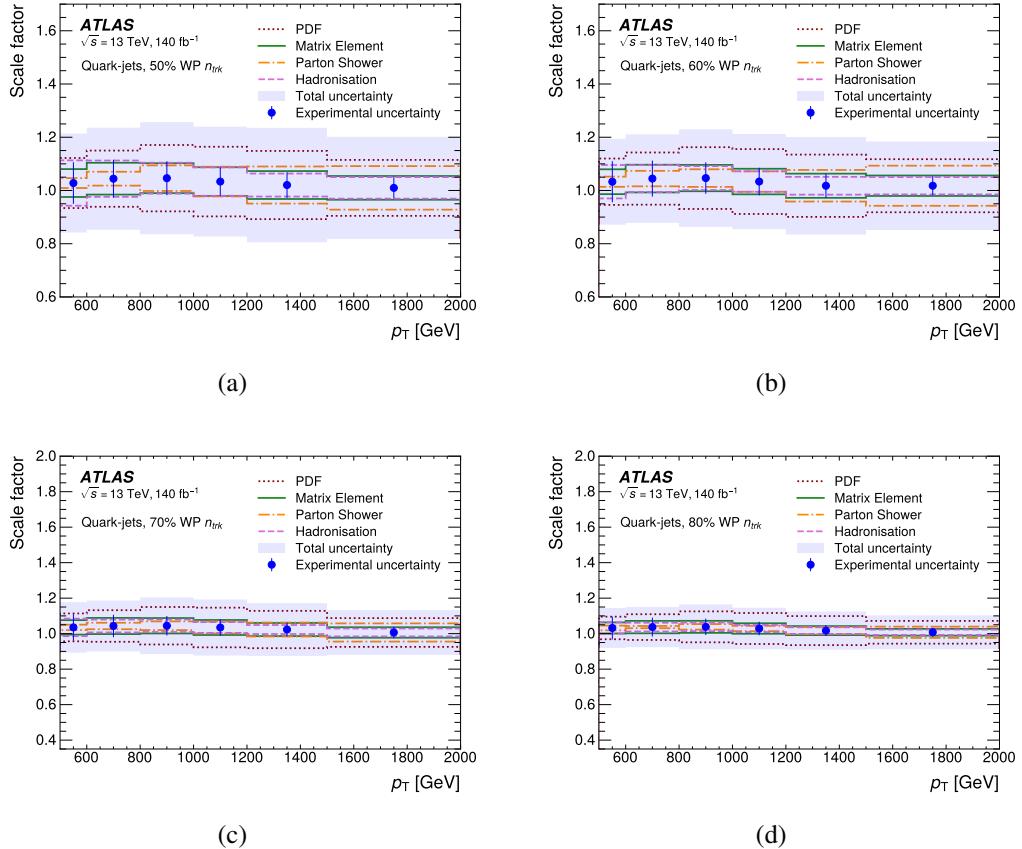


Figure 5.46 The SF with total and leading systematic uncertainty on the jet tagging variable N_{trk} obtained by PYTHIA 8 MCs as a function of jet p_T for quark-jets at each WP.

The calibration of quark/gluon jets taggers

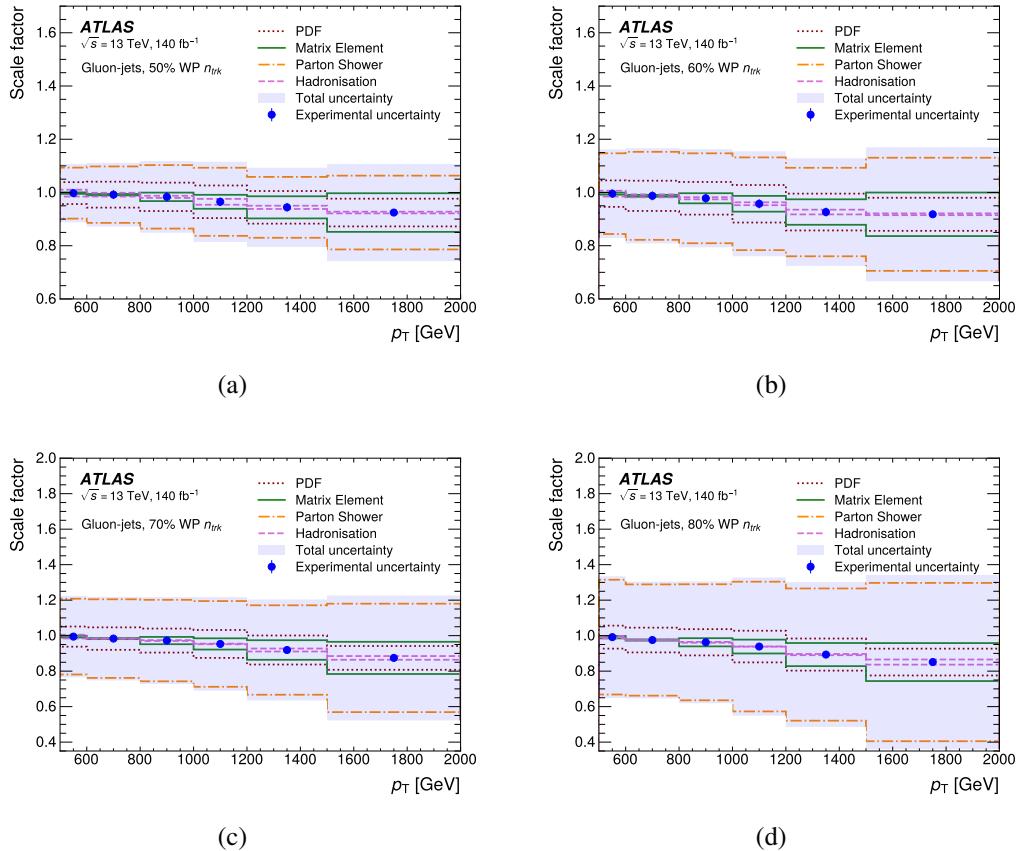


Figure 5.47 The SF with total and leading systematic uncertainty on the jet tagging variable N_{trk} obtained by PYTHIA 8 MCs as a function of jet p_{T} for gluon-jets at each WP.

The calibration of quark/gluon jets taggers

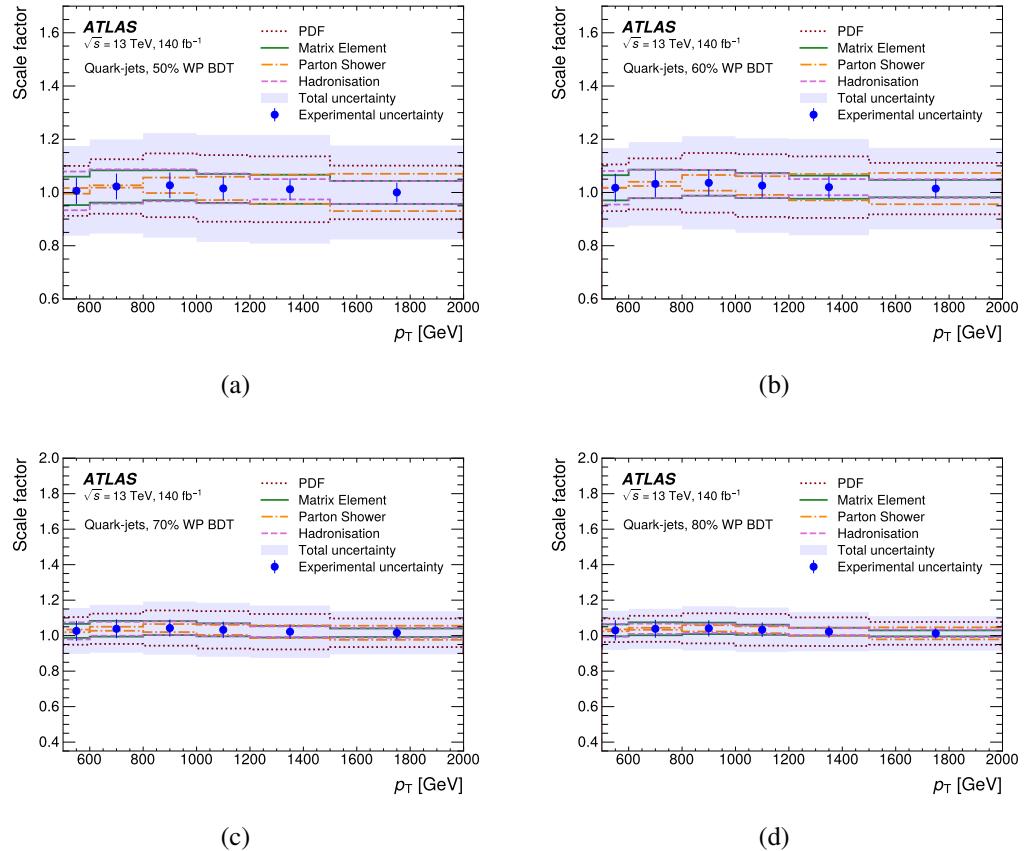


Figure 5.48 The SF with total and leading systematic uncertainty on the jet tagging variable BDT obtained by PYTHIA 8 MCs as a function of jet p_T for quark-jets at each WP.

The calibration of quark/gluon jets taggers

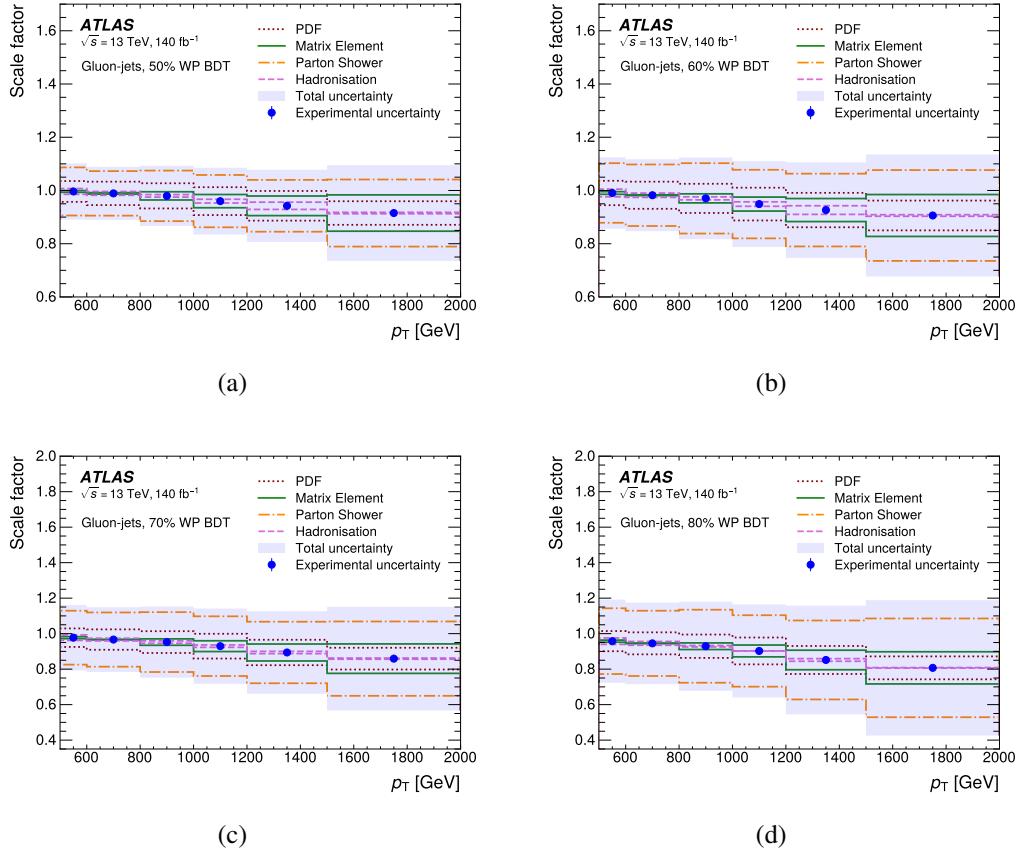


Figure 5.49 The SF with total and leading systematic uncertainty on the jet tagging variable BDT obtained by PYTHIA 8 MCs as a function of jet p_T for gluon-jets at each WP.

The calibration of quark/gluon jets taggers

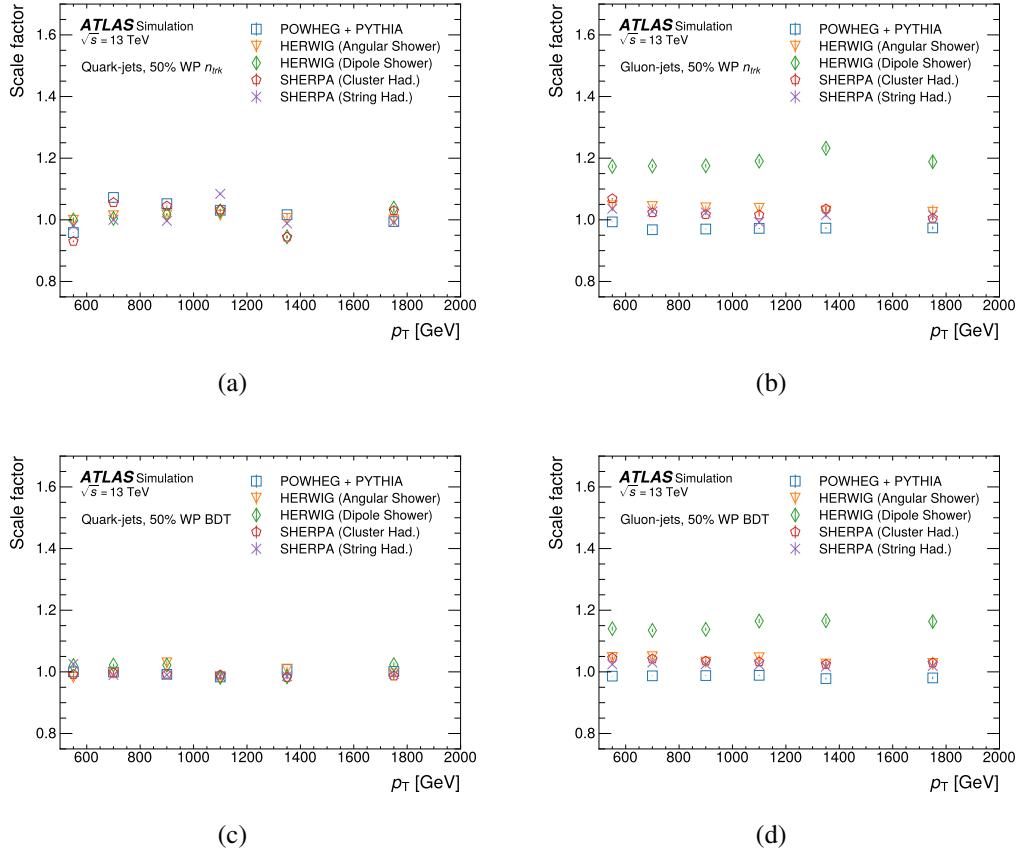


Figure 5.50 The MC-to-MC SF of the N_{trk} , (a) and (b), and BDT, (c) and (d), as a function of jet p_T for quark-jets (left) and gluon-jets (right) at the 50% WP. The vertical error bars show the statistical uncertainty.

The calibration of quark/gluon jets taggers

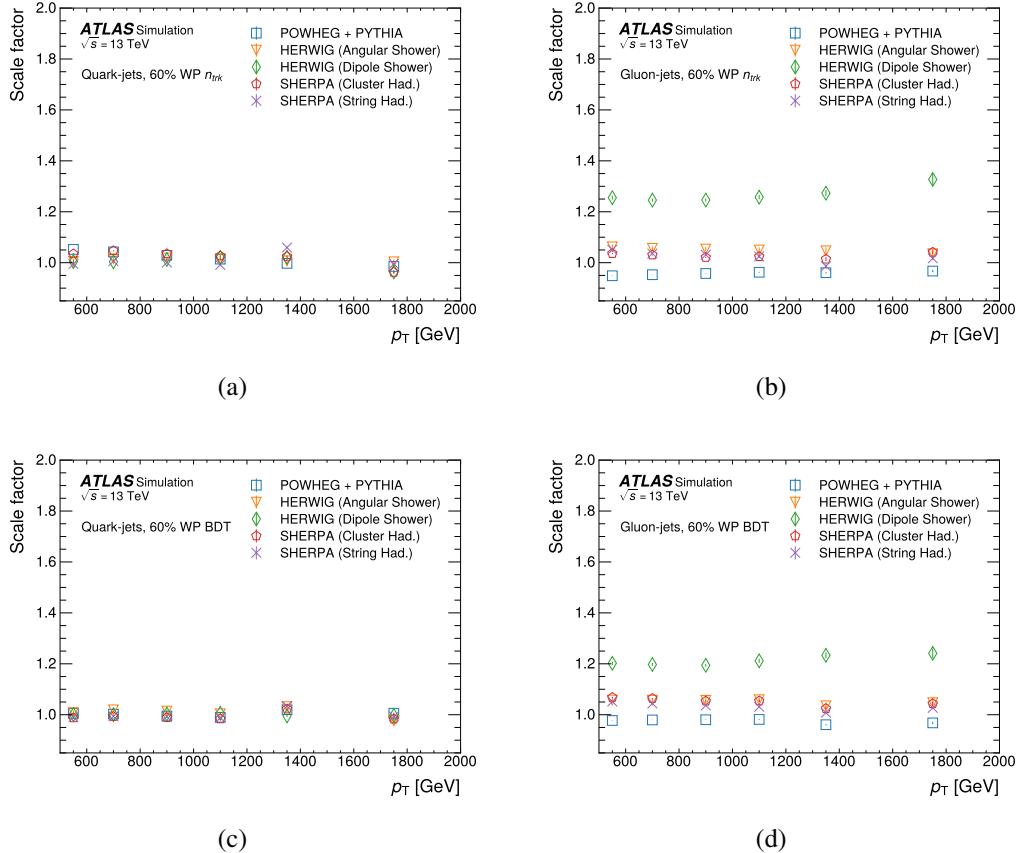


Figure 5.51 The MC-to-MC SF of the N_{trk} , (a) and (b), and BDT, (c) and (d), as a function of jet p_T for quark-jets (left) and gluon-jets (right) at the 60% WP. The vertical error bars show the statistical uncertainty.

The calibration of quark/gluon jets taggers

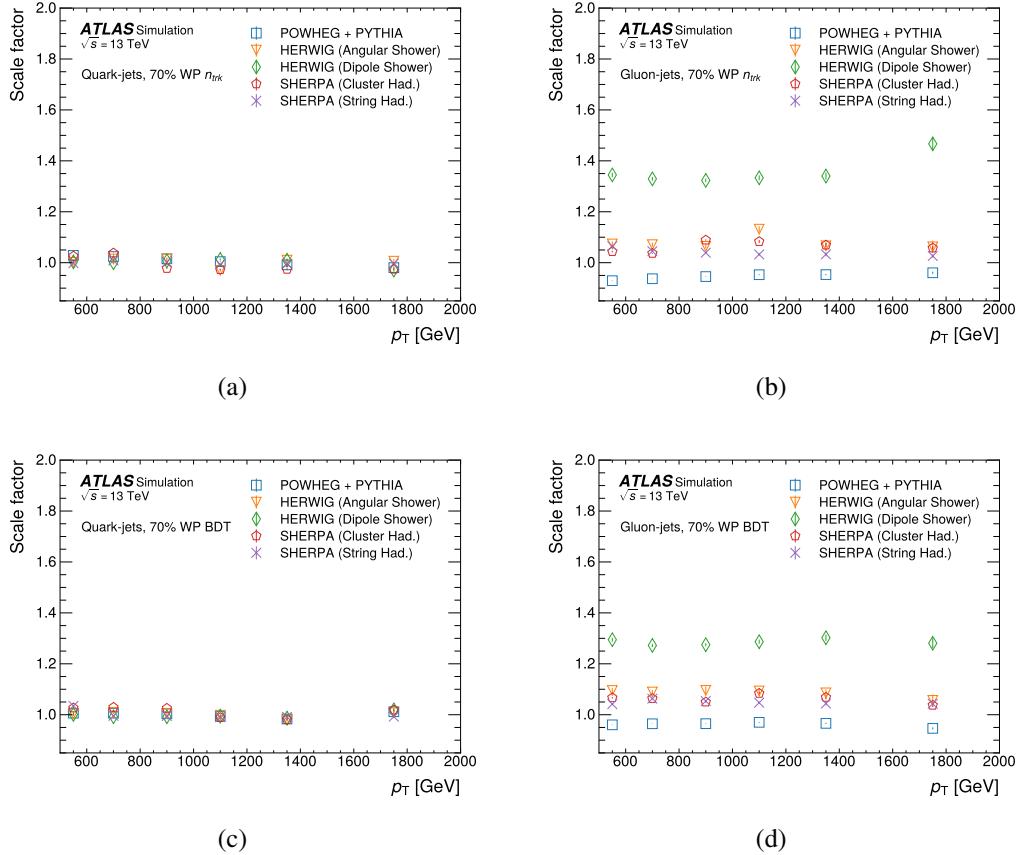


Figure 5.52 The MC-to-MC SF of the N_{trk} , (a) and (b), and BDT, (c) and (d), as a function of jet p_T for quark-jets (left) and gluon-jets (right) at the 70% WP. The vertical error bars show the statistical uncertainty.

The calibration of quark/gluon jets taggers

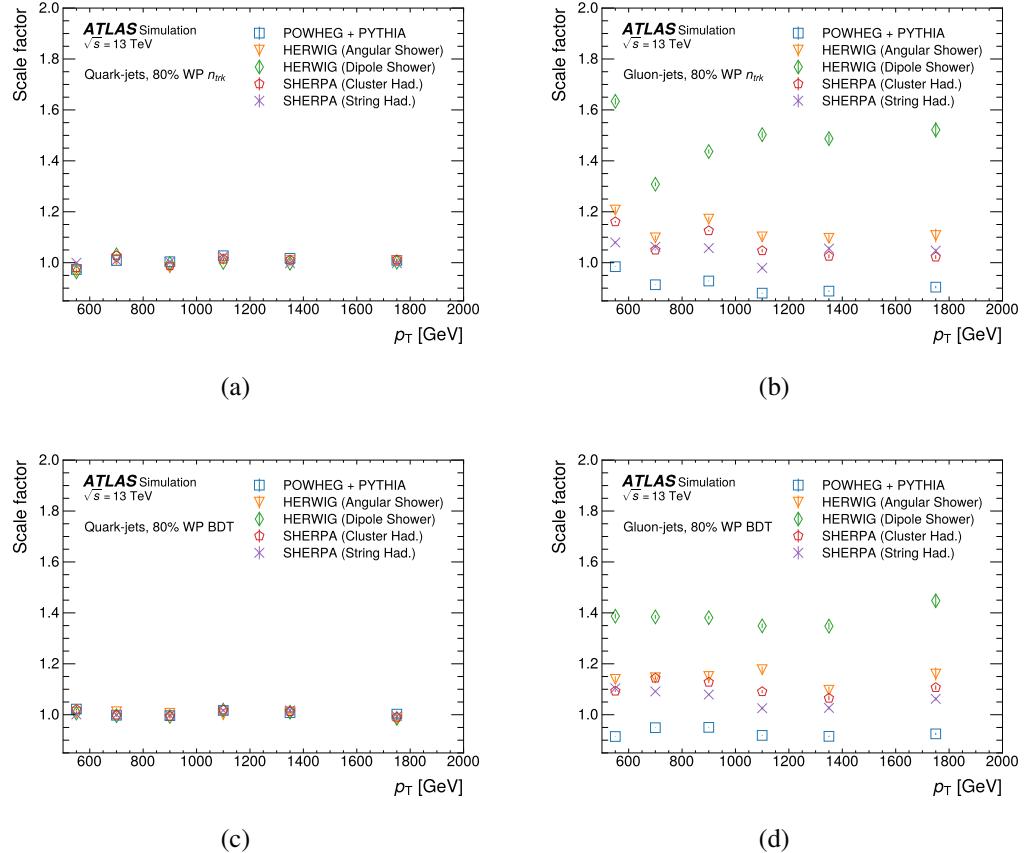


Figure 5.53 The MC-to-MC SF of the N_{trk} , (a) and (b), and BDT, (c) and (d), as a function of jet p_T for quark-jets (left) and gluon-jets (right) at the 80% WP. The vertical error bars show the statistical uncertainty.

1257

6 Search for new phenomena in dijet events

1258 As described in Section 2, the heavy resonance predicted by many BSM play a key role
1259 in understanding many fundamental phenomena. The narrow heavy resonance which
1260 decays into two gluons final state at the LHC, appears to be two hadronic jets in the
1261 detector. Produced by the QCD processes, the dijet events have a smoothly falling dis-
1262 tribution of the invariant mass m_{jj} , whereas two jets appear to be a resonance in the
1263 m_{jj} spectrum. As a result, searches for dijet resonance are one of the flagship exotics
1264 analyses in ATLAS.

1265 Besides, on the assumption that the resonant sample can be classified according to
1266 the type of parton that initiated the jets, the sensitivity of searches for new resonance
1267 can be improved by identifying the types of partons through which the potentially new
1268 particle interact. One of simplest examples of such tagging is gluon-tagging one or more
1269 of the jets. The jet tagging procedure based on the number of charged tracks with trans-
1270 verse momentum p_T above 500 GeV is described in Section. 5. The m_{jj} spectrum of
1271 background is estimated from the data, which is used for the search in three categories:
1272 inclusive, single-gluon, and double-gluon tagged dijet systems. The inclusive m_{jj} spec-
1273 trum is thus considered as control region for quark/gluon studies.

1274 This chapter describes searches for new heavy particles decay in dijet final state
1275 as originating from gluons or quarks, a technique of quark/gluon tagging is employed
1276 to enhance the sensitivity to the results. The search performed uses full Run 2 data
1277 at $\sqrt{s} = 13$ TeV, with higher integrated luminosity compared to previous one (Run 1),
1278 significantly improvements in the understanding of systematic uncertainties are expected.
1279 On the other hand, cross section upper limits will be set if no significantly resonances
1280 are observed.

1281

The simplified procedures in this analysis is performed as following:

1282

- Search for high-mass resonances in the untagged (inclusive), single-gluon tagged,
1283 and two-gluon tagged categories with dijet events.
- If significant resonances are found, claim something interesting, else the upper
1284 limits are set.
- Model independent upper-limits are set on resonance cross sections in inclusive,
1285 single-gluon tagged, and two-gluon tagged categories.

- 1288 • For the specific resonance model, set lower limits on the relevant scales in inclu-
1289 sive, single-gluon tagged, and two-gluon tagged categories. dijet systems.

1290 **6.1 Monte Carlo models**

1291 . This section outlines benchmark models for both background from the QCD and
1292 for new physics signals that encapsulated in the models chosen: Strings, graviton and
1293 QBH. Full Run 2 data are used to produce EXOT2 skimmed samples used in this analy-
1294 sis [77].

1295 **6.1.1 QCD background**

1296 QCD processes from the MC are simulated at LO and NLO in SM perturbative
1297 theory. Due to the large range in cross section of QCD sample [78], the samples are thus
1298 sliced based on the leading jet p_T , to obtain comparable statistical precision across the
1299 jet p_T range of interest.

1300 **6.1.2 Kaluza-Klein Graviton**

1301 For the RS KK graviton samples considered in this study, we focus on $k/\bar{M}_{Pl} = 0.2$.
1302 These samples encompass both gluon-gluon and quark-quark initial states, with decays
1303 exclusively to gluons or bottom quarks.

1304 The signal templates for the KK gravitons are generated with different mass val-
1305 ues using the PYTHIA 8 event generator. These simulations utilize the A14 tune and
1306 NNPDF2.3 PDF set.

1307 Figure 6.54 shows the Graviton to gg invariant mass distribution for the considered
1308 mass points.

1309 **6.1.3 Quantum Black Hole**

1310 In our study, we employ the QBH model for the purpose of comparing limits with
1311 the previous iteration of the analysis. The feasibility of producing QBHs at the LHC
1312 is contingent upon the presence of sufficiently large extra dimensions within the uni-
1313 verse [90]. This model posits that the energy scale of quantum gravity M_D , at which
1314 QBHs are generated, diminishes as the number of these large extra dimensions, denoted

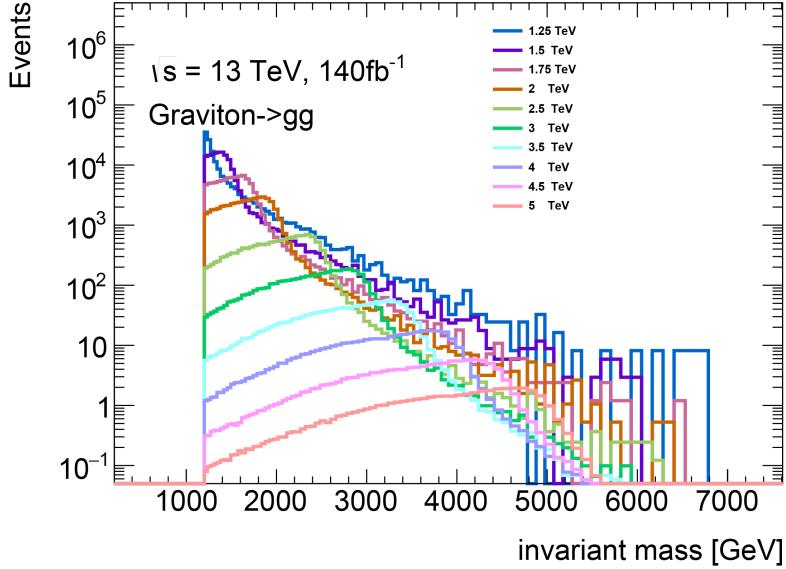


Figure 6.54 (a) Invariant mass distribution for the Graviton to gg samples

as n , increases. Consequently, a larger n permits lower mass scales at which QBHs can be formed.

Two-body isotropic final state is expected by the QBH decay at the LHC, where the M_D energy threshold could be reached [91]. Therefore the quantum gravitational effects can be probed by searches on m_{jj} spectrum. To simulate events involving quantum black holes with $n = 6$, we utilize the BlackMax [92] MC generator. This MC generator facilitates the simulation of QBH events within the $n = 6$ framework.

6.1.4 Gaussian resonances

A model-independent signal as Gaussian [93] are used to expand the sensitivity of the search to new signals that may be detectable with this analysis but not currently theoretically described. Besides, a model-independent signal could help to evaluate and compare the strength of different analyses without bias, as the case where specific models are applied and leads less sensitive to the search.

Therefore, model-independent fit function tests are produced based on model-independent signal resonances. Because this analysis is sensitive to the shape of resonance, specific models with different shapes would influence the results strongly. In general, a model-independent signal is a good feature of the analysis which verify the ability to distinguish different signal models, although the model-independent limits are still influenced by the

1333 shape of the resonance in an implicit way. The motivation to choose a Gaussian reso-
 1334 nance as a proxy is the fact that it is similar to the ‘average’ signal with specific width.
 1335 Besides, the shape of reconstructed jet p_T of any realistic signal without very specific
 1336 model is produced approximately as a Gaussian resonance, without applied JER. Hence
 1337 it is straightforward to use Gaussian resonances to represent any realistic resonance.

1338 The general form of Gaussian distribution is:

$$f(x) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2} \quad (6.1)$$

1339 where the parameter μ is the mean or expectation of the distribution (and also its median
 1340 and mode), while the parameter σ is its standard deviation.

1341 6.2 Events selections

1342 The MC and data events are divided into three categories to perform the search:
 1343 the untagged dijet invariant mass spectrum, one-gluon tagged spectrum, and two-gluon
 1344 tagged spectrum. The evidence of BSM resonances would appear as peaks in the m_{jj}
 1345 spectrum formed by two highest p_T jets in the events. A series of specific cuts is applied
 1346 to improved the sensitivity of the searches.

1347 6.2.1 Observables and Kinematic Variables

1348 The predominant source of dijet events in the SM is two-to-two scattering though
 1349 the QCD processes. This search exams two key properties of the QCD background:

- 1350 • The background at high m_{jj} appears as a smooth and continuously falling spec-
 1351 trum.
- 1352 • The background at high energy strongly peaks in the forward region as a result
 1353 of Rutherford t - and u -channel poles in the cross sections for certain scattering
 1354 processes [94].

1355 Resonances of interest have $\cos \theta$ distributions in the detector, which in contrast to
 1356 Rutherford scattering, are either isotropic or have polynomial behaviour in $\cos \theta$ ¹, thus
 1357 a angular distribution appears. This search therefore defines a y^* to indicate the angle
 1358 separation of the jets in the selected events:

$$y^* = (y_1 - y_2)/2 \quad (6.2)$$

1359 to improve the sensitivity to higher energies where new phenomena are expected. The
 1360 variables y_1, y_2 represent the rapidity of the leading and subleading jet. The value of the
 1361 y^* cut on events is optimized for each signal as discussed in Section .6.4.1.

1362 In this analysis, jets are reconstructed with the anti- k_t algorithm with a radius pa-
 1363 rameter $R = 0.4$, as implemented in the FASTJET package [95]. The EMTopo jets, re-
 1364 constructed from topological clusters via procedures described in Section .4.1, are used.
 1365 The standard *Loose* cut is applied to jet quality as well as jet cleaning. The summarized
 1366 jet criteria are shown in Table 6.22.

¹See Ref. [94] p15 for a summary.

Parameter / Observable	Requirement
Algorithm	anti- k_t
R-parameter	0.4
Input Constituent	EMTopo
p_T	>150 GeV
$ \eta $	<2.1

Table 6.22 Jet selection criteria used in this analysis.

6.2.2 Baseline selection

The triggers used in this analysis is HLT_j420. Besides, two single-jet trigger HLT_j225_gsc420_boffperf_split is also used as the unprescaled trigger for full Run 2 data. Both triggers have the threshold of $p_T > 420$ GeV of the jets, while the GSC is applied to the HLT_j225_gsc420_boffperf_split to the trigger turn-on improvement. A turn-on based on the m_{jj} spectrum is found to be much powerful than the cut requirement of the leading jet p_T , where the m_{jj} cut imposes a soft cut on the leading and subleading jet, respectively [96]. More details are shown in Section ??.

The baseline event selection is applied for all categories. The GRL and various flags that indicate the status of detector when taking data are provided by the ATLAS Data Quality (DQ) group, are applied to ensure the data integrity. Primary vertex requirement is also included to ensure good quality jets. The

- All jets with $p_T > 150$ GeV pass *Loose* cleaning cuts
- Passes the lowest unprescaled single-jet trigger: HLT_j420
- Jet multiplicity ≥ 2
- Leading jet $p_T > 380$ GeV and subbeading jet $p_T > 150$ GeV
- Leading jet $|\eta| < 2.1$ and subbeading jet $|\eta| < 2.1$
- $|\Delta\phi|$ between two jets: $|\Delta\phi| > 1.0$
- $m_{jj} > 1100$ GeV

Additional kinematic criteria are applied according to the distributions of signals, in order to optimize the search potential, are then discussed in Section 6.4.1.

6.3 Quark-Gluon Sample Selection

1389 . The sensitivity of the search on the resonant is expected to increase by distin-
 1390 guishing the type of parton that initiated the jets. The parton types of dijet events as a
 1391 function of m_{jj} from the MC with a PYTHIA8.186 at LO NNPDF2.3 PDFs is shown in
 1392 Figure 6.55, suggesting that the search for new resonance can be improved by tagging
 1393 quark and gluon jets.

1394 In this section we present the search for new particles using the full Run 2 $\sqrt{s} =$
 1395 13 TeV dataset with quark and gluon tagging method.

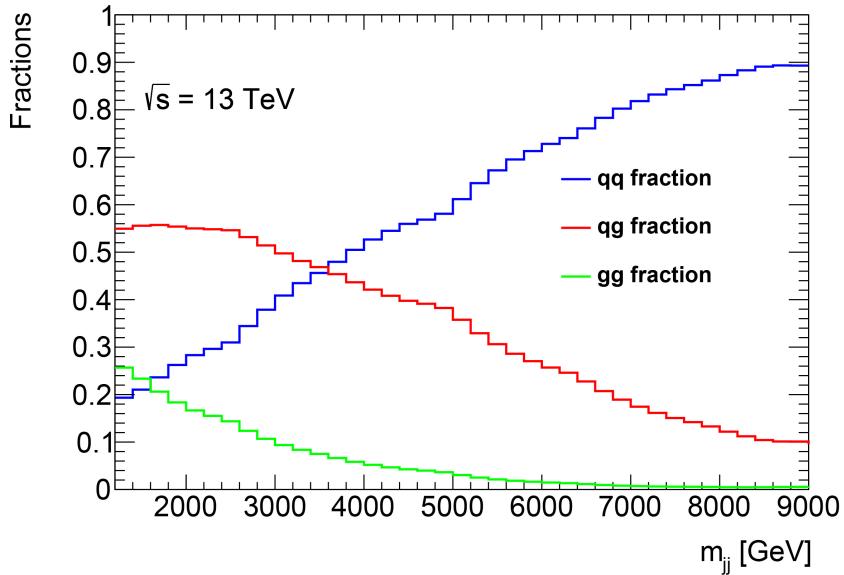


Figure 6.55 The fraction of dijet events that are initiated by quark-quark events (blue), quark-gluon events (green) and gluon-gluon events (red) in simulated data.

1396 Previous study in ATLAS has shown that the jets can be tagged quark or gluon
 1397 jets based on the number of charged tracks associated with the jets with p_T above 500
 1398 MeV. Samples with enhanced fractions of quark or gluon initiated jets can be created by
 1399 using a selection based on the charged-particle constituent multiplicity N_{trk} . As shown in
 1400 Figure 6.56, where PYTHIA 8 generator is used for MC to ensure a good agreement with
 1401 the distribution of N_{trk} in data within the ID acceptance $|\eta| < 2.1$.

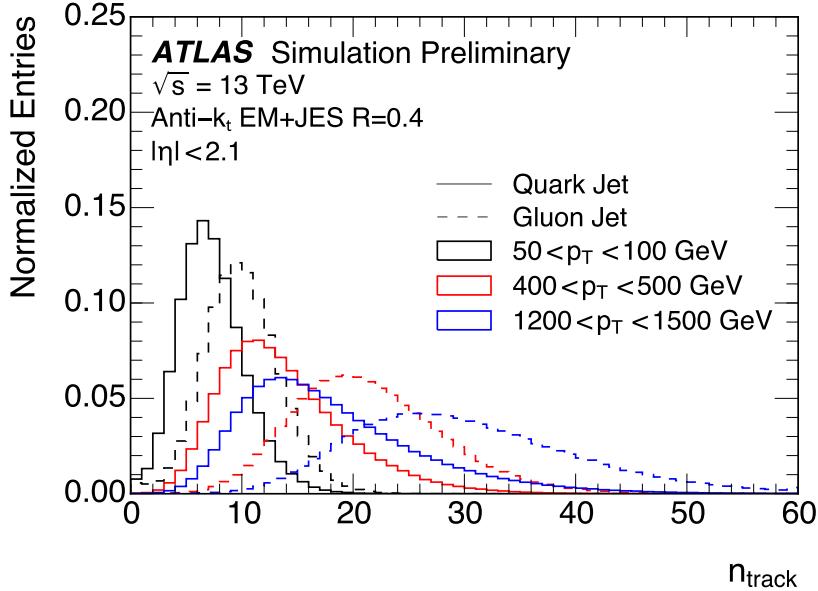


Figure 6.56 Distribution of the jet reconstructed track multiplicity (N_{trk}) in different p_{T} ranges with the PYTHIA 8 MC samples and processes with a full simulation of the ATLAS detector. Tracks are required to have $p_{\text{T}} > 500$ MeV and pass quality criteria described in Ref. [47].

1402 6.3.1 Selection Criteria

1403 The selection criteria for an quark-enriched jet sample was chosen so that 60%
 1404 quark-initiated purity is achieved in each jet p_{T} bin. However, discontinuities in the m_{jj}
 1405 spectrum would occur when such criteria is applied to the high mass ($p_{\text{T}} > 5000$ GeV),
 1406 leads to difficulties presented in resonance search.

A selection criteria is thus built as a linear function of the $\ln(p_{\text{T}})$, results in a smooth m_{jj} distribution. A jet is tagged as being more likely to be quark-initiated if N_{trk} is less than the threshold n_q and more likely to be gluon-initiated if N_{trk} is greater than the threshold n_g :

$$N_{\text{trk}} \leq n_q \text{ quark-initiated sample} \quad (6.3)$$

$$N_{\text{trk}} \geq n_g \text{ gluon-initiated sample}$$

1407 where

$$n_{q(g)} = c_{q(g)} + m_{q(g)} \ln(p_{\text{T}}) \quad (6.4)$$

1408 parameters $m_{q(g)}$ and $c_{q(g)}$ are constants obtained from the MC samples, these are founded
 1409 by finding the value of N_{trk} that corresponds to a given efficiency for truth quark and gluon

1410 jets in p_T bins, and chosen to defined suitable subsamples, the p_T here is in units of GeV.

1411 For each p_T bin, the number of tracks N_{trk} that closest to the given selection effi-
 1412 ciency is found. Because the N_{trk} is an integer number of track thus does not correspond
 1413 exactly to the selection efficiency, a linear interpolation is carried out between the given
 1414 efficiencies of the selected bin and the closest bin of it, to correct the fractional number
 1415 of tracks that corresponds to the selection efficiency, the corresponding uncertainty is
 1416 evaluated as binomial distribution.

1417 The jet p_T bin edges are divided into 480, 500, 520, 540, 560, 580, 600, 625, 650,
 1418 700, 750, 800, 900, 1000, 1400, 1600, 1800, 2000, 2500, 3000, 3500, 4000, 5000, 6000
 1419 GeV. An example of the cumulative distribution of N_{trk} for truth quark- and gluon-jets at
 1420 the p_T range of 800 - 900 GeV is shown in Figure 6.57.

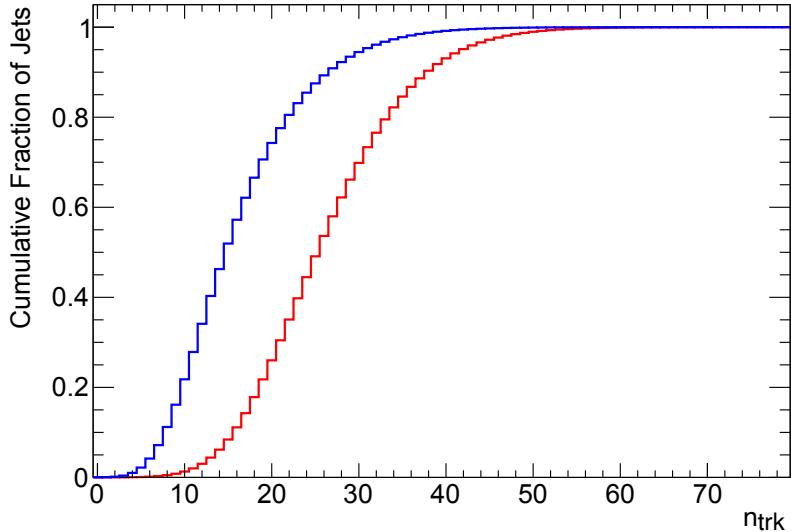


Figure 6.57 The cumulative distribution of N_{trk} for truth quark- (blue) and gluon- (red) jets satisfying $800 < p_T < 900$ GeV.

1421 The coefficients for Equation 6.4 are determined for quark and gluon selection ef-
 1422 ficiencies ranging from 65% to 95% in increments of 5%. The plot showcasing the N_{trk}
 1423 values corresponding to selection efficiencies of 70%, 75%, and 80% is depicted in Fig-
 1424 ure 6.58, along with the optimal fit employing Equation 6.4. The constants' values for
 1425 both quark and gluon selections are summarized in Tables 6.23 and 6.24. For a selec-
 1426 tion efficiency of 75%, the fitting yields a χ^2 of 33.5 (quark selection) and 2.6 (gluon
 1427 selection) for 21 degrees of freedom.

1428 Notably, the N_{trk} value that satisfies the selection efficiency attains a plateau above

1429 4000 GeV, suggesting the potential presence of a saturation effect. To validate these
 1430 findings, the data is subjected to an alternative fit function. An alternative fit function is
 1431 derived as a cross check:

$$n_{q(g)} = c + m \ln(p_T) + n \sqrt{\ln(p_T)}. \quad (6.5)$$

1432 which improve the χ^2 of the fit in a selection efficiency of 75% from 33.5 to 25.1 in
 1433 quark-selection, and from 2.6 to 1.6 in gluon-selection. Figure 6.59 shows the alternative
 1434 fit for quark and gluon selections. The values of the constants for both quark and gluon
 1435 selections are summarised in Tables 6.25 and 6.26.

1436 The values of the constants for both quark and gluon selections are summarised in
 Tables 6.23 and 6.24.

Truth- <i>q</i> selection efficiency	Truth- <i>g</i> selection efficiency	<i>c</i>	<i>m</i>
0.95	0.732	-27.568	8.789
0.90	0.563	-21.518	7.269
0.85	0.447	-17.646	6.304
0.80	0.350	-14.956	5.610
0.75	0.278	-12.600	5.022
0.70	0.221	-10.691	4.536
0.65	0.174	-8.990	4.105

Table 6.23 Values of constants m and c from Equation. 6.4 such that $N_{\text{trk}} \leq n_q$ for truth quark jets for a range of efficiencies from 65 to 95%.

1437

Truth- <i>g</i> selection efficiency	Truth- <i>q</i> selection efficiency	<i>c</i>	<i>m</i>
0.95	0.586	-7.541	3.233
0.90	0.456	-8.980	3.779
0.85	0.377	-10.419	4.230
0.80	0.320	-11.964	4.659
0.75	0.274	-13.376	5.047
0.70	0.234	-14.937	5.446
0.65	0.202	-16.466	5.834

Table 6.24 Values of constants m and c from Equation 6.4 such that $N_{\text{trk}} \geq n_g$ for truth quark jets for a range of efficiencies from 65 to 95%.

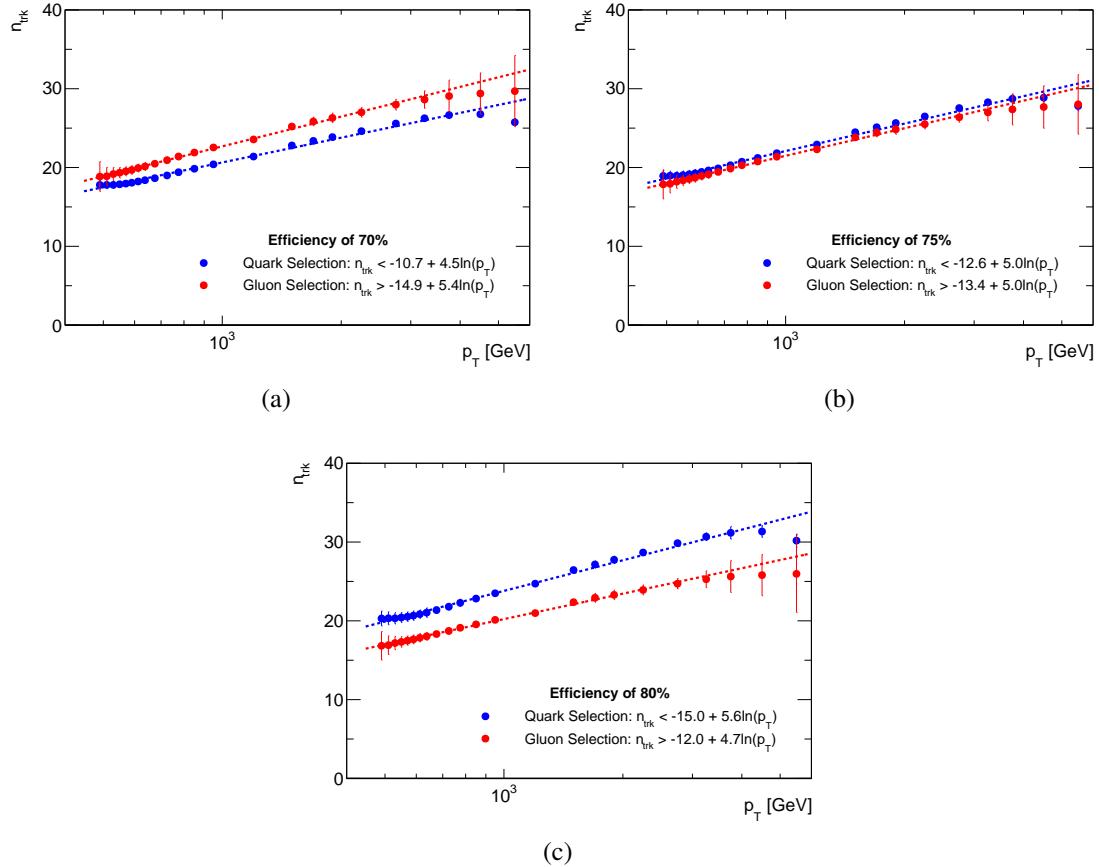


Figure 6.58 The values of N_{trk} for (a) 70%, (b) 75% and (c) 80% quark (blue) and gluon (red) selection efficiencies in each p_T bin along with the best fit to Equation 6.4.

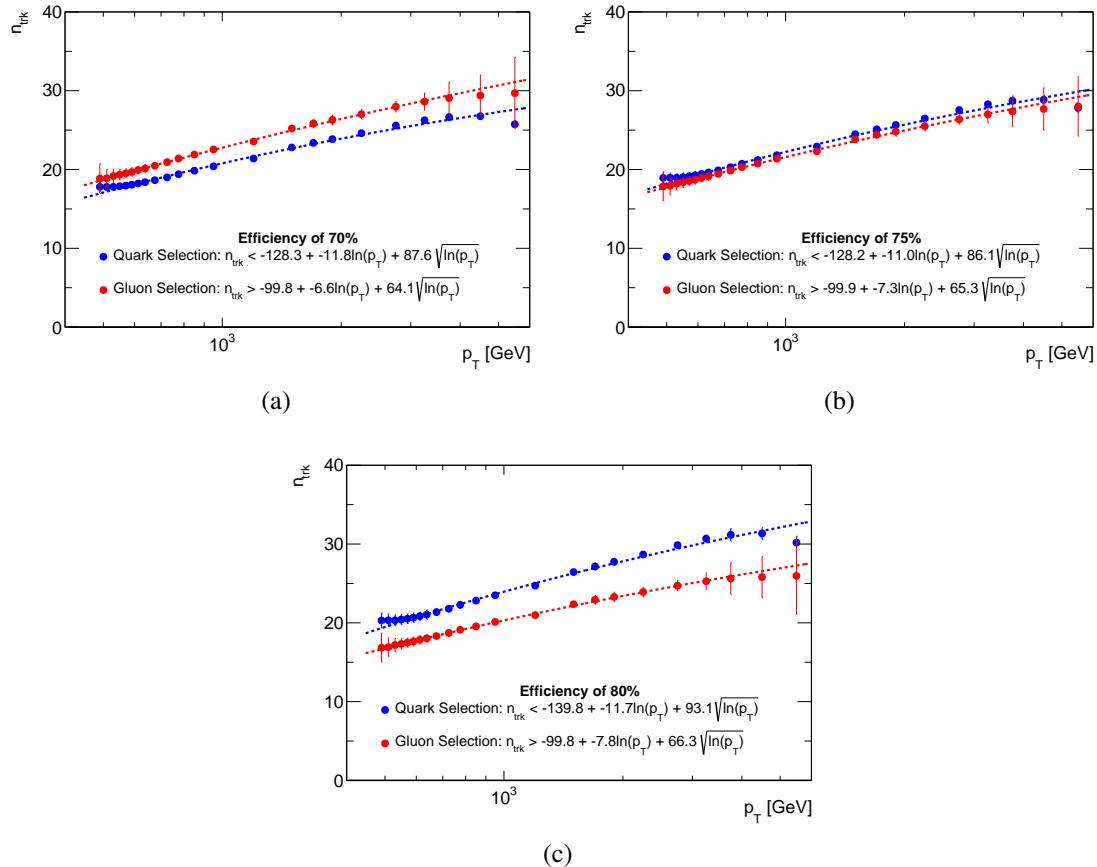


Figure 6.59 The values of N_{trk} for (a) 70%, (b) 75% and (c) 80% quark (blue) and gluon (red) selection efficiencies in each p_T bin along with the best fit to Equation 6.5.

Truth- q selection efficiency	Truth- g selection efficiency	c	m	n
0.80	0.350	-139.822	-11.714	93.100
0.75	0.278	-128.174	-11.001	86.141
0.70	0.221	-128.255	-11.755	87.604

Table 6.25 Values of constants m and c from Equation 6.5 such that $N_{\text{trk}} \leq n_q$ for truth quark jets for a range of efficiencies from 70 to 80%.

Truth- g selection efficiency	Truth- q selection efficiency	c	m	n
0.80	0.320	-99.796	-7.839	66.301
0.75	0.274	-99.949	-7.271	65.347
0.70	0.234	-99.774	-6.640	64.077

Table 6.26 Values of constants m and c from Equation 6.5 such that $N_{\text{trk}} \geq n_g$ for truth quark jets for a range of efficiencies from 70 to 80%.

1438 6.4 Signal Optimisation

1439 6.4.1 y^* Cut Optimisation

1440 In QCD, t -channel in 2-to-2 scattering is the dominant process. Thus the dijet pro-
 1441 duction from the QCD is proportional to $(1 - \cos \theta^*)^{-2}$. However the distribution of
 1442 $\cos \theta^*$ is supposed to be flat for H' signal, which means the y^* of H' signal will peak at 0
 1443 while that of QCD background will minimize at 0.

1444 The significance is defined as:

$$1445 S = \sqrt{\sum_i 2 \left[(S_i + B_i) \cdot \ln \left(1 + \frac{S_i}{B_i} \right) - S_i \right]} \quad (6.6)$$

1446 where S_i (B_i) is the number of signal (background) events in bin i . The calculation of
 1447 such significance only include the bins where signal samples have 95% of the area under
 1448 the distribution, not include the entire m_{jj} distribution.

1449 For some signal samples where S_i is small ($S_i \ll 10^{-5}$) thus the logarithm functions
 1450 do not have enough precision in equation 6.6. An approximation is introduced as follows:

$$1450 S = \sqrt{\sum_i 2 \sum_{n=1}^6 \frac{(-S_i)^{n+1}}{n(n+1)B_i^n}} \quad (6.7)$$

1451 which is accurate up to 10 decimal places around $\frac{S_i}{B_i} = 10^{-5}$ and even more precise for
 1452 smaller $\frac{S_i}{B_i}$.

1453 Figure. 6.60 shows the significance of Graviton signal as a function of y^* cut. The
 1454 significance peaks at about 0.6, so the optimal cut for the Graviton search is $|y^*| < 0.6$.
 1455 Table. 6.27 shows the y^* cut corresponding to the peak significance value for Graviton at
 1456 each mass point, and the range in y^* cut around the peak that gives a significance ≥ 0.99

1457 Figure. 6.61 shows the significance of QBH signal as a function of y^* cut. The
 1458 maximum significance is at about 0.9, so the optimal cut for the QBH search is $|y^*| < 0.9$.
 1459 Table. 6.28 shows the y^* cut corresponding to the peak significance value for the QBH at
 1460 each mass point, and the range in y^* cut around the peak that gives a significance ≥ 0.99

1461 However, further study have provided that using multiple signal regions was an over
 1462 optimisation, so in the analysis, $|y^*| < 0.8$ is used.

Search for new phenomena in dijet events

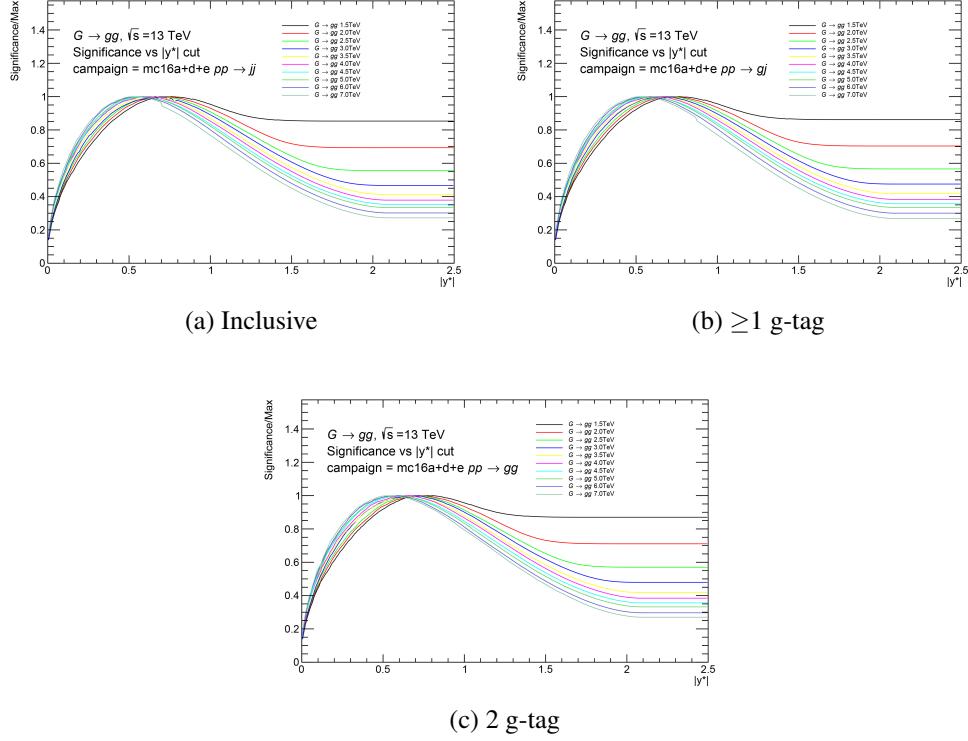


Figure 6.60 Graviton significance as a function y^* cut in the case of (a) Inclusive, (b) ≥ 1 g-tag, (c) 2 g-tag.

Graviton Mass (TeV)	Optimal Selection			Peak Width
	Inclusive	≥ 1 g tag	2 g tag	
1.5	0.77	0.77	0.78	0.65–0.87
2.0	0.71	0.74	0.72	0.65–0.83
2.5	0.67	0.69	0.70	0.61–0.80
3.0	0.66	0.66	0.66	0.60–0.77
3.5	0.64	0.65	0.65	0.57–0.73
4.0	0.63	0.64	0.64	0.55–0.73
4.5	0.59	0.59	0.59	0.53–0.69
5.0	0.59	0.59	0.59	0.50–0.69
6.0	0.57	0.57	0.60	0.49–0.66
7.0	0.53	0.53	0.56	0.47–0.63

Table 6.27 $|y^*|$ selection leading to the maximum significance value calculated using Equation 6.6.

Search for new phenomena in dijet events

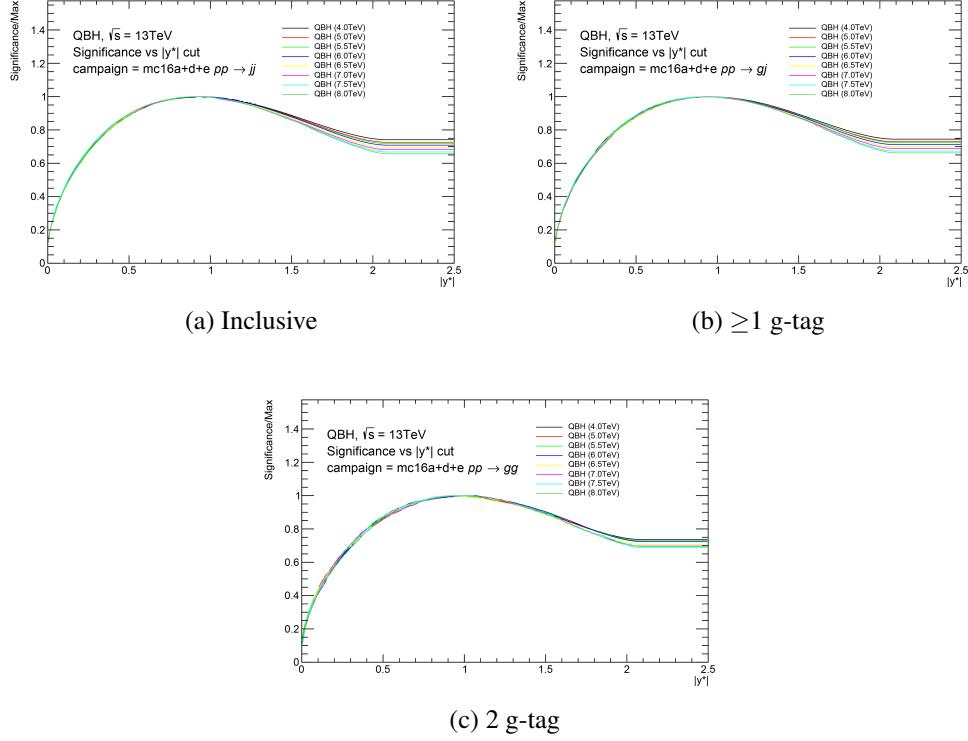


Figure 6.61 QBH significance as a function y^* cut in the case of (a) Inclusive, (b) ≥ 1 g-tag, (c) 2 g-tag.

QBH Mass (TeV)	Optimal Selection			Peak Width
	Inclusive	≥ 1 g tag	2 g tag	
4.0	0.92	0.95	1.01	0.81–1.11
5.0	0.95	0.95	0.95	0.81–1.09
5.5	0.94	0.96	0.94	0.81–1.09
6.0	0.92	0.96	1.01	0.81–1.09
6.5	0.91	0.91	0.93	0.81–1.06
7.0	0.93	0.97	0.94	0.82–1.07
7.5	0.92	0.94	0.93	0.79–1.08
8.0	0.92	0.96	0.99	0.82–1.09

Table 6.28 $|y^*|$ selection leading to the maximum significance value calculated using Equation 6.6.

1463 **6.4.2 Optimised Selection**

1464 In addition to the baseline selection described in Section 6.2.2, optimized cuts are
1465 applied to different tagging regions to improve the search potential with good tracking
1466 efficiency.

1467 The following additional cuts are applied for the the inclusive samples.

- 1468 • $|y^*| < 0.8$
- 1469 • $m_{jj} > 1200 \text{ GeV}$

1470 The following additional cuts are for quark-gluon tagging.

- 1471 • $|\eta| < 2.1$ (both jets) for track acceptance
- 1472 • ≥ 1 gluon tagged (75% working point)
- 1473 • 2 gluons tagged (75% working point)

1474 where the 75% gluon selection criteria is applied as: $N_{\text{trk}} > -7.3 + 4.2 \ln(p_T)$, with jet
1475 p_T in GeV.

1476 **6.4.3 Selected Kinematic Plots**

1477 In this section a selection of kinematic and monitoring plots processed with sam-
1478 ples passed the gluon-gluon selection criteria are shown in Figure 6.62, 6.63, 6.64. The
1479 distributions of kinematics in MC are consistent with full dataset.

Search for new phenomena in dijet events

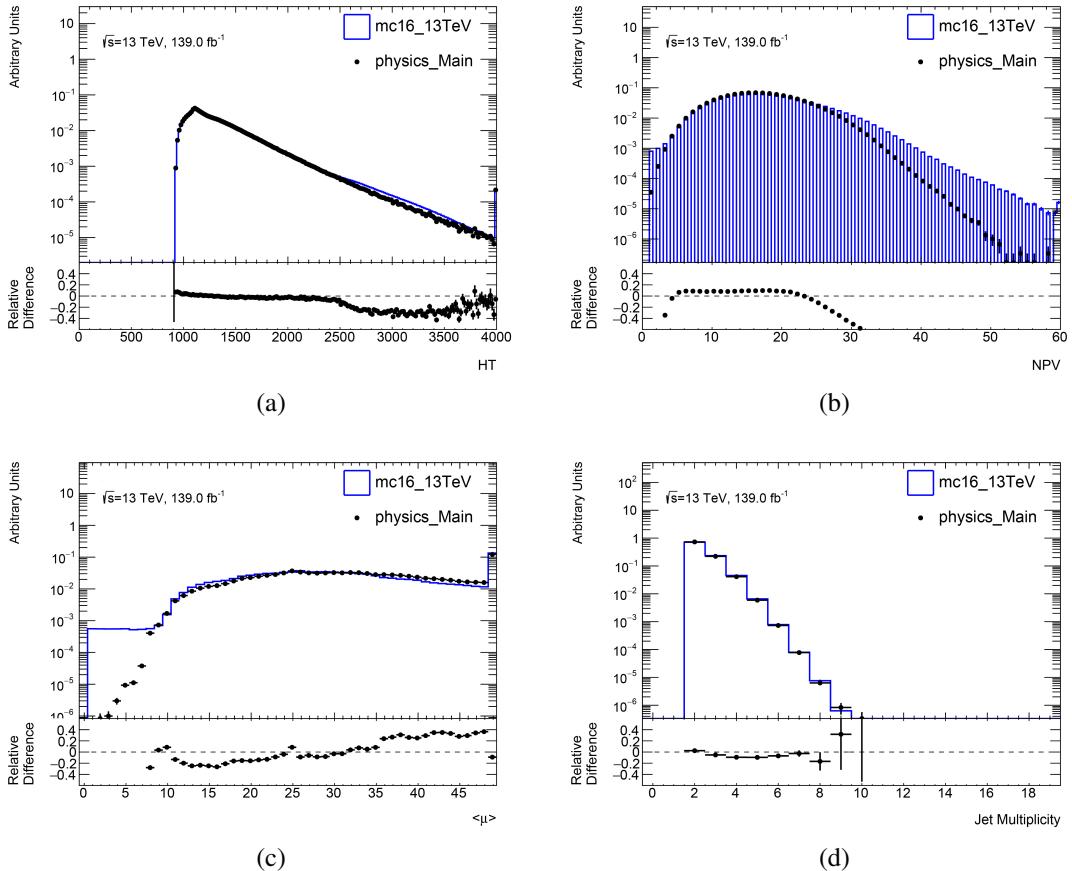


Figure 6.62 Monitoring plots for the gluon-gluon selection. (a) scalar p_T sum of all parton-level jets (H_T), (b) number of primary interaction vertices (NPV), (c) average interactions per bunch crossing, and (d) number of jets.

Search for new phenomena in dijet events

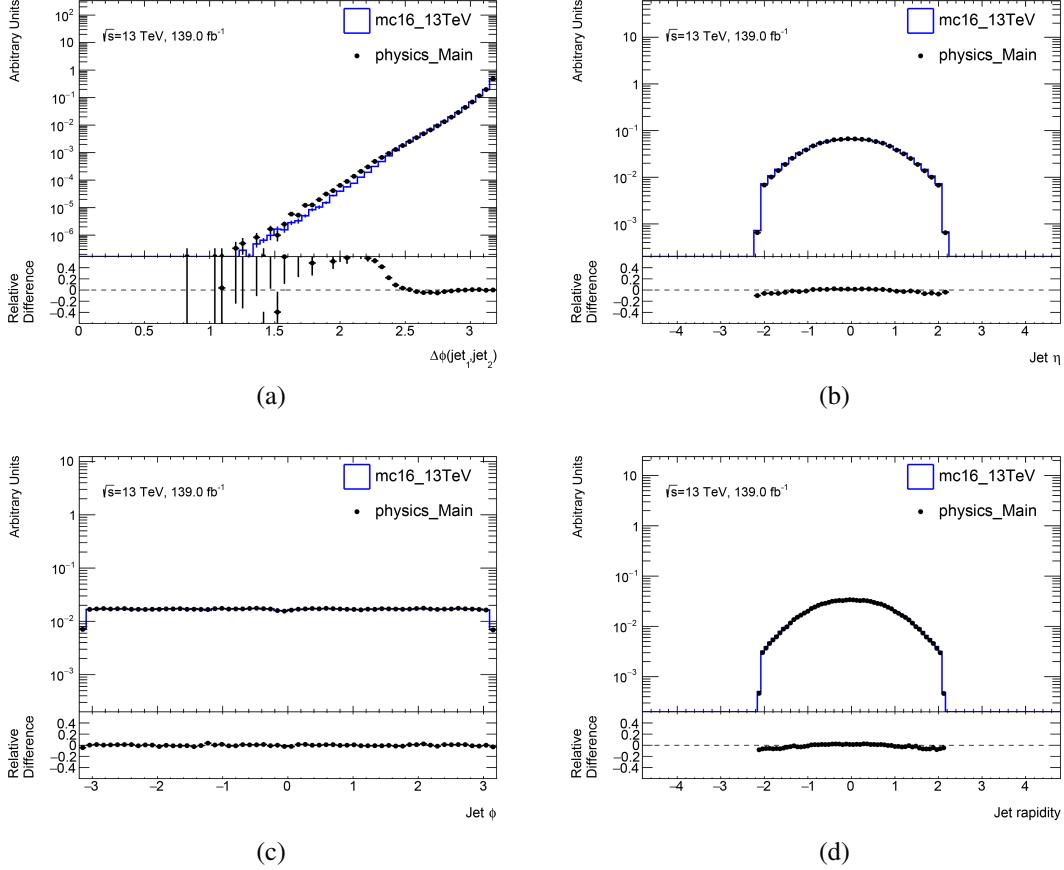


Figure 6.63 Monitoring plots on the gluon-gluon sample. (a) $\Delta\phi$ between the two jets, (b) jet η , (c) jet ϕ , and (d) jet rapidity.

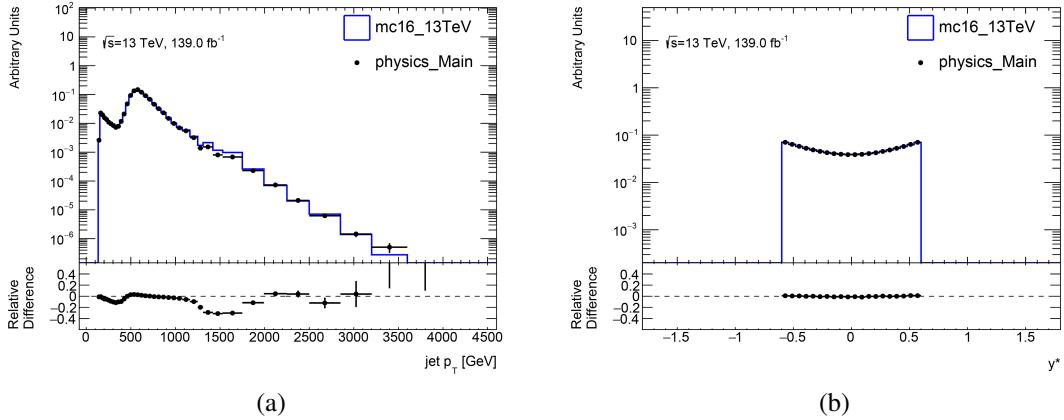


Figure 6.64 Monitoring plots on the gluon-gluon sample. (a) jet p_T , (b) y^* .

1480 6.5 Statistical Framework

1481 6.5.1 Fitting Framework

1482 The fitting framework used to parameterise QCD background is based on XML
 1483 Analytic Workspace Builder [97] (`xmlAnaWSBuilder`), which employs one-dimensional
 1484 observables to create RooFit [98] workspaces. The workflow of the framework is sum-
 1485 marised in Figure 6.65.

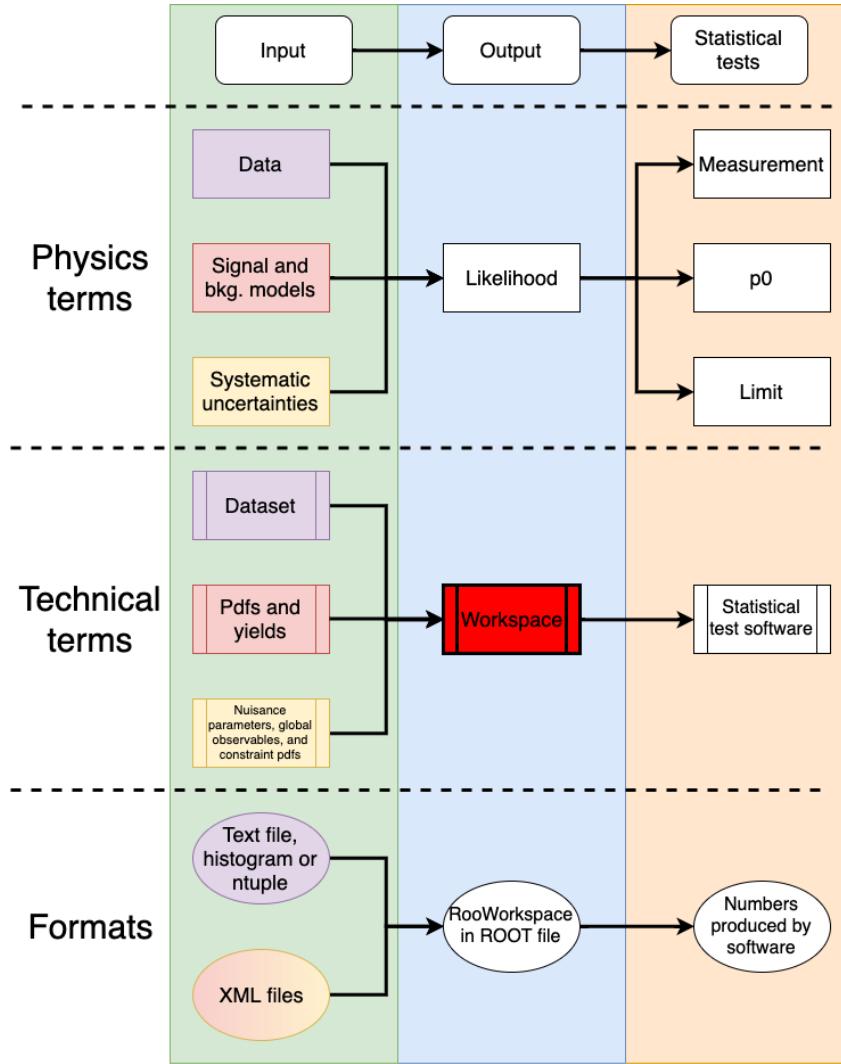


Figure 6.65 Workflow of the `XmlAnaWSBuilder`.

1486 The xRooFit framework [99] that based on RooFit data fitting package is used for
 1487 data fitting. Modifications are needed so that it can integrate over binned data, as RooFit
 1488 evaluates its fit functions using the centre value of each bin rather than the actual average

mass in each bin. As a result, significant biases could occur in the fit results [100]. Recent developments introduce a new class of `RooBinSamplingPdf` in to `RooFit` package, which solve such issue.

6.5.2 Statistical Method

In this analysis, the discriminating variable is set to the dijet invariant mass m_{jj} , and the distribution of it is used as a probability density function (pdf) to build the likelihood function.

6.5.2.1 Parametric background models

The distribution of m_{jj} of background is parameterized by

$$f_b(m_{jj}; \mathbf{p}_b) = f_b(m_{jj}; p_1, p_2, p_3, p_4, p_5) = p_1 \left(1 - \frac{m_{jj}}{\sqrt{s}}\right)^{p_2} \left(\frac{m_{jj}}{\sqrt{s}}\right)^{p_3 + p_4 \ln\left(\frac{m_{jj}}{\sqrt{s}}\right) + p_5 \left[\ln\left(\frac{m_{jj}}{\sqrt{s}}\right)\right]^2}, \quad (6.8)$$

where \mathbf{p}_b are free parameters determined by fitting to data (or pseudo data), and $\sqrt{s} = 13$ TeV. In some cases, $p_5 = 0$ is taken. We will assume Equation (6.8) is normalized to unity as needed.

Given that we are employing a binned likelihood approach and working with histograms, it becomes essential to determine the average count of events in the i th bin, arising from both the signal and background contributions:

$$s_i = s_{\text{tot}} \int_{\text{bin } i} f_s(m_{jj}; \mathbf{p}_s) dm_{jj}, \quad (6.9)$$

$$b_i = b_{\text{tot}} \int_{\text{bin } i} f_b(m_{jj}; \mathbf{p}_b) dm_{jj}, \quad (6.10)$$

where f_s and f_b are pdfs of m_{jj} for the signal and background, respectively. The quantities s_{tot} and b_{tot} represent the total mean numbers of signal and background events. The variable b_{tot} is an additional nuisance parameter. The signal normalization s_{tot} is not treated as a parameter that can be adjusted, but rather is set to the value determined by the nominal signal model. The parameter can be expressed as $s_{\text{tot}} = \sigma L \epsilon$, where σ is fixed by the model cross section, and L and ϵ represent the nominal luminosity and total acceptance times efficiency, respectively.

1511 **6.5.2.2 Uncertainties**

1512 In this analysis, there are six sources of systematic uncertainties on the signal stud-
1513 ied:

1514 δL an uncertainty on the integrated luminosity of the data sample,

1515 $\delta \epsilon$ an uncertainty on the signal efficiency times acceptance,

1516 δt an uncertainty on the gluon-tag efficiency,

1517 δE_{JER} an uncertainty on the jet energy resolution, and

1518 δE_{JES} an uncertainty on the jet energy scale.

1519 δS an uncertainty due to spurious signals.

1520 All these uncertainties are treated as shape uncertainties except for δL which is a normal-
1521 ization uncertainty. These uncertainties are associated to nuisance parameters denoted
1522 by $\alpha_L, \alpha_\epsilon, \alpha_t, \alpha_{E_{\text{JER}}}, \alpha_{E_{\text{JES}}}, \alpha_S$, respectively, and the values of the auxiliary measurements
1523 by $\theta_b, \theta_L, \theta_\epsilon, \theta_t, \theta_{E_{\text{JER}}}, \theta_{E_{\text{JES}}}, \theta_S$, respectively.

1524 **6.5.2.3 Likelihood function definition**

1525 A binned likelihood is used in this analysis. Consider the m_{jj} histogram of $\mathbf{n} =$
1526 (n_1, \dots, n_N) events, the likelihood function without uncertainties is built as:

$$\mathcal{L}(\mu; b_{\text{tot}}, \mathbf{p}_s, \mathbf{p}_b) = \prod_{i=1}^N \frac{(\mu s_i + b_i)^{n_i}}{n_i!} e^{-(\mu s_i + b_i)}, \quad (6.11)$$

1527 where the parameter of interest (POI) μ is the signal strength parameter, b_i is the num-
1528 ber of background events in the i bin, s_i is the number of signal events in the i bin.

1529 Background-only hypothesis corresponding to $\mu = 0$, whereas nominal signal hypoth-
1530 esis corresponding to $\mu = 1$.

1531 The full likelihood function with uncertainties included is defined as:

$$\begin{aligned} \mathcal{L}(\mu; b_{\text{tot}}, \mathbf{p}_s, \mathbf{p}_b, \boldsymbol{\alpha}_s) &= \prod_{i=1}^N \frac{(\mu_i^T)^{n_i}}{n_i!} e^{-\mu_i^T} N_i(\alpha_L; \theta_L, \delta_L) N_i(\alpha_\epsilon; \theta_\epsilon, \delta \epsilon) \\ &\quad \cdot N_i(\alpha_t; \theta_t, \delta E_t) N_i(\alpha_{E_{\text{JER}}}; \theta_{E_{\text{JER}}}, \delta E_{\text{JER}}) \end{aligned} \quad (6.12)$$

$$\cdot N_i(\alpha_{E_{\text{JES}}}; \theta_{E_{\text{JES}}}, \delta E_{\text{JES}}) N_i(\alpha_s; \theta_s, \delta_s), \quad (6.13)$$

1532 where μ_i^T is the total number of expected event in the i bin, which is given by:

$$\mu_i^T = \mu s_i \eta_i^L(\alpha_L) \eta_i^\epsilon(\alpha_\epsilon) \eta_i^t(\alpha_t) \eta_i^{E_{\text{JER}}}(\alpha_{E_{\text{JER}}}) \eta_i^{E_{\text{JES}}}(\alpha_{E_{\text{JES}}}) + b_i. \quad (6.14)$$

1533 The parameter $\eta^s(\alpha_s)$ are response functions for uncertainty s , and the subsidiary mea-
1534 surements are constrained by the $N(\alpha; \theta, \delta)$ functions.

1535 In this analysis, constraint functions are built from standard Gaussians, together
1536 with uncertainties that mapped in the response functions. Luminosity uncertainty is
1537 fitted by a log-normal response function, the JER and JES uncertainties are given by
1538 Gaussian and asymmetric response functions, respectively. For each bin, a vertical inter-
1539 polation strategy called piece-wise linear method is used independently. In the case of
1540 the asymmetric error, the polynomial interpolation and exponential extrapolation method
1541 is used.

1542 The parameters $(\mu, N_b, p_s, p_b, \alpha_L)$ are fixed from the fit to data (pseudo-data) and
1543 are common for all bins, whereas parameters $(\alpha_\epsilon, \alpha_t, \alpha_{E_{\text{JER}}}, \alpha_{E_{\text{JES}}}, \alpha_s)$ are different from
1544 bin to bin.

1545 For simplicity in notation, the 18 nuisance parameters are written as the vector α ,
1546 where six of them have corresponding uncertainties. The simplified likelihood function
1547 is written as:

$$\mathcal{L}(\mu; \alpha) = \prod_{i=1}^N \frac{[\mu_i^T(\mu, \alpha)]^{n_i}}{n_i!} e^{-\mu_i^T(\mu, \alpha)} \prod_{s=1}^6 G_{i,s}(\alpha_s). \quad (6.15)$$

1548 6.5.2.4 Statistical Method

1549 A hypothesis test is used for estimating the compatibility between data and a theo-
1550 retical hypothesis, where the pseudo datasets are generated according to a given hypoth-
1551 esis, and compared to the tested dataset in terms of a test statistic.

1552 The procedure is demonstrated as follows: first, the agreement between the col-
1553 lected data and the null hypothesis is evaluated through a hypothesis test. The null hy-
1554 pothesis ($\mu = 0$) posits that only the SM background is present. If the data does not
1555 exhibit any substantial excess under this hypothesis test, the subsequent step involves es-
1556 tablishing an exclusion limit for the targeted signal model on the resonance cross section
1557 for m_{jj} . In this scenario, the hypothesis transforms into a signal + background assump-

1558 tion, leading to the construction of a test statistic based on the signal + background PDF
 1559 of the discriminating variable.

1560 The statistical measurement's p-value serves as a quantification of the degree of
 1561 agreement or discrepancy between a hypothesis and the observed data. Mathematically,
 1562 it represents the integral of the distribution of the test statistic from the value obtained
 1563 for the dataset in question to infinity. This value characterizes the probability of achiev-
 1564 ing the observed outcomes assuming the null hypothesis. A lower p-value indicates a
 1565 higher degree of statistical significance for the observed incompatibility. For instance,
 1566 if the p-value of the data is below 0.05, it signifies that the likelihood of the observed
 1567 data aligning with the hypothesis is less than 5%. This prompts the assertion that the
 1568 hypothesis can be excluded at the 95% confidence level (CL).

1569 **6.5.2.5 Test statistic and p-value definitions**

1570 A binned maximum likelihood (ML) fitting method is used to extract the signal,
 1571 together with profile likelihood ratio test statistic. The test statistics used for claiming a
 1572 positive signal is defined as:

$$q_0 = \begin{cases} -2 \ln \frac{\mathcal{L}(0, \hat{\alpha}(0))}{\mathcal{L}(\hat{\mu}, \hat{\alpha})} & \hat{\mu} \geq 0, \\ 0 & \hat{\mu} < 0. \end{cases} \quad (6.16)$$

1573 and the test statistic used for evaluating the upper limits is given as:

$$\tilde{q}_\mu = \begin{cases} -2 \ln \frac{\mathcal{L}(\mu, \hat{\alpha}(\mu))}{\mathcal{L}(0, \hat{\alpha}(0))} & \hat{\mu} < \mu, \\ -2 \ln \frac{\mathcal{L}(\mu, \hat{\alpha}(\mu))}{\mathcal{L}(\hat{\mu}, \hat{\alpha})} & 0 \leq \hat{\mu} \leq \mu, \\ 0 & \hat{\mu} > \mu. \end{cases} \quad (6.17)$$

1574 where the parameter μ represents the signal strength associated with the hypothesis being
 1575 tested. The maximum likelihood (ML) estimators that optimize the likelihood function
 1576 \mathcal{L} without constraints are referred to as $\hat{\mu}$ for the signal strength and $\hat{\alpha}$ for the other pa-
 1577 rameters. The parameter $\hat{\alpha}$ represents the conditional ML estimator of α that maximizes
 1578 \mathcal{L} while considering a specific value of μ .

1579 The p-value corresponding to the background-only hypothesis is expressed as:

$$p_0 = \int_{q_{0,\text{obs}}}^{\infty} f(q_0|0) dq_0. \quad (6.18)$$

1580 The values of \tilde{q}_μ are calculated for different values of μ by fitting a dataset where

1581 the pseudo data is represented by μ' . This calculation of \tilde{q}_μ is conducted for each pseudo
 1582 dataset at various selected signal mass points, resulting in a distribution of \tilde{q}_μ denoted as
 1583 $f(\tilde{q}_\mu | \mu = \mu')$. As a result, a p-value for the tested dataset is determined based on this
 1584 distribution:

$$p_{\mu'} = \int_{\tilde{q}'_{\mu,\text{obs}}}^{\infty} f(\tilde{q}_\mu | \mu = \mu') dq_\mu, \quad (6.19)$$

1585 the term $\tilde{q}'_{\mu,\text{obs}}$ represents the computed value of the test statistic based on the dataset
 1586 being tested. These p-values are also referred to as p_{s+b} , which signifies that they are
 1587 associated with the signal plus background hypothesis.

1588 6.5.2.6 Generation of pseudo-data

1589 The PDF of a certain model is used for generating the pseudo datasets. Signal +
 1590 background pseudo datasets are utilized to estimate the observed confidence level (CL) of
 1591 a signal + background hypothesis, while background-only pseudo datasets are employed
 1592 for expected CL estimations.

1593 During the generation of pseudo datasets, all parameters in the PDF are set to their
 1594 nominal values. The expected event counts in each bin follow a Poisson distribution.
 1595 Nuisance parameters (NPs), which represent systematic uncertainties, are treated ac-
 1596 cording to the "unconditional ensemble" approach: for each pseudo dataset, the values
 1597 of α_i (associated with the NPs) are drawn from their respective constraint terms, and
 1598 these values are used in both the likelihood \mathcal{L} and the computation of \tilde{q}_μ .

1599 6.5.2.7 Definition of exclusion limit

1600 The data is interpreted by the modified frequentest method (CL_s method), where
 1601 p-value is modified to take into account downward background fluctuations and quoted
 1602 as CL_s . The definition of CL_s is:

$$CL_s = \frac{p_{s+b}}{1 - p_b}, \quad (6.20)$$

1603 where $p_{b(s+b)}$ is the integrated value of the background-only (signal + background) dis-
 1604 tribution from zero to $\tilde{q}_\mu^{\text{obs}}$. Thus $1 - p_b$ is also referred to as the confidence level of the
 1605 background-only hypothesis (CL_b). The CL_s limit claims exclusion at 95% CL when
 1606 $CL_s = 0.05$.

1607 6.5.2.8 Implementation

1608 The statistical approach employed in this analysis differs slightly from previous
 1609 dijet analyses and aligns with the current trigger-level analysis. In previous approaches,
 1610 a background model devoid of NPs was fitted to the data, and the resulting background
 1611 fit parameters were employed (and held constant) in subsequent likelihood fits involving
 1612 nuisance parameters. However, in this analysis, the background fit parameters are treated
 1613 as unconstrained NPs within the complete likelihood framework used in all fits.

1614 To create the RooFit workspaces, the XML Analytic Workspace Builder is utilized.
 1615 The xRooFit tool processes these workspaces and performs operations like setting limits,
 1616 among others, using classes from the RooFit and RooStats libraries.

1617 6.5.3 Background Estimation

1618 In the resonant search the SM background of the m_{jj} spectrum is established
 1619 through a functional fitting procedure applied to the data. Refs. [101, 102, 103, 104,
 1620 105, 106]) have found that a parametric function of the form

$$f(x) = p_1(1-x)^{p_2}x^{p_3+p_4 \ln x + p_5 (\ln x)^2}, \quad (6.21)$$

1621 where $x \equiv m_{jj} / \sqrt{s}$, accurately describes dijet mass distribution predicted by leading and
 1622 next-to-leading-order QCD Monte Carlo. In the ATLAS Run 2 analysis with 139.0 fb^{-1}
 1623 of data [107, 96], the four parameter version of the function ($p_5 = 0$) was found to
 1624 sufficiently described the data. The introduction of gluon tagging may require more
 1625 parameters to properly describe the full invariant mass spectrum.

1626 To avoid introducing any potential bias due to the selection of a specific background
 1627 function, an alternative functional form is employed. This alternative form is inspired by
 1628 the one used by the UA2 experiment [108, 109] when observing the decay of W and Z
 1629 bosons into two jets, followed by a subsequent search.

$$f(x) = p_1 x^{p_2} \exp(p_3 x + p_4 x^2). \quad (6.22)$$

1630 6.5.4 Analysis Strategy

1631 The analysis begins with the utilization of skimmed ntuples, which are the result
 1632 of applying the event selection criteria outlined in Section 6.4.2. These ntuples serve as

1633 the basis for generating pseudo-data using the background-only model. Subsequently,
 1634 a 4-parameter ($p_5 = 0$) fit function described by Equation 6.21 is employed to fit this
 1635 pseudo-data. The fit to the data is deemed satisfactory if it meets the following criterion:

- 1636 • Global χ^2 p -value > 0.05

1637 If the conditions mentioned above are satisfied, the background is chosen for the
 1638 purpose of upper limit estimations. Conversely, if the criteria are not met, the 5-parameter
 1639 version of Equation 6.21 is employed for background fitting and is subjected to the same
 1640 selection criterion. If the fit using the 5-parameter function also fails to meet the cri-
 1641 teria, the analysis reduces the range of the window and repeats the fitting process with
 1642 the 5-parameter function to see if a satisfactory fit can be achieved. If this attempt still
 1643 does not meet the criteria, the analysis switches to an alternative option for generating
 1644 pseudo-data. Once a fit satisfying the criteria is obtained, the fit function undergoes var-
 1645 ious validation tests to ensure the appropriateness of the fit strategy. The flowchart of
 1646 Figure 6.66 shows the analysis strategy.

1647 **6.5.5 Spurious Signal Tests**

1648 The spurious signal test is designed to estimate the difference between the signal
 1649 yields from the fit and the expected signal yields that given by fitting a known template
 1650 signal model on a smooth background distribution. Such difference is considered as fit
 1651 bias and defined as S_{spur} :

$$S_{\text{spur}} = S_{\text{fit}} - S_{\text{template}} \quad (6.23)$$

1652 It is crucial to verify the stability of the fit when applied to a background-only
 1653 distribution. In this context, no signal is intentionally introduced into the yields, ensuring
 1654 that the extracted number of signal events remains zero. In the spurious signal test, S_{spur}
 1655 is determined by fitting a model comprising both signal and background components
 1656 onto a background-only template. The corresponding uncertainty from the fit is denoted
 1657 as σ_{fit} . Both the spurious signal S_{spur} and its associated uncertainty σ_{fit} are expected to be
 1658 consistent with zero.

1659 The estimation of the spurious signal is consequently conducted through these pseudo-
 1660 experiments. The mean value across all experiments is calculated, and a total of 100
 1661 pseudo-experiments have been employed. For each individual signal hypothesis, the

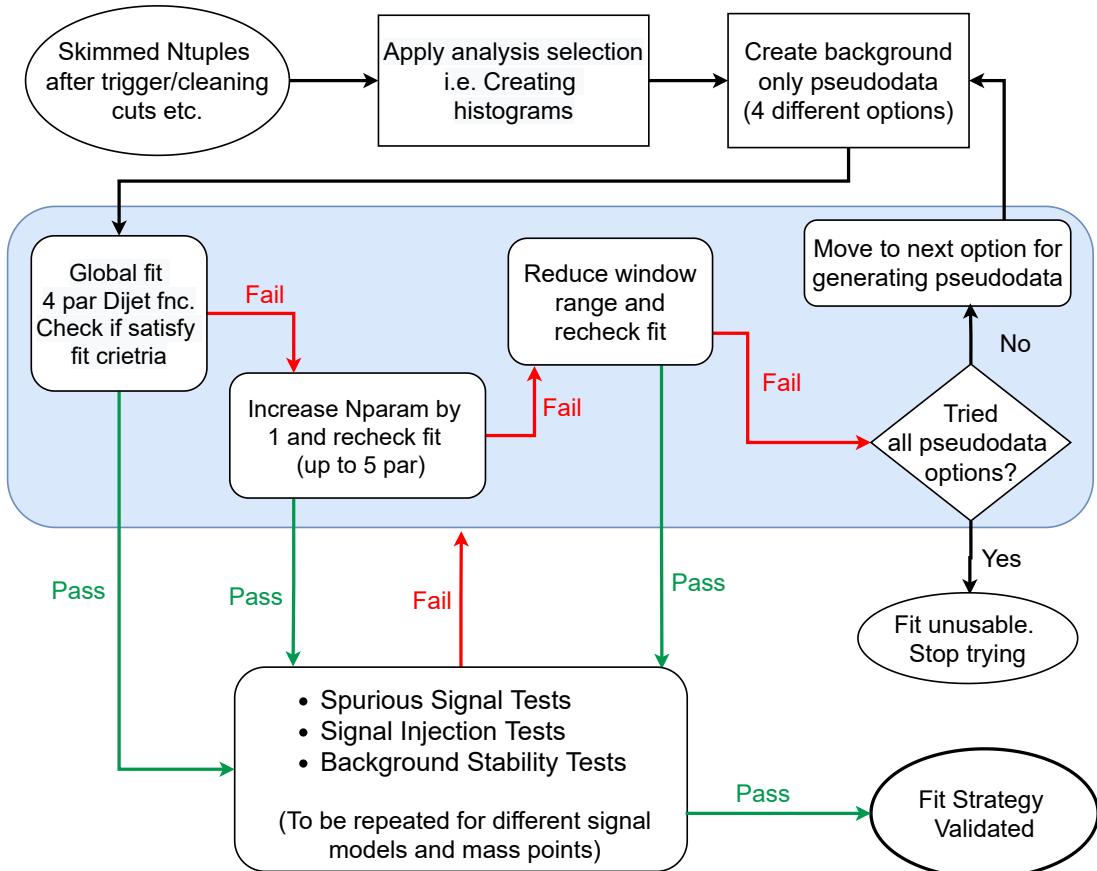


Figure 6.66 Analysis top-level flowchart.

1662 assessment of spurious signals is conducted at various mass points. This is done in
 1663 individually for each signal hypothesis and at each mass point. The outcomes of the
 1664 model-independent tests for Gaussian signals, considering different masses and widths,
 1665 are consolidated in Table 6.29 for the 1 gluon-tagged category and in Table 6.30 for the
 1666 2 gluon-tagged category.

1667 Following the recommendations of the Statistical PUB Note [110], the spurious
 1668 signal is required to be

$$S_{\text{spur}} < (20\% - 50\%) \sigma_{\text{fit}} \quad (6.24)$$

1669 The idea criteria is when the spurious signal satisfy: $S_{\text{spur}} < 30\% \sigma_{\text{fit}}$, but can be
 1670 loosen up to 50% σ_{fit} . Most of the tested mass points and widths satisfy the spurious
 1671 signal criteria.

Mass TeV	Width percentage [%]	Median ± Rms		Ratio $S_{\text{spurious}}/\text{Uncertainty}$
		S_{spurious}	± Uncertainty	
2	5	0.19 2	± 802.85 2	2.36E-042
2	10	3.35 2	± 1313.792	2.55E-032
2	15	154.92 2	± 1666.6 2	0.093 2
3	5	1.76 2	± 249.13 2	7.06E-032
3	10	82.55 2	± 520.85 2	0.158 2
3	15	344.74 2	± 803.85 2	0.429 2
4	5	48.42 2	± 112.34 2	0.431 2
4	10	115.89 2	± 200.83 2	0.577 2
4	15	2.02 2	± 242.15 2	8.34E-032
5	5	0.021 2	± 31.77 2	6.61E-042
5	10	0.012 2	± 31.96 2	3.75E-042
5	15	0.006 2	± 18.98 2	3.16E-042
6	5	7.82E-042 ± 5.54 2		1.41E-042
6	10	2.84E-042 ± 5.93 2		4.79E-052
6	15	3.62E-042 ± 5.79 2		6.25E-052
7	5	8.65E-042 ± 2.66 2		3.25E-042
7	10	1.6E-04 2	± 2.59 2	6.18E-052
7	15	8.34E-052 ± 2.71 2		3.08E-052

Table 6.29 Spurious Signal tests using Gaussian signals for 1 gluon tagged category.

Mass TeV	Width percentage [%]	Median ± Rms $S_{\text{spurious}} \pm \text{Uncertainty}$	Ratio $S_{\text{spurious}}/\text{Uncertainty}$
2	5	179.84 2 ± 635.08 2	0.283 2
2	10	757.07 2 ± 1265.99 2	0.598 2
2	15	1666.24 2 ± 2126.08 2	0.784 2
3	5	1.83E-032 ± 85.31 2	2.14E-05 2
3	10	0.27 2 ± 125.63 2	2.15E-03 2
3	15	0.021 2 ± 113.74 2	1.85E-04 2
4	5	1.91E-032 ± 25.6 2	7.46E-05 2
4	10	3.55E-032 ± 38.68 2	9.18E-05 2
4	15	1.50E-032 ± 27.01 2	5.55E-05 2
5	5	2.72E-042 ± 7.13 2	3.81E-05 2
5	10	9.99E-052 ± 5.57 2	1.79E-05 2
5	15	2.1E-04 2 ± 4.72 2	4.45E-05 2
6	5	1.37E-042 ± 1.92 2	7.14E-05 2
6	10	1.47E-042 ± 3.25 2	4.52E-05 2
6	15	6.49E-052 ± 2.59 2	2.51E-05 2
7	5	1.88E-042 ± 1.19 2	1.58E-04 2
7	10	1.17E-042 ± 1.17 2	1.0E-04 2
7	15	7.83E-052 ± 1.20 2	6.53E-05 2

Table 6.30 Spurious Signal tests using Gaussian signals for 2 gluon tagged category.

6.5.6 Fit Stability Tests

The fit stability tests are employed to assess the behaviour of the background fit function under different scenarios: when applied to the background-only template and the signal + background template. A comparison is made between the fit results obtained from these two templates. Ideally, the background fit function should yield consistent outcomes in both cases. The results of these fit stability tests are presented in Table 6.31 through Table 6.32, encompassing various signal strengths and mass points.

Notably, the background estimation derived from the signal + background fit (B_1) aligns with the background estimation obtained from the background-only fit (B_2), indicating good agreement between the two approaches.

Mass (TeV)	Width (percentage)	Signal Strength	B_1 from S+B fit	B_2 from B-only fit
			Mean \pm Rms	Mean \pm Rms
2	5	1	20062716.452 \pm 4370.572	20064025.612 \pm 4003.072
2	5	3	20063730.272 \pm 4882.092	20067248.182 \pm 4003.142
2	5	5	20062961.532 \pm 4521.622	20070470.902 \pm 4003.362
5	5	1	20062414.492 \pm 4005.802	20062458.642 \pm 4003.052
5	5	3	20062420.852 \pm 4002.942	20062547.112 \pm 4003.092
5	5	5	20062420.962 \pm 4002.822	20062635.822 \pm 4003.252
5	10	1	20062435.182 \pm 4010.372	20062483.502 \pm 4002.872
5	10	3	20062448.752 \pm 4007.222	20062622.262 \pm 4002.952
5	10	5	20061413.122 \pm 3682.052	20062761.082 \pm 4003.122
7	5	1	20062420.382 \pm 4002.682	20062420.292 \pm 4002.982
7	5	3	20062422.562 \pm 4002.862	20062432.082 \pm 4003.082
7	5	5	20062422.862 \pm 4002.982	20062444.092 \pm 4003.202

Table 6.31 Fit Stability tests using Gaussian signals for 1 gluon tagged category.

Mass (TeV)	Width (percentage)	Signal Strength	B_1 from S+B fit		B_2 from B-only fit	
			Mean ± Rms	Mean ± Rms	Mean ± Rms	Mean ± Rms
2	5	1	3901512.922 ± 2163.272	3902240.712 ±	2048.042	
2	5	3	3901530.762 ± 2166.982	3903253.552 ±	2047.372	
2	5	5	3901621.902 ± 2291.012	3905032.952 ±	2050.682	
5	5	1	3901529.752 ± 2049.312	3901559.922 ±	2046.182	
5	5	3	3901528.522 ± 2049.152	3901589.412 ±	2044.932	
5	5	5	3901533.992 ± 2047.482	3901621.882 ± 3901586.682		
5	10	1	3901536.862 ± 2047.402	3901566.442 ±	2048.232	
5	10	3	3901535.712 ± 2054.622	3901616.492 ±	2050.262	
5	10	5	3901538.472 ± 2049.542	3901670.562 ±	2047.942	
7	5	1	3901531.272 ± 2047.302	3901538.452 ±	2049.162	
7	5	3	3901540.722 ± 2068.732	3901542.752 ±	2048.462	
7	5	5	3901533.132 ± 2052.642	3901540.092 ±	2048.942	

Table 6.32 Fit Stability tests using Gaussian signals for 2 gluon tagged category.

1682 6.6 Systematic uncertainties

1683 Indeed, obtaining uncertainties for a q/g tagger built upon track multiplicity poses
 1684 challenges, particularly in the higher p_T range. This difficulty is partly attributed to the
 1685 limited statistics available beyond 1 TeV, where fewer gluon-jets are present due to their
 1686 tendency to be produced at lower masses compared to quark-jets. Consequently, an issue
 1687 arises in equations that necessitate the average number of tracks in quark- or gluon-jets to
 1688 facilitate calculations. The scarcity of data points at higher p_T values hampers the robust
 1689 estimation of these averages, contributing to the uncertainty challenge in this context.

1690 The determination of the fraction of jets classified as quark- or gluon-initiated jets
 1691 is accomplished through the ratio f_q^f/f_g^c , where the superscript f (c) designates the jet
 1692 with the higher (lower) η value in simulated dijet events. These fractions are derived by
 1693 convolving parton distribution functions with matrix element calculations. The number
 1694 of charged tracks events in the jet with higher η can be described by the following system
 1695 of equations [47]:

$$\langle n_{\text{charged}}^f \rangle = f_q^f \langle n_{\text{charged}}^q \rangle + f_g^f \langle n_{\text{charged}}^g \rangle \quad \langle n_{\text{charged}}^c \rangle = f_q^c \langle n_{\text{charged}}^q \rangle + f_g^c \langle n_{\text{charged}}^g \rangle. \quad (6.25)$$

1696 These equations require two samples with different fractions of quark- and gluon-
 1697 jets. While theoretically valid even at high p_T values, their applicability diminishes in the
 1698 high p_T regime due to the exceedingly small fractions of gluon jets. Notably, the main
 1699 sources of uncertainty stem from discrepancies in the MC modelling and the challenges
 1700 associated with reconstructing charged tracks within jets. This is especially relevant as
 1701 the separation between tracks is comparable to the resolution of the detector. Conse-
 1702 quently, the efficiency of the tagger relies on the accurate resolution of tracks for precise
 1703 N_{trk} determination, which in turn is constrained by available statistics.

1704 They systematic uncertainty can be estimated by using pure MC simulations and
 1705 is expected to be substantial, yet smaller than that obtained from data at the edges of
 1706 the mass range. This technique is particularly effective where statistics are not limited,
 1707 such as in the central region of the p_T distribution. Such an approach has proven to be
 1708 the optimal choice. To extend the uncertainties into the higher p_T regime, particle-level
 1709 effects and MC reconstruction effects are incorporated. These uncertainties pertain to
 1710 "in-situ" considerations, making it reasonable to employ them during an extrapolation

1711 procedure.

1712 The procedure is performed at constant p_T ranges, as N_{trk} depends only on p_T and
1713 the parton type that initiating jets, uncertainties can be computed by comparing the dis-
1714 tribution of N_{trk} in bins of jet p_T , which generated from different simulation models.
1715 Thus different type of MC generators could introduce underlying uncertainties to the re-
1716 sults. Details on different types of uncertainties and the samples used to estimate them
1717 are described in Section [5.7](#).

1718

6.7 Results

1719 The untagged, 1-g tagged and 2-g tagged upper limits on Graviton models are shown
 1720 in Figures 6.67, and on QBH models are given in Figures 6.68. The observed limit in
 1721 2-g tagged region gives higher m_{jj} than that in 1-g tagged and untagged regions.

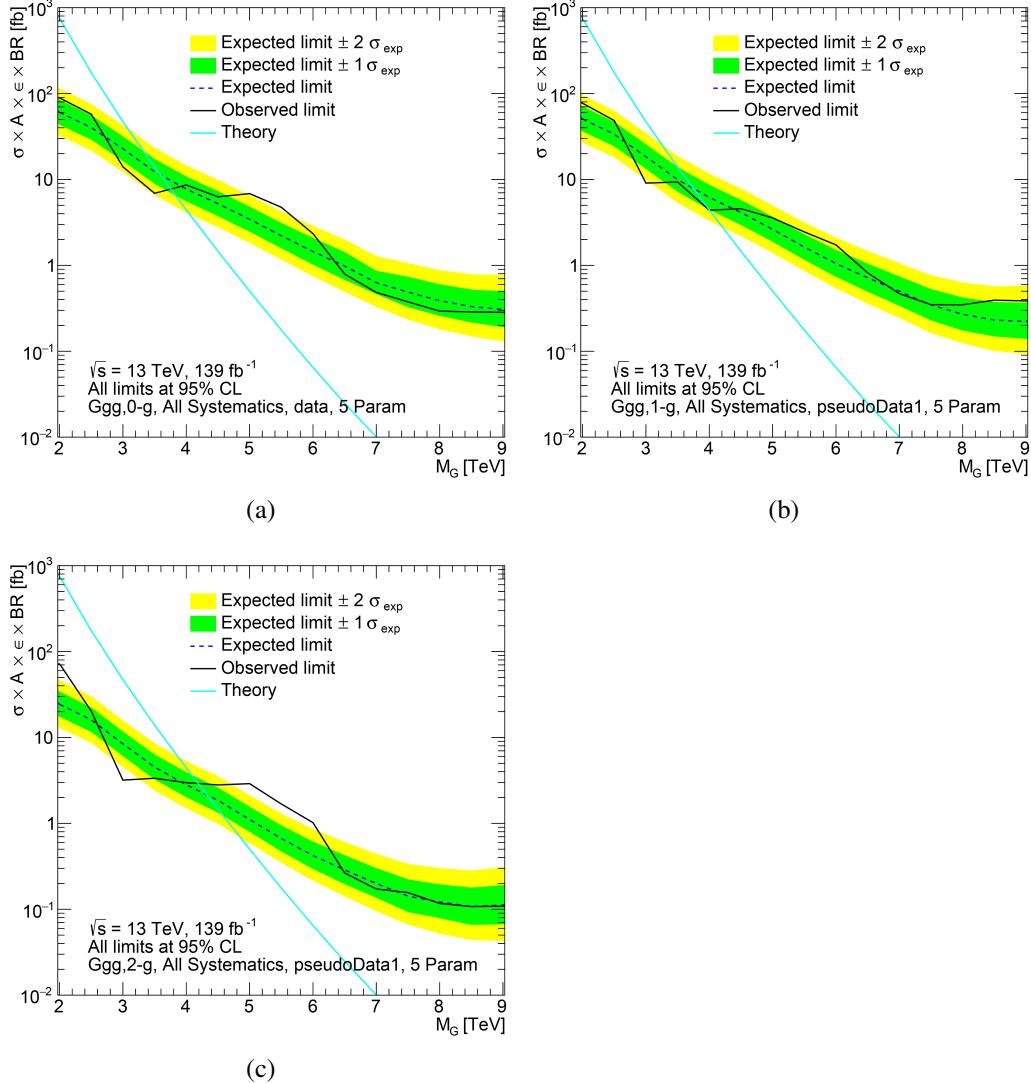


Figure 6.67 Upper limits set in the untagged (a), 1-g tagged (b) and 2-g (c) tagged Signal Region using Graviton model with systematics included using the full 139fb^{-1} Run-2 dataset.

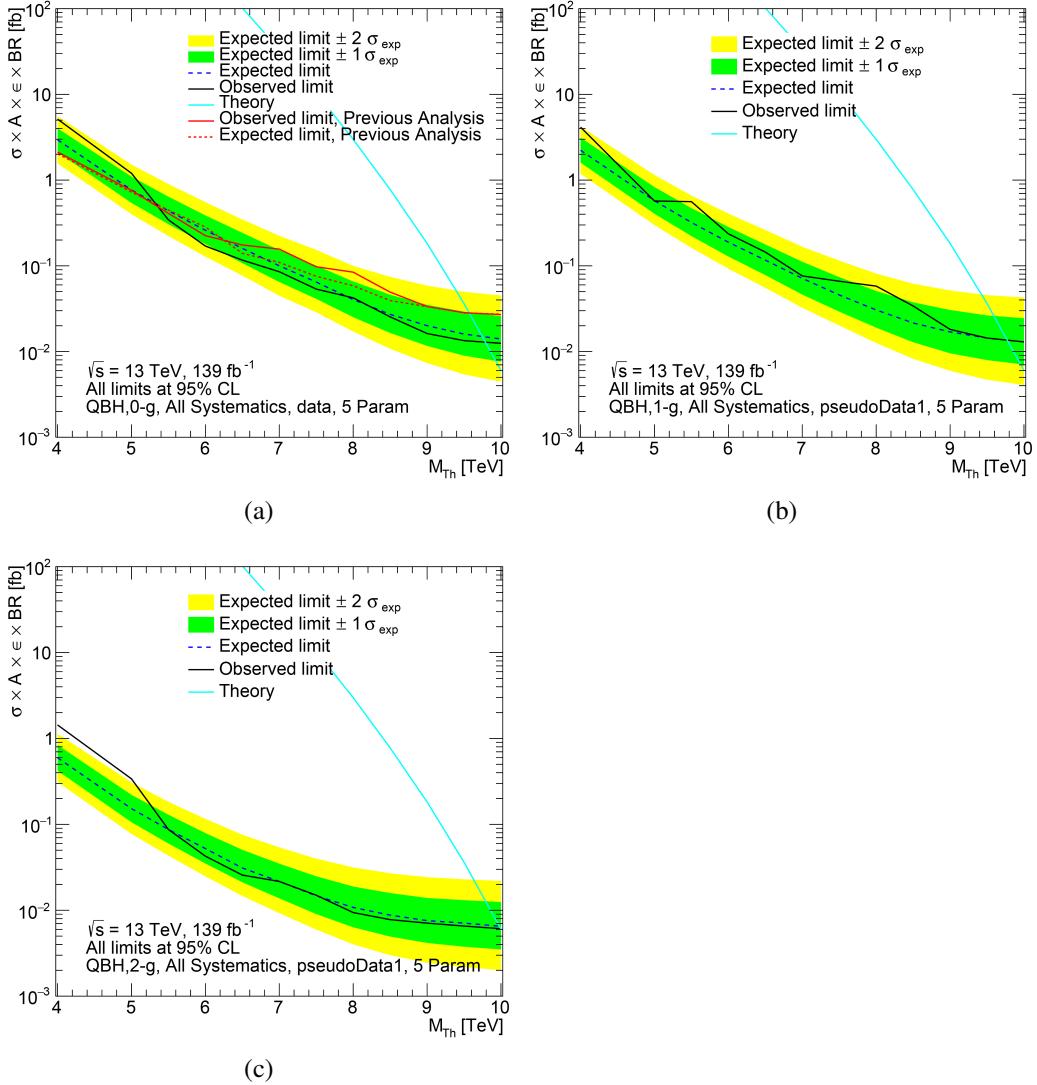


Figure 6.68 Upper limits set in the untagged (a), 1-g tagged (b) and 2-g (c) tagged Signal Region using QBH model with systematics included using the full 139fb^{-1} Run-2 dataset.

1722 7 Conclusions

1723 From 2015 to 2018, the proton-proton collision at the LHC have achieved an unprece-
1724 dented centre-of-mass energy of $\sqrt{s} = 13$ TeV, with a total integrated luminosity of 140
1725 fb^{-1} that have been recorded by the ATLAS experiment. Such huge amount of collision
1726 data allow scientists test models beyond the SM in a more efficient way, leading a deeper
1727 understanding of physics beyond the SM.

1728 This thesis presents the search for new resonances that potentially decay into a pair
1729 of jets using the data collected by the ATLAS detector during 2015-2018. Resonances
1730 predicted by the BSM can decay into quarks and/or gluons, by introducing jet taggers,
1731 the sensitivity of the search could be significantly increased. This study leverages the
1732 extensive dataset recorded between 2015 and 2018 to extend the taggers' applicability
1733 to high-energy jets. Two distinct jet tagging methods are explored: a tagger centred on
1734 the charged-particle jet constituent multiplicity (N_{trk}), and a BDT-based tagger, which
1735 integrates various individual jet substructure observables.

1736 The matrix method is adopted to estimate the distribution shapes of the tagging
1737 variables for quark- and gluon-jets. This entails combining information from samples
1738 enriched with quark- and gluon-jets, acquired from a selection of dijet events charac-
1739 terized by jet p_T ranging from 500 GeV to 2 TeV. The considered variables exhibit a
1740 satisfactory agreement with the MC simulations, with discrepancies relative to data mea-
1741 surements being less than 25% across various defined regions.

1742 The BDT-tagger demonstrates superior performance over the N_{trk} -only tagger in
1743 distinguishing quark-jets from gluon-jets within the jet p_T range of 500 GeV to 1200
1744 GeV. Above this range, the performance of the two taggers becomes comparable. The
1745 evaluation of tagger performance differences between data and MC samples is facilitated
1746 through the data-to-MC SFs. Four working points of 50%, 60%, 70%, 80% together with
1747 all systematics are provided so that analyses can use it based on their own interest. These
1748 factors are measured across varying jet- p_T intervals, exhibiting a range from 0.92 to 1.02,
1749 with a cumulative uncertainty of approximately 20%. The primary contributor to this
1750 uncertainty stems from divergent modelling choices within MC simulations, constituting
1751 approximately 18% for both taggers. To account for variations between different MC
1752 generators, MC-to-MC SFs are also presented, ranging from 0.9 to 1.1 for the majority
1753 of MC samples.

Conclusions

1754 The q/g taggers developed in this study and the associated measurement of their SFs
1755 hold relevance for various analyses. These applications encompass SM measurements
1756 that rely on accurate jet origin identification, as well as BSM physics searches that can
1757 capitalize on heightened sensitivity to the presence of new particles. This thesis performs
1758 the searches on m_{jj} spectrum. Benchmark models graviton and QBH are tested. Because
1759 no significant excess in data are found, a upper limit is set to each model.

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