

Graph Neural Network Flavour Tagging and Boosted Higgs Measurements at the LHC

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Declaration

I, Samuel John Van Stroud confirm that the work presented in this thesis is my own. Where information has been derived from other sources, I confirm that this has been indicated in the thesis.

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Abstract

This thesis presents investigations into the challenges of, potential improvements to, and the application of b -jet identification at the ATLAS experiment at the Large Hadron Collider (LHC). A focus is placed on the high transverse momentum regime, which is a critical region in which to study the Standard Model, but within which successful b -jet identification becomes difficult.

As b -jet identification relies on the successful reconstruction of charged particle trajectories (tracks), the tracking performance is investigated and potential improvements are assessed. Track reconstruction becomes increasingly difficult at high transverse momentum due to the increased multiplicity and collimation of tracks, and also due to the presence of displaced tracks that may occur as the result of the decay of a long-flying b -hadron. The investigations revealed that the track quality selections applied during track reconstruction are suboptimal for tracks inside high transverse momentum b -jets, motivating future studies into the optimisation of these cuts.

To improve b -tagging performance two novel techniques are employed: the classification of the origin of tracks and the application of graph neural networks. An algorithm has been developed to classify the origin of tracks, which allows a more optimal collection of tracks to be selected for use in other algorithms. A graph neural network (GNN) jet flavour tagger has also been developed. This tagger requires only tracks and jet variables as inputs, making a break from previous algorithms, which relied on the outputs of several other algorithms. This model is trained to simultaneously predict the jet

flavour, track origins, and track-pair compatibility (i.e. vertexing), and demonstrates markedly improvements in b -tagging performance, both at low and high transverse momenta. The closely related task of c-jet identification also benefits from these methods.

Analysis of high transverse momentum $H \rightarrow b\bar{b}$ decays, where the Higgs boson is produced in association with a vector boson, was also performed using 139 fb^{-1} of 13 TeV proton-proton collision data from Run 2 of the LHC. The analysis is described, with a focus on the detailed modelling studies performed by the author. The analysis measured provided first measurements in this channel of the Higgs boson production in two high transverse momentum regions. The impact of applying the improved GNN-based b -tagging algorithms to the analysis is also studied.

Impact Statement

impact statement 500 words [link to ucl info](#)

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² Chapter 1

³ Introduction

- ⁴ This thesis describes various efforts in improving the understanding of the Higgs boson and its coupling to heavy flavour quarks, primarily through the improvement of the algorithms used to reconstruct and analyse jets.
- ⁷ Chapter 2 describes the theoretical foundations of the work presented in the rest of the thesis.
- ⁹ Chapter 3 describes the ATLAS detector at the CERN accelerator complex. Details of reconstructed physics objects are also provided.
- ¹¹ Chapter 4 provides an overview of tracking and *b*-tagging at ATLAS, and studies into the challenges of high transverse momentum *b*-tagging.
- ¹³ Chapter 5 describes a tool to predict the origins of tracks. The tool is used to improve *b*-tagging performance by the identification and removal of fake tracks before their input to the *b*-tagging algorithms.
- ¹⁶ Chapter 6 introduces a novel monolithic approach to *b*-tagging using graph neural networks and auxiliary training objectives.
- ¹⁸ Chapter 7 describes the measurement of the associated production of a Higgs boson decaying into a pair of *b*-quarks at high transverse momentum.
- ²⁰ Chapter 8 contains some concluding remarks.

- 21 The author's contribution to the work presented in this thesis is as follows.
- 22 **Tracking:** The author was been an active member of the Cluster and Tracking
23 in Dense Environments group for the duration of their qualification task on the
24 understanding of tracking performance at high transverse momentum. The author
25 played a key role in software r22 validation studies for the tracking group, including
26 the validation of the quasi-stable particle interaction simulation and the radiation
27 damage Monte-Carlo simulation. The author helped design and improve several
28 tracking software frameworks, and contributed to heavy flavour tracking efficiency
29 studies in dense environments.
- 30 ***b*-tagging:** The author has been an active member of the Flavour Tagging group
31 since September 2014. The author played a key role in investigating the performance
32 of the low level taggers at high transverse momentum and led studies into the
33 labelling and classification of track origins. Based on work by Jonathan Shlomi,
34 the author helped develop a new flavour tagging algorithm which offers a large
35 performance improvement with respect to the current state of the art. The author
36 was the primary editor of a public note associated with this work [2], and also
37 contributed to the proliferation of GN1 to the trigger, High Luminosity LHC, and
38 $X \rightarrow bb$ use cases. The author also played a key role in software r22 validation
39 studies for the Flavour Tagging group, including the validation of the quasi-stable
40 particle interaction simulation. The author maintains and contributes to various
41 software frameworks used in the Flavour Tagging group, and contributes to group
42 documentation.
- 43 **Higgs:** The author was an active member of the Boosted VHbb analysis group. The
44 author performed various studies deriving systematic uncertainties for the $V+jets$
45 and diboson backgrounds. The author also produced and maintained samples, ran fit
46 studies and cross checks, and gave the diboson unblinding approval talk to the Higgs
47 group. The author also contributed to the developement of the analysis software.

⁴⁸ Chapter 2

⁴⁹ Theoretical Framework

⁵⁰ The Standard Model (SM) of particle physics is the theory describing all known
⁵¹ elementary particles and their interactions via three of the four fundamental forces.
⁵² Developed by merging the successful theories of quantum mechanics and relativity
⁵³ in the second half of the 20th century, the SM's position today at the centre of our
⁵⁴ understanding of the nature of the Universe is firmly established by an unparalleled
⁵⁵ level of agreement between the predictions from the model and experimental results
⁵⁶ [3, 4].

⁵⁷ The SM has predicted the discovery of the top and bottom quarks [5–7], the W
⁵⁸ and Z bosons [8], and the tau neutrino [9]. The last missing piece of the SM to be
⁵⁹ discovered was the Higgs boson, first theorised in the 1960s [10–12], and eventually
⁶⁰ observed at the LHC in 2012 [13, 14]. After its discovery, much ongoing work has
⁶¹ been carried out performing detailed measurements of its mass and interactions with
⁶² other particles.

⁶³ In this chapter, an overview of the SM is given in Section 2.1, and a more detailed
⁶⁴ discussion of the Higgs sector and Higgs phenomenology is provided in Section 2.2.

⁶⁵ 2.1 The Standard Model

⁶⁶ The SM is formulated in the language of Quantum Field Theory (QFT). In this
⁶⁷ framework, particles are localised excitations of corresponding quantum fields, which
⁶⁸ are operator-valued distributions across spacetime.

Central to QFT is the Lagrangian density which describes the kinematics and dynamics of a field. Observations of conserved quantities are linked, via Noether's theorem, to symmetries which are expressed by the Lagrangian. Alongside Global Poincaré symmetry, the SM Lagrangian observes a local non-Abelian $SU(3)_C \otimes SU(2)_L \otimes U(1)_Y$ gauge symmetry. Gauge symmetries leave observable properties of the system unchanged when the corresponding gauge transformations are applied to the fields. The full Lagrangian of the SM can be broken up into distinct terms corresponding to the different sectors, as in Eq. (2.1). An overview of each sector is given in the following chapters.

$$\mathcal{L}_{\text{SM}} = \mathcal{L}_{\text{EW}} + \mathcal{L}_{\text{QCD}} + \mathcal{L}_{\text{Higgs}} + \mathcal{L}_{\text{Yukawa}} \quad (2.1)$$

The SM provides a mathematical description of how three of the four fundamental forces interact with the matter content of the Universe. The SM contains 12 spin-1/2 fermions, listed in Table 2.1, and five bosons listed in Table 2.2.

Generation	Leptons			Quarks		
	Flavour	Mass [MeV]	Charge [e]	Flavour	Mass [MeV]	Charge [e]
First	e	0.511	-1	u	2.16	$2/3$
	ν_e	$< 1.1 \times 10^{-6}$	0	d	4.67	$-1/3$
Second	μ	105.7	-1	c	1.27×10^3	$2/3$
	ν_μ	< 0.19	0	s	93.4	$-1/3$
Third	τ	1776.9	-1	t	173×10^3	$2/3$
	ν_τ	< 18.2	0	b	4.18×10^3	$-1/3$

Table 2.1: The fermions of the SM [15]. Three generations of particles are present. Also present (unlisted) are the antiparticles, which are identical to the particles up to a reversed charge sign.

80

2.1.1 Quantum Electrodynamics

Quantum electrodynamics (QED) is the relativistic quantum theory which describes the interaction between the photon and charged matter. Consider a Dirac spinor field $\psi = \psi(x)$ and its adjoint $\bar{\psi} = \psi^\dagger \gamma^0$, where ψ^\dagger denotes the Hermitian conjugate of ψ . The field ψ describes fermionic spin-1/2 particle, for example an electron. The

Name	Symbol	Mass [GeV]	Charge [e]	Spin
Photon	γ	$< 1 \times 10^{-27}$	$< 1 \times 10^{-46}$	1
Charged Weak boson	W^\pm	80.377 ± 0.012	± 1	1
Neutral Weak boson	Z	91.1876 ± 0.0021	0	1
Gluon	g	0	0	1
Higgs	H	125.25 ± 0.17	0	0

Table 2.2: The bosons of the SM [15]. The photon, weak bosons and gluons are gauge bosons arising from gauge symmetries, and carry the four fundamental forces of the SM. The recently discovered Higgs boson is the only fundamental scalar particle in the SM.

⁸⁶ Dirac Lagrangian density is

$$\mathcal{L}_{\text{Dirac}} = \bar{\psi}(i\cancel{\partial} - m)\psi, \quad (2.2)$$

⁸⁷ where $\cancel{\partial} = \gamma^\mu \partial_\mu$ denotes the contraction with the Dirac gamma matrices γ^μ (summation over up-down pairs of indices is assumed). Application of the Euler-Lagrange equation on Eq. (2.2) yields the Dirac equation

$$(i\cancel{\partial} - m)\psi = 0. \quad (2.3)$$

⁹⁰ Suppose some fundamental symmetry that requires invariance under a local $U(1)$
⁹¹ gauge transformation

$$\psi \rightarrow \psi' = \psi e^{-iq\alpha(x)}, \quad (2.4)$$

⁹² where α varies over every spacetime point x . Under this transformation, the Dirac
⁹³ equation transforms as

$$(i\cancel{\partial} - m)\psi e^{-iq\alpha(x)} + q\cancel{\partial}\alpha(x)\psi e^{-iq\alpha(x)} = 0. \quad (2.5)$$

⁹⁴ For the Dirac equation to remain invariant under the transformation in Eq. (2.4),
⁹⁵ a new field A_μ which transforms as $A_\mu \rightarrow A'_\mu = A_\mu + \partial_\mu \alpha(x)$ must be added. The
⁹⁶ transformed interaction term

$$-q\cancel{A}\psi \rightarrow -q\cancel{A}\psi e^{-iq\alpha(x)} - q\cancel{\partial}\alpha(x)\psi e^{-iq\alpha(x)} \quad (2.6)$$

⁹⁷ will then cancel the asymmetric term in Eq. (2.5) as required. The $U(1)$ invariant
⁹⁸ Lagrangain can therefore be constructed by adding an interaction between ψ and
⁹⁹ A_μ to Eq. (2.2). For completeness, the kinetic term for the new field A_μ is
¹⁰⁰ also added in terms of $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$, which is trivially invariant under the
¹⁰¹ transformation in Eq. (2.4). The interaction term is typically absorbed into the
¹⁰² covariant derivative $D_\mu = \partial_\mu + iqA_\mu$, thus named as it transforms in the same way as
¹⁰³ the field ψ . Collecting these modifications to Eq. (2.2) yields the QED Lagrangain

$$\mathcal{L}_{\text{QED}} = -\frac{1}{4}F_{\mu\nu}F^{\mu\nu} + \bar{\psi}(iD^\mu - m)\psi. \quad (2.7)$$

¹⁰⁴ The quadratic term $A_\mu A^\mu$ is not invariant and therefore the field A_μ must be
¹⁰⁵ massless. Requiring invariance under local $U(1)$ gauge transformations necessitated
¹⁰⁶ the addition of a new field A_μ , interpreted as the photon field, which interacts with
¹⁰⁷ charged matter. In the SM, the QED Lagrangian is absorbed into the electroweak
¹⁰⁸ sector, discussed in Section 2.1.3.

¹⁰⁹ 2.1.2 Quantum Chromodynamics

¹¹⁰ Quantum Chromodynamics (QCD) is the study of quarks, gluons and their interactions.
¹¹¹ Quarks and gluons carry colour charge, which comes in three kinds, called
¹¹² red, green and blue. While the $U(1)$ symmetry group in Section 2.1.1 was Abelian,
¹¹³ the QCD Lagrangian is specified by requiring invariance under transformations from
¹¹⁴ the non-Abelian $SU(3)$ group, making it a Yang-Mills theory [16] which requires the
¹¹⁵ addition of self-interacting gauge fields. The infinitesimal $SU(3)$ group generators
¹¹⁶ are given by $T_a = \lambda_a/2$, where λ_a are the eight Gell-Mann matrices. These span the
¹¹⁷ space of infinitesimal group transformations and do not commute with each other,
¹¹⁸ instead satisfying the commutation relation

$$[T_a, T_b] = if_{abc}T_c, \quad (2.8)$$

¹¹⁹ where f_{abc} are the group's structure constants. Consider the six quark fields $q_k = q_k(x)$.
¹²⁰ Each flavour of quark q_k transforms in the fundamental triplet representation, in
¹²¹ which each component of the triplet corresponds to the colour quantum number
¹²² for red, green and blue colour charged respectively. $G_{\mu\nu}^a$ are the eight gluon field

123 strength tensors, one for each generator T_a , defined as

$$G_{\mu\nu}^a = \partial_\mu A_\nu - \partial_\nu A_\mu - g_s f^{abc} A_\mu^b A_\nu^c, \quad (2.9)$$

124 where A_μ^a are the gluon fields and g_s is the strong coupling constant. The covariant
125 derivative is written as

$$D_\mu = \partial_\mu + i g_s T_a A_\mu^a. \quad (2.10)$$

126 The full QCD Lagrangian is then given by

$$\mathcal{L}_{\text{QCD}} = -\frac{1}{4} G_{\mu\nu}^a G_a^{\mu\nu} + q_k (i \not{D} - m_k) q_k. \quad (2.11)$$

127 Cubic and quartic terms of the gauge fields A_μ^a appear in the Lagrangian, leading to
128 the gluon's self interaction.

129 The QCD coupling constant g_s varies, or “runs”, with energy. At lower energy
130 scales (and corresponding larger distance scales) the interaction is strong. This
131 leads to quark confinement, whereby an attempt to isolate individual colour-charged
132 quarks requires so much energy that additional quark-antiquark are produced. At
133 higher energy scales (and corresponding smaller distance scales), asymptotic freedom
134 occurs as the interactions become weaker, allowing perturbative calculations to be
135 performed. Hadrons are bound states of quarks. They are invariant under $SU(3)$
136 gauge transformations (i.e. are colour-charge neutral, or *colourless*).

137 2.1.3 The Electroweak Sector

138 The weak and electromagnetic forces are unified in the Glashow-Weinberg-Salam
139 (GWS) model of electroweak interaction [17–19]. The Lagrangian is specified by
140 requiring invariance under the symmetry group $SU(2)_L \otimes U(1)_Y$, as motivated by a
141 large amount of experimental data. Here, $SU(2)_L$ is referred to as weak isospin and
142 $U(1)_Y$ as weak hypercharge.

- 143 The generators of $SU(2)_L$ are $T_a = \sigma_a/2$, where σ_a are the three Pauli spin matrices
144 which satisfy the commutation relation

$$[T_a, T_b] = i\varepsilon_{abc}T_c. \quad (2.12)$$

- 145 The generator of $U(1)_Y$ is $Y = 1/2$. Each generator corresponds to a gauge field,
146 which, after symmetry breaking (discussed in Section 2.2), give rise to the massive
147 vector bosons, W^\pm and Z , and the massless photon. The massive vector bosons
148 are the carriers of the weak force. Due to the mass of the force carriers, the weak
149 force has a short range and so it appears weak even though its intrinsic strength is
150 comparable to that of QED.

- 151 The charge operator Q can be written as a combination of the third $SU(2)_L$ generator
152 and the $U(1)_Y$ generator as in

$$Q = T_3 + Y. \quad (2.13)$$

- 153 The weak force violates parity conservation [20–22], i.e. invariance under parity
154 transformations (mirror reflections). Only left handed fermions participate in the
155 weak interaction. Since there is no other force through which neutrinos interact with
156 other particles, there are no right handed neutrinos in the standard model.

157 2.2 The Higgs Mechanism

- 158 The Brout-Englert-Higgs mechanism (henceforth just “Higgs mechanism”) is the
159 mechanism through which the fundamental particles of the SM acquire mass [10–12].
160 Experimentally it was known that the weak force had a weak effective strength,
161 which was suggestive of a massive mediating gauge particle. However, directly
162 adding mass to the weak gauge bosons violates the non-Abelian symmetry of the
163 SM. Instead, the gauge bosons can gain mass through the interaction with a scalar
164 Higgs field which results from the spontaneous breakdown of symmetry as discussed
165 in Section 2.2.1. Similarly, the Higgs mechanism gives mass to the fermions, as
166 discussed in Section 2.2.2. Section 2.2.3 described some basic phenomenology of the
167 Higgs particle relevant to hadron colliders.

¹⁶⁸ 2.2.1 Electroweak Symmetry Breaking

¹⁶⁹ Spontaneous symmetry breaking (SSB) is a key part of the Higgs mechanism. It
¹⁷⁰ is the transition of a physical system from a state of manifest symmetry to a state
¹⁷¹ of hidden, or *broken*, symmetry. In particular, this applies to physical systems
¹⁷² where the Lagrangian observes some symmetry, but the lowest energy vacuum states
¹⁷³ do not exhibit that same symmetry. In other words, the symmetry is broken for
¹⁷⁴ perturbations around the vacuum state.

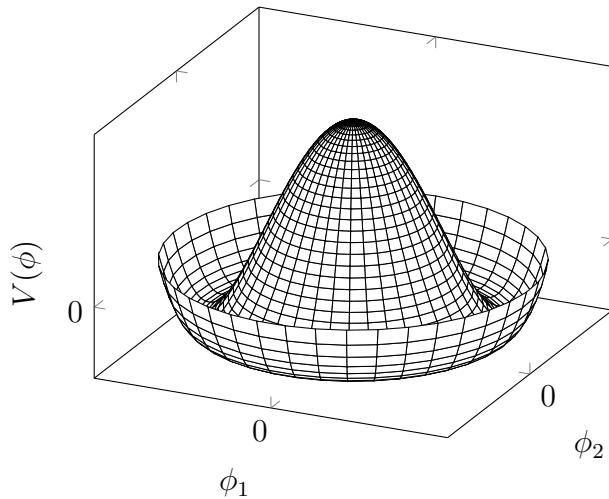


Figure 2.1: The Higgs potential $V(\phi)$ of the complex scalar field singlet $\phi = \phi_1 + i\phi_2$, with a choice of $\mu^2 < 0$ leading to a continuous degeneracy in the true vacuum states. A false vacuum is present at the origin. The SM Higgs mechanism relies on a complex scalar doublet with a corresponding 5-dimensional potential.

¹⁷⁵ Consider gauge fields from the local $SU(2)_L \otimes U(1)_Y$ symmetry group discussed in
¹⁷⁶ Section 2.1.3 coupled to a complex scalar field $\phi = \phi(x)$. The scalar field ϕ transforms
¹⁷⁷ as a weak isospin doublet. Omitting the kinetic term of the gauge fields, and writing
¹⁷⁸ $\phi^2 \equiv \phi^\dagger \phi$, the Lagrangian is

$$\mathcal{L}_{\text{Higgs}} = (D_\mu \phi)^\dagger (D^\mu \phi) - [\mu^2 \phi^2 + \lambda \phi^4], \quad (2.14)$$

¹⁷⁹ where the covariant derivative is given by

$$D_\mu = \partial_\mu + igA_\mu^a T^a + ig' B_\mu, \quad (2.15)$$

and T^a are the generators of $SU(2)$. The potential term $V(\phi)$ is made up of a quadratic and quartic term in the scalar field ϕ , which each contain an arbitrary parameter, respectively λ and μ . The quartic term gives the field self-interaction, and cannot be negative as this would lead to a potential that was unbounded from below. The quadratic term can be positive or negative. In the case where the quadratic term is positive, it is interpreted as a mass term for the scalar field. By choosing $\mu^2 < 0$ the field becomes unphysical due to its negative mass. In order to obtain a physical interpretation of the Lagrangian in Eq. (2.14) for the case where $\mu^2 < 0$, the field ϕ is expanded around the vacuum state. The vacuum expectation value (VEV) is the expected value of the field ϕ which minimises the potential $V(\phi)$ (equivalently the expected value of the field operator ϕ when the system is in a vacuum state, $|\langle \phi \rangle_0|^2 \equiv |\langle 0 | \phi | 0 \rangle|^2 \equiv \phi_0^2$). Minimising the potential gives a VEV of

$$\phi_0^2 = -\mu^2/\lambda = v^2. \quad (2.16)$$

Due to the shape of the potential in Fig. 2.1, there is a degeneracy in the direction that the complex doublet ϕ points. As all the different vacuum states minimise the potential and therefore yield identical physics, one can arbitrarily choose the state to lie along the second component of the doublet. Application of Eq. (2.13) shows this choice is manifestly invariant under the charge operator. This allows the identification of the unbroken subgroup $U(1)_Q$, under which the ground state is invariant. The generator of $U(1)_Q$ is the charge operator Q .

Adding the particle content back to the theory by expanding the field around the vacuum state, and making a transformation to the unitary gauge to remove unphysical Nambu-Goldstone modes (which arise in the context of global symmetries [23, 24]), yields

$$\phi = \frac{1}{\sqrt{2}} \begin{bmatrix} 0 \\ v + H \end{bmatrix}, \quad (2.17)$$

where H is a real scalar field, the *true vacuum* Higgs field. Substituting this into Eq. (2.14) and identifying physical fields from the quadratic terms of linear combinations of unphysical fields, one can write the physical fields W_μ^\pm , Z_μ and A_μ

206 in terms of the original fields A_μ^a and B_μ . This gives

$$W_\mu^\pm = \frac{1}{\sqrt{2}}(A_\mu^1 \mp iA_\mu^2) \quad \begin{bmatrix} A_\mu \\ Z_\mu \end{bmatrix} = \begin{bmatrix} \cos \theta_W & \sin \theta_W \\ -\sin \theta_W & \cos \theta_W \end{bmatrix} \begin{bmatrix} B_\mu \\ A_\mu^3 \end{bmatrix}. \quad (2.18)$$

207 where θ_W is the weak mixing angle defined by

$$\cos \theta_W = \frac{g}{\sqrt{g^2 + g'^2}}. \quad (2.19)$$

208 The corresponding masses of the now massive vector bosons can be read off as

$$m_W = \frac{1}{2}gv \quad m_Z = \frac{m_W}{\cos \theta_W}, \quad (2.20)$$

209 while the photon remains massless. The Higgs mass is $m_H = v\sqrt{\lambda} = \mu$.

210 This is the Higgs mechanism. It maintains the renormalisability and unitarity of
211 the SM whilst allowing the weak vector bosons to acquire mass. In summary, an
212 unphysical complex scalar field ϕ with a nonzero VEV leads to spontaneous symmetry
213 breaking. Due to the non-Abelian symmetry breaking, would-be massless Nambu-
214 Goldstone modes, which arise after expansion around the true vacuum state, are
215 exactly cancelled out by making a local gauge transformation to the unitary gauge,
216 and instead are absorbed by the vector bosons, allowing them to acquire mass.

217 This sector of the SM contains four fundamental parameters that must be determined
218 from experiment. These can be specified by the Lagrangian parameters g , g' , v
219 and λ or the physically measurable parameters m_Z , $\sin \theta_W$, m_H and e . In the
220 local neighbourhood around the true vacuum, the macroscopic symmetry of the
221 system is not realised, and therefore the physical particles do not obey the original
222 symmetry. However, information about the symmetry is retained through some
223 additional constraints on the parameters of the theory. Prior to symmetry breaking,
224 the potential contained two terms and two constants. After symmetry breaking
225 there are three terms but still only two constants that relate these terms. This is the
226 vestige of the original symmetry.

227 Spontaneous symmetry breaking has modified the original symmetry group of the SM
228 $SU(2)_L \times U(1)_Y \rightarrow SU(3)_C \otimes U(1)_Q$. Three broken generators from the symmetry
229 group $SU(2)_L \times U(1)_Y$ have been absorbed into the definition of the physical weak

230 vector bosons, giving them mass. The same methodology can be used to generate
231 the fermion masses, as shown in the next section.

232 2.2.2 Fermionic Yukawa Coupling

233 Adding the masses of the fermions by hand breaks the gauge invariance of the
234 theory. Instead, we can use a Yukawa coupling between the fermion fields and the
235 Higgs field in order to generate mass terms after spontaneous electroweak symmetry
236 breakdown [18]. In this way, the fermion masses are determined by both the respective
237 couplings to the Higgs field and the VEV of the Higgs field itself, which sets the
238 basic mass scale of the theory.

239 The Higgs field ϕ transforms as an $SU(2)$ doublet with $Y = 1/2$, as does the left-
240 handed fermion field ψ_L . The right-handed fermion field ψ_R transforms as an $SU(2)$
241 singlet.

242 Lepton Masses

243 The renormalisable and gauge invariant coupling between a fermionic field ψ and a
244 scalar Higgs field ϕ can be written as

$$\mathcal{L}_{\text{Yukawa}} = -g_f(\bar{\psi}_L \phi \psi_R + \bar{\psi}_R \phi^\dagger \psi_L). \quad (2.21)$$

245 where $\psi_L = (\nu_L, e_L)$ and $\psi_R = e_R$ for the first generation leptons. After spontaneous
246 symmetry breaking (see Section 2.2.1), the scalar Higgs field in unitary gauge
247 Eq. (2.17) consists of a VEV and the true vacuum Higgs field H . Substituting this
248 in to Eq. (2.21) yields

$$\mathcal{L}_{\text{Yukawa}} = -\frac{v g_e}{\sqrt{2}} \bar{e} e - \frac{g_e}{\sqrt{2}} \bar{e} H e, \quad (2.22)$$

249 using $\bar{e} e = (\bar{e}_L + \bar{e}_R)(e_L + e_R) = \bar{e}_L e_R + \bar{e}_R e_L$. The VEV component of ϕ provides
250 the first term in Eq. (2.22) which is quadratic in the electron field, and can therefore
251 be identified as the electron mass term. An interaction term between the electron
252 field e and the true vacuum Higgs field H is also present. Mass is generated for the
253 other lepton generations in the same way.

254 **Quark Masses**

255 The down-type quarks acquire their mass analogous to the leptons, with $\psi_L = (u_L, d_L)$
256 and $\psi_R = d_R$ for the first quark generation. Mass is generated for the up-type quarks
257 using the conjugate field to ϕ which transforms under $SU(2)$ as a doublet with
258 $Y = -1/2$. The conjugate field $\tilde{\phi}$ is constructed as

$$\tilde{\phi} = i\sigma_2 \phi^\dagger = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} \begin{bmatrix} \phi_1^\dagger \\ \phi_2^\dagger \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} v + H \\ 0 \end{bmatrix}, \quad (2.23)$$

259 and transforms in the same way as ϕ . This field can be used to write an additional
260 Yukawa coupling which provides mass for the up-type quarks in a similar way as
261 before.

$$\mathcal{L}_{\text{Yukawa}}^{\text{up}} = -g_q (\bar{\psi}_L \tilde{\phi} \psi_R + \bar{\psi}_R \tilde{\phi}^\dagger \psi_L) \quad (2.24)$$

262 Considering the first generation of up-type quarks with $\psi_L = (u_L, d_L)$ and $\psi_R = u_R$,
263 substitution into Eq. (2.24) yields

$$\mathcal{L}_{\text{Yukawa}}^{\text{up}} = -\frac{vg_u}{\sqrt{2}} \bar{u}u - \frac{g_u}{\sqrt{2}} \bar{u}Hu. \quad (2.25)$$

264 The Yukawa terms mix quarks of different generations of lepton and quark. Physical
265 particles are detected in their mass eigenstates q , which diagonalise the mass matrix,
266 but interact via the weak interaction according to their weak eigenstates \tilde{q} , which
267 are superpositions of the mass eigenstates. This feature of the weak sector leads to
268 mixing between different generations of quarks and leptons. Quark mixing can be
269 expressed using the Cabibbo-Kobayashi-Maskawa (CKM) matrix, which specifies the
270 strength of flavour-changing weak currents. The entries in the matrix are enumerated
271 as

$$\begin{bmatrix} \tilde{d} \\ \tilde{s} \\ \tilde{b} \end{bmatrix} = \begin{bmatrix} V_{ud} & V_{us} & V_{ub} \\ V_{cd} & V_{cs} & V_{cb} \\ V_{td} & V_{ts} & V_{tb} \end{bmatrix} \begin{bmatrix} d \\ s \\ b \end{bmatrix}, \quad (2.26)$$

272 where the size of the elements $|V_{pq}|^2$ measures the probability of a transition between
273 states p and q .

²⁷⁴ 2.2.3 Higgs Sector Phenomenology

²⁷⁵ As previous discussed in this section, the Higgs field plays a key role in the SM,
²⁷⁶ giving mass to fundamental particles. The strength of the coupling between the
²⁷⁷ Higgs field and another particle is proportional to that particle's mass. This fact
²⁷⁸ dictates which production mechanisms and decay modes are dominant at the LHC.
²⁷⁹ The cross sections for different production mechanisms at a centre of mass energy
²⁸⁰ $\sqrt{s} = 13 \text{ TeV}$ are shown as a function of the Higgs mass m_H in Fig. 2.3. Higgs boson
²⁸¹ production occurs mainly through four modes, shown in Fig. 2.2. The dominant
²⁸² production mode is gluon-gluon fusion ($pp \rightarrow H$), which is predominantly mediated
²⁸³ by a virtual top quark loop. Vector boson fusion ($pp \rightarrow qqH$) is the second most
²⁸⁴ dominant production mechanism, in which a pair of W or Z bosons fuse to produce
²⁸⁵ a Higgs after being radiated by two quarks, which also occur in the final state. Next
²⁸⁶ most common is the associated production of a Higgs boson and a vector boson
²⁸⁷ ($pp \rightarrow VH$), in which a pair of quarks fuse to produce a single W or Z boson which
²⁸⁸ radiates a Higgs. The final of the four leading production modes is top quark fusion,
²⁸⁹ in which two gluons each radiate a quark-antiquark pair, and a quark from each pair
²⁹⁰ fuses to produce a Higgs boson.

²⁹¹ Although gluon-gluon fusion is the dominant production mode, for hadronic decays
²⁹² of the Higgs boson the associated production with a vector boson has the advantage
²⁹³ of leading to a more conspicuous final state due to the likelihood of the vector bosons
²⁹⁴ decaying leptons. Leptons provide a clean signals to detect and trigger on.

²⁹⁵ Since the Higgs boson couples proportional to mass as already mentioned, decays
²⁹⁶ to heavier particles are favoured. The branching ratios of different Higgs boson
²⁹⁷ decay modes are shown as a function of m_H in Fig. 2.4. Approximately 58% of the
²⁹⁸ time the Higgs boson decays to a pair of b -quarks, the dominant decay mode. The
²⁹⁹ next heaviest fermions are the tau lepton and the c -quark, decays to pairs of these
³⁰⁰ particles happen approximately an order of magnitude less often. Decays to pairs
³⁰¹ of vector bosons are via a virtual off shell Higgs boson only. While the $H \rightarrow \gamma\gamma$ and
³⁰² $H \rightarrow ZZ$ branching ratios are small compared with fermionic decay modes (around
³⁰³ 0.2% for $H \rightarrow \gamma\gamma$), these decay channels were instrumental in the initial discovery of
³⁰⁴ the Higgs due to the low level of background processes which mimic the final state.

³⁰⁵ This thesis presents a measurement of the Higgs bosons production rate using events
³⁰⁶ with a Higgs boson produced in association with vector boson and decaying to a pair

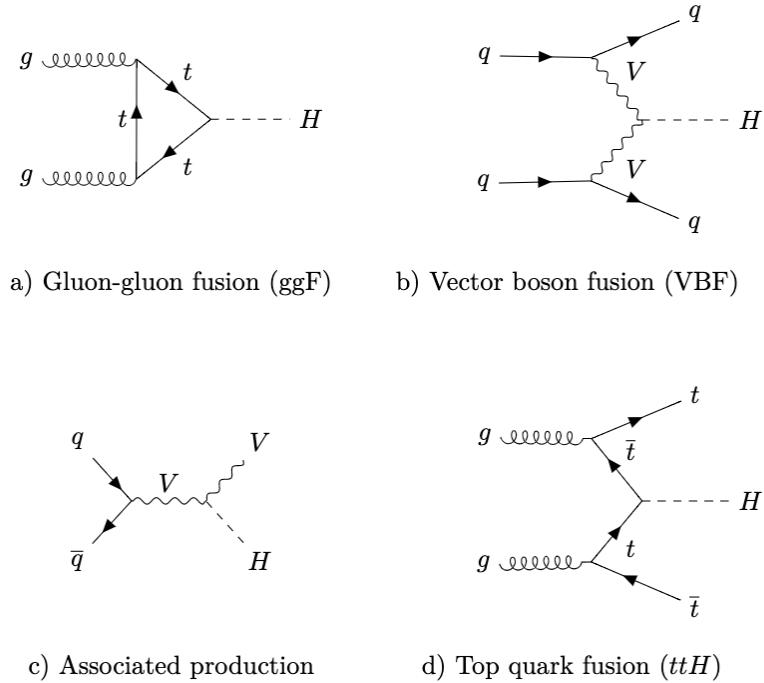


Figure 2.2: Diagrams for the four main Higgs boson production modes at the LHC for a Higgs mass $m_H = 125$ GeV at a centre of mass energy $\sqrt{s} = 13$ TeV.

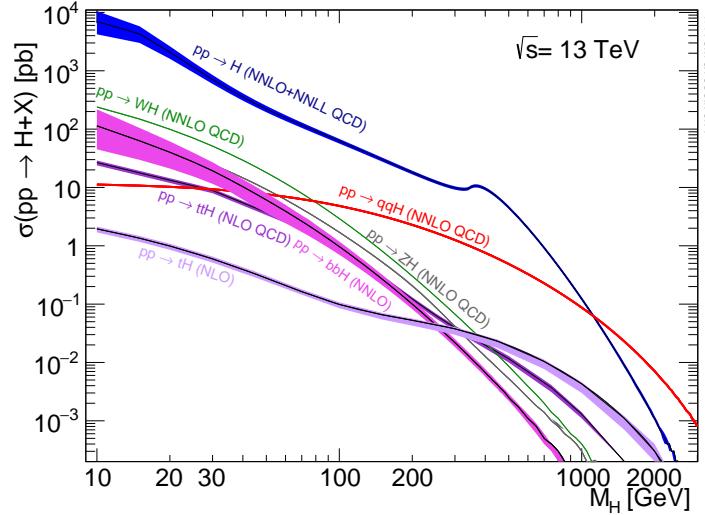


Figure 2.3: Higgs boson production cross sections as a function of Higgs mass (m_H) at $\sqrt{s} = 13$ TeV [25]. Uncertainties are shown in the shaded bands. At $m_H = 125$ GeV, Higgs boson production is dominated by gluon-gluon fussion, vector boson fusion, associated production with vector bosons, and top quark fusion.

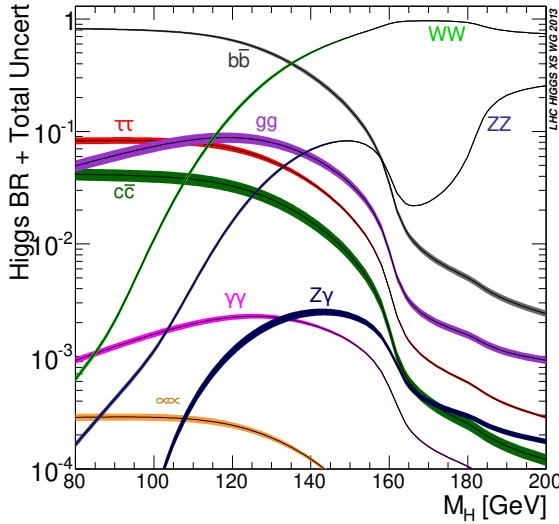


Figure 2.4: Higgs boson branching ratios as a function of Higgs mass (m_H) at $\sqrt{s} = 13 \text{ TeV}$ [25]. Uncertainties are shown in the shaded bands. At $m_H = 125 \text{ GeV}$, the Higgs predominantly decays to a pair of b -quarks, around 58% of the time. The leading subdominant decay mode is to a pair of W bosons.

of b -quarks, i.e. $pp \rightarrow VH(bb)$. The $H \rightarrow b\bar{b}$ decay mode directly probes the Higgs coupling to the second generation fermions, and more specifically to the bottom quark. This coupling was first observed in 2018 [26, 27]. Ongoing work measuring the coupling strengths, in particular in the high energy regime, is the focus of the analysis presented in this thesis in Chapter 7.

₃₁₂ Chapter 3

₃₁₃ The Large Hadron Collider and the
₃₁₄ ATLAS Detector

₃₁₅ Since the completion of its construction in 2008, the Large Hadron Collider (LHC) [28]
₃₁₆ at CERN has extended the frontiers of particle physics through its unprecedented
₃₁₇ energy and luminosity. The LHC accelerates protons around a 27 km ring until they
₃₁₈ are travelling just 3 m s^{-1} slower than the speed of light, at which point they
₃₁₉ are made to collide. The protons travel round the ring 11,000 times per second in
₃₂₀ two concentric beams, which are guided by superconducting magnets cooled using
₃₂₁ liquid helium to -271.3°C (1.9 K). The beams travel in opposite directions around
₃₂₂ the ring and are crossed at four locations so that collisions between protons can
₃₂₃ take place. Around these collision points four specialised detectors, ALICE [29],
₃₂₄ CMS [30], LHCb [31] and ATLAS [32], are located to capture information about the
₃₂₅ products of the collisions.

₃₂₆ In this chapter, a brief overview of the LHC and the accelerator complex at CERN
₃₂₇ is given in Section 3.1. The coordinate system used at the ATLAS detector and
₃₂₈ other common definitions are introduced in Section 3.2. Next, an overview of the
₃₂₉ different detector systems is provided in Section 3.3, and finally descriptions of
₃₃₀ various commonly used reconstructed objects is given in Section 3.4.

3.1 The Large Hadron Collider

The LHC is operated in multi-year *runs* during which beams of protons are circulated and collided. Between runs there are periods of shutdown while the accelerator and detector machinery is maintained and upgraded. Run 1 began in 2010 when the LHC collided proton bunches, each containing more than 10^{11} particles, 20 million times per second, providing 7 TeV proton-proton collisions at instantaneous luminosities of up to $2.1 \times 10^{32} \text{ cm}^{-2} \text{ s}^{-1}$. The centre-of-mass energy was increased to 8 TeV towards the end of Run 1 in 2012. Run 2, which spanned in 2015–2018, further increased the the proton-proton collision energy to 13 TeV. During Run 2 the bunch spacing was reduced, leading to a collision rate of 40 MHz. Over the course of Run 2 a total usable integrated luminosity of 139 fb^{-1} was recorded. 2022 marked the beginning of Run 3 which, with a higher center of mass energy and peak luminosity, is expected to culminate in the approximate tripling of the dataset size. A summary of key information about each run is listed in Table 3.1.

Period	Year	\sqrt{s} [TeV]	$\langle\mu\rangle$	Bunch spacing [ns]	Luminosity [$\text{cm}^{-2} \text{ s}^{-1}$]
Run 1	2010–2012	7–8	18	50	8×10^{33}
Run 2	2015–2018	13	34	25	$1\text{--}2 \times 10^{34}$
Run 3	2022–2025	13.6	50	25	2×10^{34}

Table 3.1: Overview of the different LHC runs [33,34]. The average number of interactions per bunch-crossing is denoted as $\langle\mu\rangle$ (see Section 3.2.3), and is here averaged over the entire run. Numbers for Run 3 are preliminary and are only provided to give an indication of expected performance.

An overview of the accelerator complex at CERN is shown in Fig. 3.1. The LHC is at the final stage of a chain of accelerators which incrementally step-up the energy of incoming protons. The first accelerator is Linac4, a linear accelerator which accelerates negative hydrogen ions to an energy of 160 MeV. Upon leaving Linac4, the ions are stripped of both electrons and the resulting protons are fed into the Proton Synchrotron Booster (PSB), which increases the energy of the protons to 2 GeV. The protons leaving the PSB are passed to the Proton Synchrotron (PS), which increases the energy to 26 GeV, and then from the PS to the Super Proton Synchrotron (SPS) which further increases the energy to 450 GeV. Finally, the proton

354 beams are injected in the LHC where they are accelerated to their final energy of
 355 6.5 TeV (for Run 2).

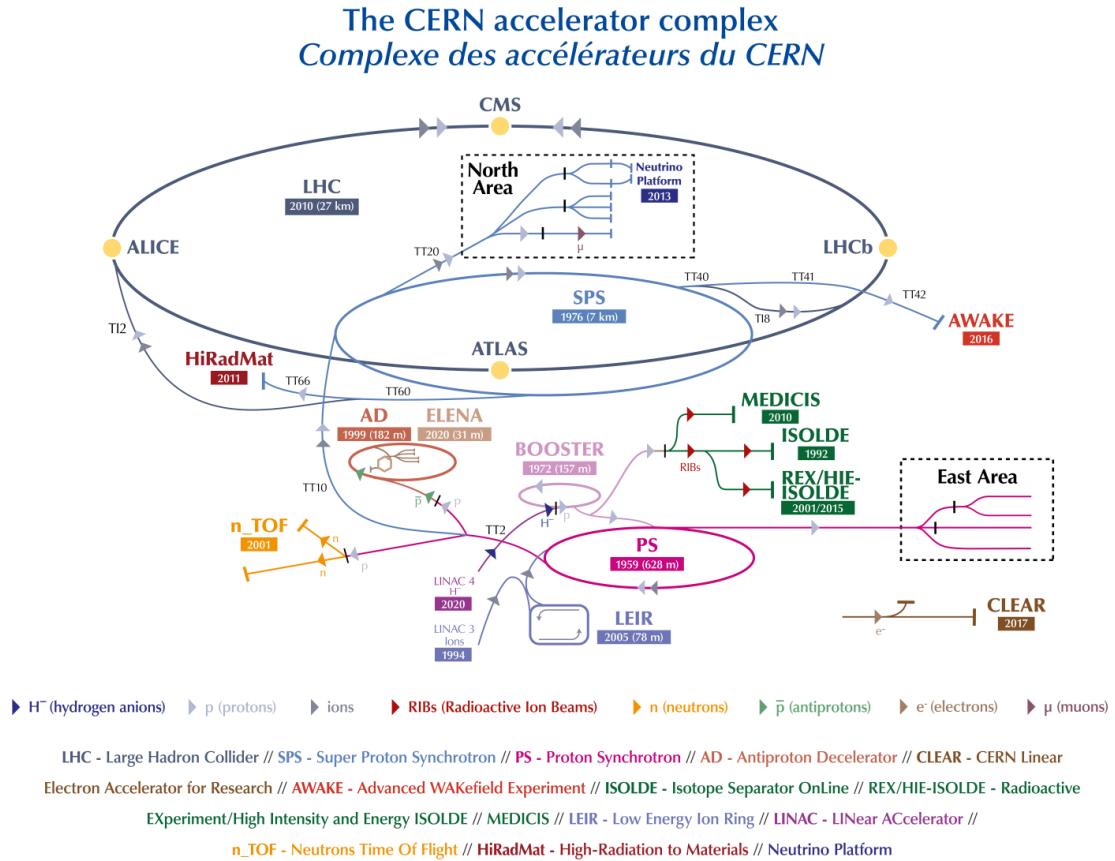


Figure 3.1: An overview of the CERN accelerator complex [35]. The LHC is fed by a series of accelerators starting with Linac4. Next are the Proton Synchrotron Booster, the Proton Synchrotron, and finally the Super Proton Synchrotron which injects protons into the LHC.

356 3.2 Coordinate System & Collider Definitions

357 In Section 3.2.1, the coordinate system used at ATLAS is introduced. The parameter-
 358 isation used for the specifying the trajectory of charged particle tracks is described in
 359 Section 3.2.2, and definitions for some frequently occurring concepts and quantities
 360 is provided in Section 3.2.3.

361 3.2.1 ATLAS Coordinate System

362 The origin of the coordinate system used by ATLAS is the nominal interaction point
 363 in the centre of the detector. As shown in Fig. 3.2, the z -axis points along the
 364 direction the beam pipe, while the x -axis points from the interaction point to the
 365 centre of the LHC ring, and the y -axis points upwards. The transverse plane lies
 366 in x - y while the longitudinal plane lies along the z -axis. A cylindrical coordinate
 367 system with coordinates (r, ϕ) is used in the transverse plane, where r is the radius
 368 from the origin and ϕ is the azimuthal angle around the z -axis.

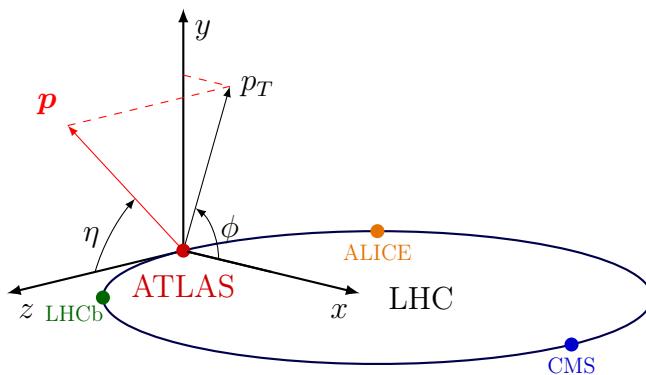


Figure 3.2: The coordinate system used at the ATLAS detector, showing the locations of the four main experiments located at various points around the LHC. The 3-vector momentum $\mathbf{p} = (p_x, p_y, p_z)$ is shown by the red arrow. Reproduced from Ref. [36].

369 The polar angle θ is commonly specified in terms of the pseudorapidity η , defined as

$$\eta = -\ln \left[\tan \left(\frac{\theta}{2} \right) \right]. \quad (3.1)$$

370 The pseudorapidity is a convenient quantity to work with as differences in η are
 371 invariant under Lorentz boosts. In addition, particle production is constant as a
 372 function of η .

373 The transverse momentum p_T of an object is the sum in quadrature of the momenta
 374 in the transverse plane

$$p_T = \sqrt{p_x^2 + p_y^2}. \quad (3.2)$$

³⁷⁵ Angular distance between two objects is measured in units of ΔR and is defined as
³⁷⁶ the sum in quadrature of the η and ϕ displacements

$$\Delta R = \sqrt{(\Delta\eta)^2 + (\Delta\phi)^2}. \quad (3.3)$$

³⁷⁷ 3.2.2 Track Parameterisation

³⁷⁸ The trajectories of charged particle tracks are parameterised as a helix which is
³⁷⁹ fully specified using five parameters: $(d_0, z_0, \phi, \theta, q/p)$. Transverse and longitudinal
³⁸⁰ impact parameters (IP) d_0 and z_0 specify the closest approach of the trajectory of
³⁸¹ a particle to the origin. The transverse IP d_0 and longitudinal IP z_0 are measured
³⁸² with respect to the hard scatter primary vertex (see Section 3.4.2). ϕ and θ are
³⁸³ the azimuthal and polar angles respectively, and q/p is the measured charge on the
³⁸⁴ track¹ divided by the scalar 3-momentum. Fig. 3.3 shows each of these parameters
³⁸⁵ diagrammatically.

³⁸⁶ Impact parameter significances are defined as the IP divided by its corresponding
³⁸⁷ uncertainty, $s(d_0) = d_0/\sigma(d_0)$ and $s(z_0) = z_0/\sigma(z_0)$. When used in flavour tagging
³⁸⁸ (see Chapter 4), track IP significances are lifetime signed according to the track's
³⁸⁹ direction with respect to the jet axis and the primary vertex [38]. The sign IP
³⁹⁰ significances is positive if the track crosses the jet axis in front of the primary vertex
³⁹¹ and negative if the crossing is behind the primary vertex.

³⁹² 3.2.3 Hadron Collider Definitions

³⁹³ Cross Section

³⁹⁴ The cross section σ is closely related to the probability of an interaction between
³⁹⁵ two colliding particles, and is analogous to an effective cross-sectional area of the
³⁹⁶ particles. The cross section of a process depends on the transition matrix element,
³⁹⁷ obtained using the Feynman rules of the theory which are derived using QFT, and a
³⁹⁸ phase space integral. At hadron colliders such as the LHC, the proton-proton cross

¹Reconstructed charged particles are assumed to have a charge of ± 1 .

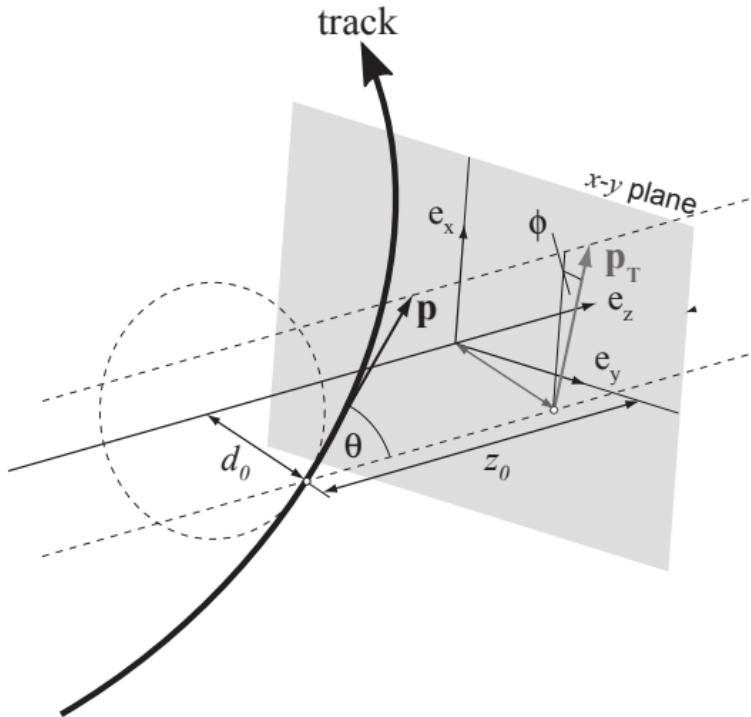


Figure 3.3: The track parameterisation used at the ATLAS detector. Five coordinates ($d_0, z_0, \phi, \theta, q/p$) are specified, defined at the track's point of closest approach to the nominal interaction point at the origin of the coordinate system. The figure shows the three-momentum \mathbf{p} and the transverse momentum p_T (defined in Eq. (3.2)). The basis vectors e_x, e_y and e_z are also shown. Reproduced from Ref. [37].

³⁹⁹ section can be factorised as

$$\sigma(pp \rightarrow X) \approx \text{PDFs} \cdot \text{partonic cross section.} \quad (3.4)$$

⁴⁰⁰ The partonic cross section can be calculated at sufficiently high energies such as
⁴⁰¹ those found at the LHC, while the parton distribution functions (PDFs) have to be
⁴⁰² extracted from experimental results.

⁴⁰³ Luminosity

⁴⁰⁴ The total number of proton-proton collisions N is related to the total pp cross σ
⁴⁰⁵ section by the integrated luminosity L , as in

$$N = \sigma L = \sigma \int \mathcal{L} dt. \quad (3.5)$$

⁴⁰⁶ The instantaneous luminosity \mathcal{L} relates the cross section to the number of collisions
⁴⁰⁷ per unit time. For two colliding bunched proton beams, it is defined as

$$\mathcal{L} = \frac{1}{\sigma} \frac{dN}{dt} = \frac{fn_1 n_2}{4\pi \sigma_x \sigma_y}, \quad (3.6)$$

⁴⁰⁸ where n_1 and n_2 are the number of protons in the colliding bunches, f is the bunch
⁴⁰⁹ crossing frequency, and σ_x and σ_y are the rms width of the beam in the horizontal
⁴¹⁰ and vertical directions.

⁴¹¹ The total luminosity recorded over the course of Run 2 is shown in Fig. 3.4. In
⁴¹² total, 139 fb^{-1} of usable physics data was collected over the three-year run. The
⁴¹³ uncertainty on the total integrated luminosity is 1.7% [39].

⁴¹⁴ Pile-up

⁴¹⁵ At the centre of the ATLAS detector, bunches of more than 10^{11} protons meet at a
⁴¹⁶ small crossing angle. Each bunch-crossing is called an *event*. There is generally at
⁴¹⁷ most one hard proton-proton scatter per event. Additional interactions are typically
⁴¹⁸ relatively soft and are known as *pile-up*. Pile-up from interactions within the same
⁴¹⁹ bunch-crossing is known as *in-time* pile-up while residual signatures from previous
⁴²⁰ bunch-crossings is known as *out-of-time* pile-up. The number of pile-up interactions

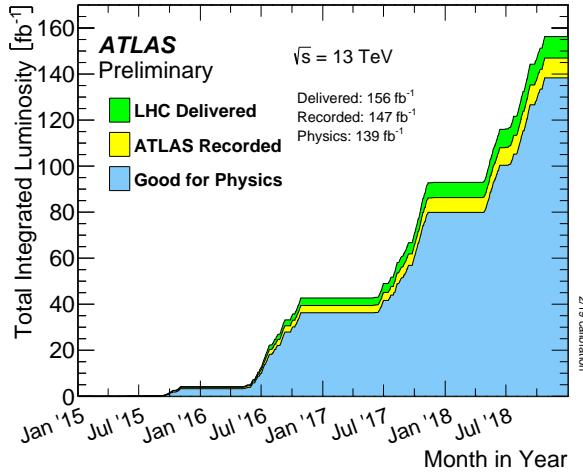


Figure 3.4: Delivered, recorded, and usable integrated luminosity as a function of time over the course of Run 2 [34]. A total of 139 fb^{-1} of collision data is labelled as good for physics, meaning all sub-detector systems were operating nominally.

is denoted μ , which is often given as a time-averaged value $\langle \mu \rangle$. Histograms showing the number of pile-up interactions over the course of Run 2 are shown in Fig. 3.5.

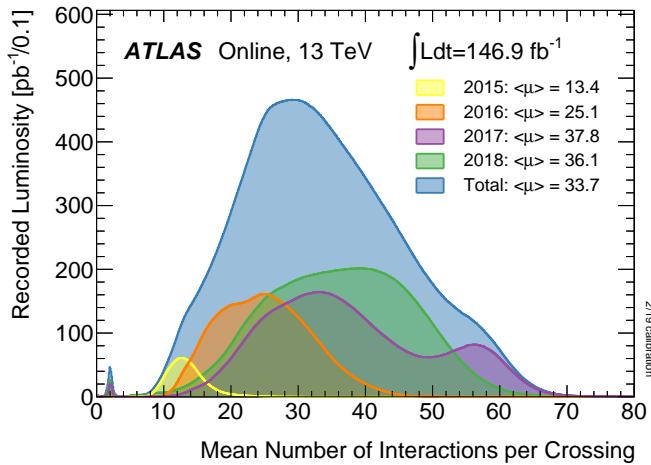


Figure 3.5: Average pile-up profiles measured by ATLAS during Run 2 [34]. Higher levels of pile-up are planned for Run 3.

423 3.3 The ATLAS Detector

424 The ATLAS² detector is made up of several specialised sub-detectors which are
425 arranged concentrically around the nominal interaction point at the centre of the
426 detector. The detector is designed to cover nearly the entire solid angle around the
427 collision point. In this section a condensed overview of each sub-detector is given, in
428 order of increasing radial distance from the point of collision. The inner tracking
429 detector is described in Section 3.3.1, the electromagnetic and hadronic calorimeters
430 in Section 3.3.2, the muon spectrometer in Section 3.3.3, and finally the trigger is
431 described in Section 3.3.4. More complete information on the detector can be found
432 in Ref. [32], while an overview of physics performance is given in [40].

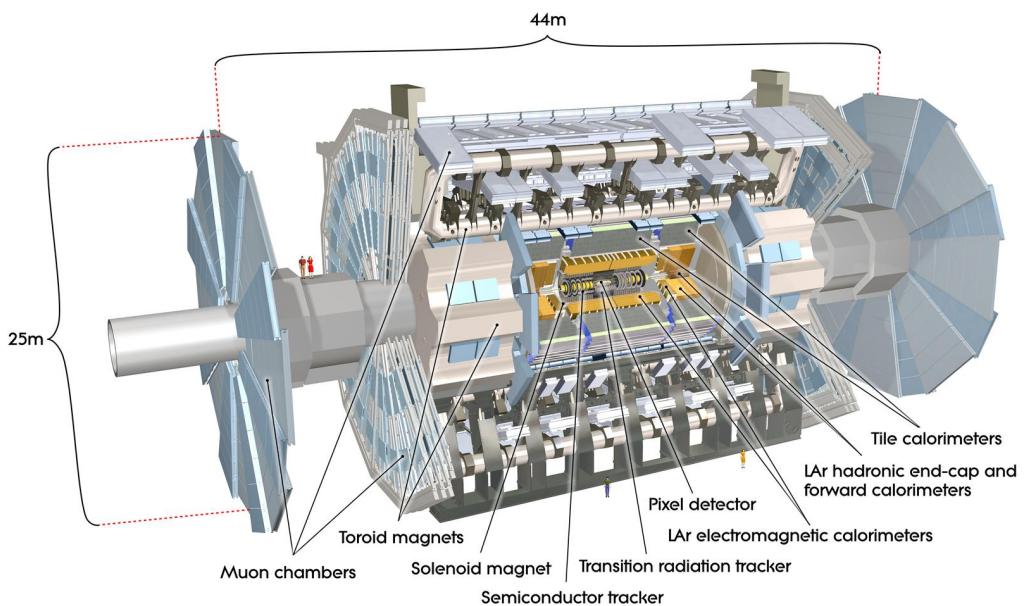


Figure 3.6: A 3D model of the entire ATLAS detector [41]. The detector is 46 m long and 25 m in diameter. Cutouts to the centre of the detector reveal the different subdetectors which are arranged in concentric layers around the nominal interaction point.

²A Toroidal LHC ApparatuS.

433 3.3.1 Inner Detector

434 The inner-detector system (ID) provides high-resolution charged particle trajectory
435 tracking in the range $|\eta| < 2.5$. The ID is immersed in a 2 T axial magnetic field,
436 produced by a superconducting solenoidal magnet, which enables the measurement
437 of particle momentum and charge. After Run 3, the ID will be replaced by the
438 ITk [42, 43].

439 The inner detector is made up of several sub-systems, shown in Figs. 3.7 and 3.8. The
440 high-granularity silicon pixel detector covers the vertex region and typically provides
441 four spacepoint measurements per track. It is followed by the silicon microstrip
442 tracker (SCT), which usually provides a further four spacepoint measurements per
443 track. These silicon detectors are complemented by the Transition Radiation Tracker
444 (TRT), which enables radially extended track reconstruction up to $|\eta| = 2.0$.

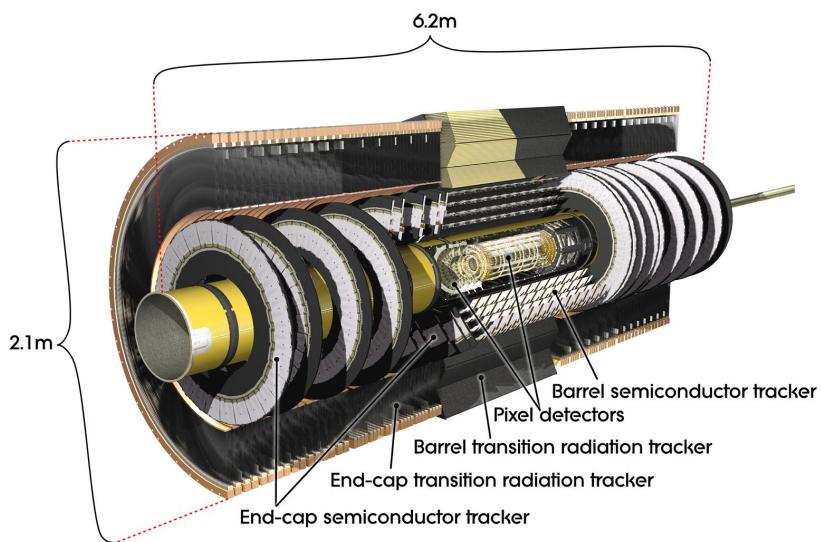


Figure 3.7: A 3D model of the ATLAS ID, made up of the pixel and SCT subdetectors, showing the barrel layers and end-cap disks [44].

445 The target inverse momentum resolution for the combined ID measurement is
446 parameterised as a function of the track transverse momentum and polar angle [40].
447 The parameterisation is given by

$$\sigma(1/p_T) = 0.36 \oplus \frac{13}{p_T \sin \theta} \text{TeV}^{-1}, \quad (3.7)$$

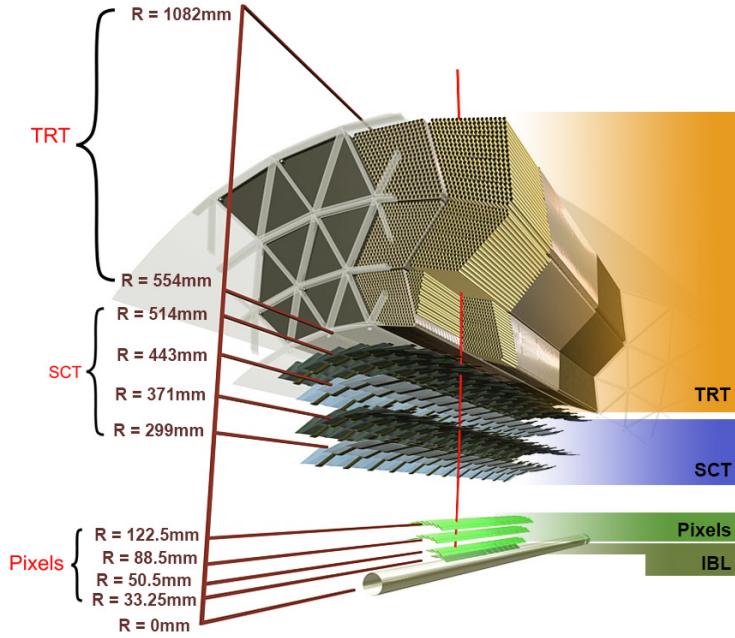


Figure 3.8: A cross-sectional view of the ATLAS ID, with the radii of the different barrel layers shown [37].

where \oplus denotes a sum in quadrature. For high- p_T tracks (e.g. $p_T \approx 100$ GeV) in the central region, $\sigma(1/p_T) \approx 0.4$ TeV $^{-1}$ corresponding to a relative error of 4%. The momentum resolution generally good enough to correctly identify the sign of the charge on particles up to the highest energies expected at the LHC. The transverse impact parameter resolution $\sigma(d_0)$ is parameterised similarly as

$$\sigma(d_0) = 11 \oplus \frac{115}{p_T \sin \theta} \mu\text{m}. \quad (3.8)$$

Pixel Detector

The silicon pixel detector is comprised of four cylindrical barrels at increasing radii from the beamline, and four disks on each side. The innermost barrel layer is the insertable B-layer (IBL), which was installed before Run 2 [45, 46] and lies approximately just 33 mm from the beam axis. The second-to-innermost layer is often referred to as the B-layer. The specification of the pixel detector determines the impact parameter resolution and the ability to reconstruct primary and secondary

vertices. The detector is required to have a high granularity (i.e. resolution) to maintain the low occupancy required to resolve nearby particles. Individual pixels are 50 μm in the transverse direction $R\phi$ and 400 μm in the longitudinal z direction (250 μm for the IBL). Cluster positions have a resolution of approximately 10 μm in $R\phi$ and 100 μm in z .

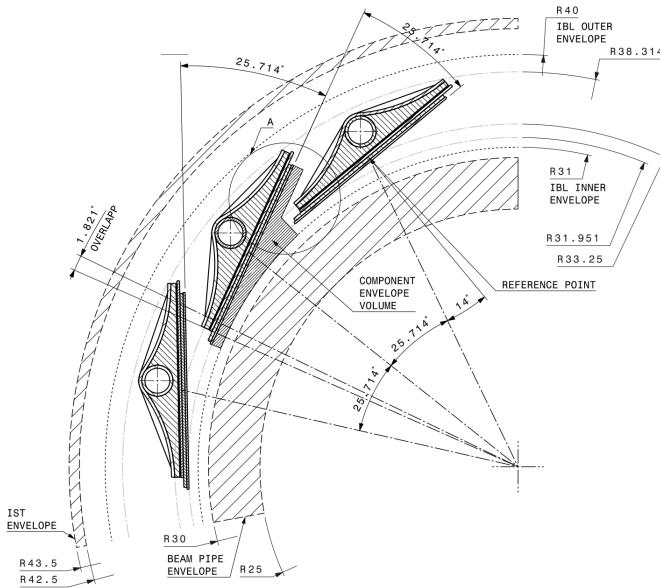


Figure 3.9: A schematic cross-sectional view of the ATLAS IBL [45].

465 Semi-Conductor Tracker (SCT)

466 The SCT is made up of four concentric barrel layers in the central region, and nine
 467 disks in each end-cap. Each layer is itself made of a pair of silicon microstrip layers,
 468 with a small stereo angle (20 mrad) between the two layers enabling the z -coordinate
 469 to be measured from a pair of strip measurements. The SCT typically provides four
 470 precision spacepoint measurements (eight strip measurements) per track in the barrel
 471 region. These have intrinsic uncertainties of 17 μm in the transverse direction $R\phi$, and
 472 580 μm in the longitudinal direction z [47]. The measurements provide a contribution
 473 to the measurement of charged particle momentum and impact parameter, along
 474 with vertex position. Charge-particle tracks can be distinguished if separated by
 475 more than $\sim 200 \mu\text{m}$.

476 Transition Radiation Tracker (TRT)

477 The TRT is a straw-tube tracker which complements the higher-resolution silicon-
478 based tracks by offering a larger number of hits per track (typically around 30) and
479 a long lever arm, which aids the accurate measurement of particle momentum. It is
480 made up of approximately 300 000 drift tubes with a diameter of 4 mm which are filled
481 with an argon/xenon gas mixture. The walls of each tube are electrically charged,
482 and a thin conducting wire runs along the center. When a charged particle traverses
483 a tube, it ionises the gas and the resulting liberated electrons drift along the electric
484 field to the wire, where an associated charge is registered. In the barrel the straws
485 run parallel to the z -axis and therefore the TRT only provides tracking information
486 in $R\phi$. Straws are arranged radially in the end-caps. The resulting two-dimensional
487 spacepoints have a resolution of approximately 120 μm . The spaces between the
488 straws are filled with a polymer which encourages the emission of transition radiation,
489 aiding electron identification.

490 3.3.2 Calorimeters

491 The calorimeter system measures the energy of incident particles over the range
492 $|\eta| < 4.9$. There are two main sub-systems: the electromagnetic calorimeter (ECal),
493 which focuses on the measurement of electrons and photons, and the hadronic
494 calorimeter (HCal), which measures the energy of hadrons. Upon entering the
495 calorimeter, incident particles will interact with the detector material to produce a
496 shower of secondary particles with reduced energies. The charge deposited in this
497 process is measured to reconstruct the energy of the initial incident particle. The
498 two calorimeter sub-systems must provide strong containment of showering particles
499 to prevent punch-through of EM and non-muon particles to the HCal and muon
500 system respectively.

501 Liquid Argon (LAr) Electromagnetic Calorimeter

502 The more granular lead/liquid-argon ECal covers the region $|\eta| < 3.2$ and is split
503 into barrel (covering $|\eta| < 1.475$) and end-cap (covering $1.375 < |\eta| < 3.2$) regions.
504 EM calorimetry works by encouraging electrons and photons to interact with electri-

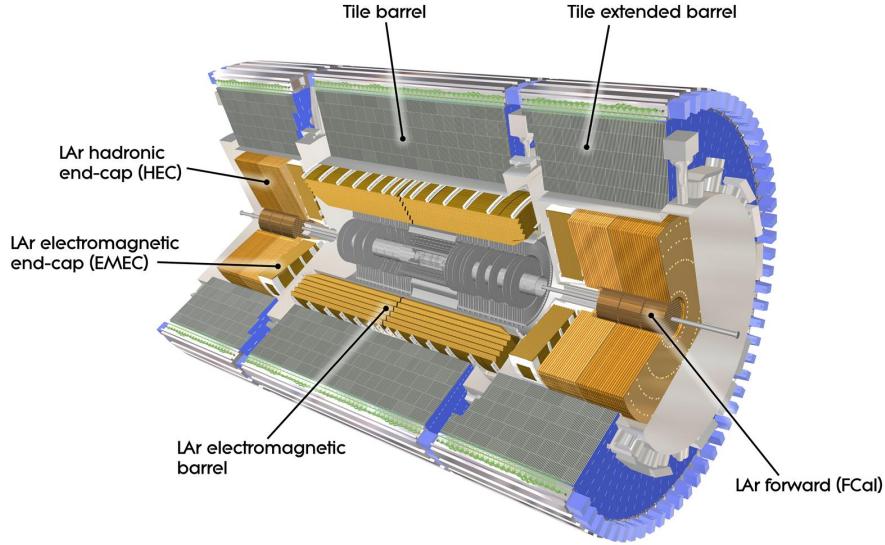


Figure 3.10: The ATLAS calorimeters [48]. The ECal uses LAr-based detectors, while the HCal uses mainly scintillating tile detectors. In the forward region the HCal also includes the LAr hadronic endcaps.

505 cally charged particles in detector material via bremsstrahlung ($e \rightarrow e\gamma$) and pair
 506 production ($\gamma \rightarrow e^+e^-$). The EM calorimeter uses lead absorber plates to initiate
 507 EM showers, resulting in secondary particles which ionise the surrounding liquid
 508 argon. The charge is collected on copper electrodes and read out. The accordion
 509 geometry of the ECal allows for a full coverage in ϕ without any azimuthal cracks.

510 The energy resolution of the LAr calorimeter is made up of a sampling and a constant
 511 term, which are summed in quadrature to produce the overall energy resolution. The
 512 sampling term contributes approximately $10\%/\sqrt{E}$, while the constant term adds an
 513 additional 0.7%. Photons with moderate transverse energy $E_T \approx 50 \text{ GeV}$ have an
 514 overall energy resolution of at most 1.6% over most of the pseudorapidity range. At
 515 lower $E_T \approx 10 \text{ GeV}$, the resolution is degraded to approximately 5%. The resolution
 516 measurements are obtained from test beam data [40].

517 Hadronic Tile Calorimeter

518 In the central barrel region with $|\eta| < 1.7$, the HCal uses a tile calorimeter with
 519 steel as an absorbing material, and scintillating tiles as the active material. Two

520 copper/liquid-argon calorimeter end-caps are also used. Incident hadrons interact
 521 via the strong and electromagnetic forces with the absorber material, mainly loosing
 522 energy due to multiple inelastic nuclear collisions. The active material captures the
 523 resulting electrons and photons to measure the energy of the incident hadron.

524 The jet energy resolution of the HCal is parameterised as a function of the jet
 525 transverse energy

$$\sigma(E_T)/E_T = 50\% \sqrt{E_T} \oplus 3\%, \quad (3.9)$$

526 corresponding to a jet energy resolution of 10% at a jet p_T of approximately 100 GeV
 527 [49].

528 3.3.3 Muon Spectrometer

529 Due to their higher mass, muons easily pass unimpeded through the ID and calorime-
 530 ters and therefore require specialised detectors for their measurement. The Muon
 531 Spectrometer (MS) is made up of dedicated tracking and triggering hardware. The
 532 precision tracking system uses three layers of monitored drift tubes with a barrel
 533 region covering $|\eta| < 1.2$ and end-caps covering $1 < |\eta| < 2.7$. The inner layers of
 534 the end-caps use cathode strip chambers to better cope with the high occupancy
 535 in the forward region. Precision tracking resolution is approximately 50 μm . The
 536 trigger system is comprised of resistive plate chambers in the barrel region covering
 537 $|\eta| < 1.0$ and thin gap chambers in the end-cap regions covering $1 < |\eta| < 2.4$. A set
 538 of three superconducting air-core toroidal magnets, each made up of eight coils, is
 539 used in each of the barrel and end-caps to deflect the muons as they pass through
 540 the MS, allowing their momentum and charge to be measured from the direction
 541 and magnitude of curvature. The toroidal magnets generate a field which is largely
 542 orthogonal to the muon trajectories which allows for maximum deflection. The
 543 transverse momentum resolution has been measured to be approximately 1.7% in the
 544 central region for low- p_T muons, increasing to 4% for high- p_T muons in the forward
 545 regions [50].

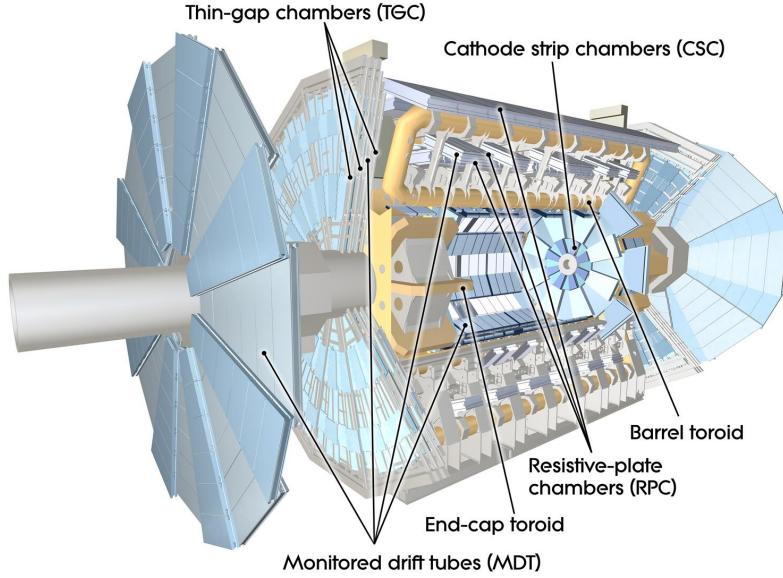


Figure 3.11: The ATLAS muon spectrometer [51].

546 3.3.4 The Trigger

547 The 25 ns bunch spacing used over the course of Run 2 corresponds to a bunch-
 548 crossing or event rate of 40 MHz (see Table 3.1). If the full information for the
 549 detector was written out for each event, this would correspond to the generation
 550 of 60 TB of data each second. This is more than can be feasibly read out from
 551 the hardware, processed and stored, requiring the use of a trigger system which
 552 quickly makes a decision about whether or not an event is potentially interesting
 553 and should be kept for further analysis. The trigger system is comprised of two
 554 levels which search for signs of electrons, muons, taus, photons, and jets, as well as
 555 events with large total or missing transverse energy. The hardware-based Level-1
 556 (L1) trigger uses coarse information from the calorimeters and MS to accept events at
 557 an average rate of 100 kHz approximately 2.5 μ s after the event. After the L1 trigger,
 558 the software-based High Level Trigger (HLT) makes use of 40 000 CPU cores to make
 559 a final selection on surviving events in approximately a few hundred milliseconds.
 560 The final event read-out rate is approximately 1.2 kHz, corresponding to 1.2 GB s^{-1}
 561 of permanent data storage. More information is provided in [52].

562 3.4 Reconstructed Physics Objects

563 Event reconstruction is the process of analysing the output from the detector to
564 determine the type and properties of particles present in an event. The reconstructed
565 event provides information about the underlying physics process that led to these
566 observable final state particles. Events passing the trigger selection (described in
567 Section 3.3.4) undergo offline reconstruction, which makes use of the full information
568 from the detector. Reconstruction and analysis of events relies on the extensive
569 ATLAS software stack, see Ref. [53] for more information.

570 Several different reconstructed objects are used for physics analyses. Objects relevant
571 to this thesis are described below.

572 3.4.1 Tracks

573 The reconstructed trajectories of charged particles are referred to as *tracks*. Track are
574 reconstructed from the energy depositions (called *hits*) left by the particles as they
575 traverse the the inner detector. Tracks are widely used for a variety of downstream
576 applications, including vertexing and jet tagging, so their accurate reconstruction
577 is a critical task. A comprehensive introduction to ATLAS tracking is available
578 in Ref. [54], while specific optimisations for dense environments are detailed in
579 Refs. [55, 56]. An overview of track reconstruction is given below.

580 Space-point Formation (Clustering)

581 When a charged particle traverses a silicon layer, charge can be collected in more
582 than one pixel or strip. This is due to the incident angle of the particles with respect
583 to the sensor, and also the drift of electrons between sensors caused by the magnetic
584 field. Clusters (also called *hits* or *space-points*) are formed by clustering neighbouring
585 pixels or strips and estimating locations of space-points using the shape and energy
586 distribution of the clusters.

587 Track Finding

588 Space-points are used to build track seeds. These are groups of three hits which
589 are geometrically compatible with being part of a track segment. A combinatorial
590 Kalman filter (KF) is used to build track candidates by extending track seeds. The
591 filter can create multiple track candidates per seed, with bifurcations along the track
592 occurring when more than one compatible space-point exists on a given layer. In
593 this way, the KF creates an excess of *track candidates*, which are only required to
594 satisfy basic quality requirements. Track candidates are allowed to reuse or *share*
595 hits freely (a single hit may be used by multiple track candidates). Typically, the
596 presence of shared hits is a predictor of a bad track due to the high granularity of
597 the ATLAS tracking detectors. At this stage, there can also be a large number of
598 incorrect hits assigned to otherwise good tracks, and additionally large number of
599 *fake* tracks, which are comprised of a majority of wrong hits and do not correspond
600 to the trajectory of any one physical particle (fake tracks are defined as those where
601 the majority of associated hits do not originate from one single truth particle, see
602 Eq. (5.8)). The low quality of tracks at this stage necessitates an ambiguity solving
603 step, in which candidates are cleaned, and the highest quality track are selected.

604 Ambiguity Solving

605 Ambiguity solving was introduced as part of the ATLAS New Tracking effort [54],
606 which was intended to improve track reconstruction performance in dense envi-
607 ronments. In the ambiguity solver, track candidates are processed individually in
608 descending order of a track score. The track score quantifies the likelihood of the
609 track corresponding to the trajectory of a real particle. Scoring uses a number of
610 variables, including the number and positions of hits (preferring hits in more precise
611 regions of the detector), the transverse momentum of the track and the track fit
612 quality. The track fit quality describes the quality of the track as the χ^2 divided
613 by the number degrees of freedom on the track. A preference for high transverse
614 momentum tracks promotes the successful reconstruction of the more physically
615 interesting energetic particles, and suppresses the large number of wrong hits assigned
616 to low momentum tracks. The ambiguity solver also penalises tracks with missing
617 hits on the innermost detector layers.

618 During the processing of a given highest-scoring track candidate, the track is cleaned
619 (whereby problematic hits are removed), and, if the resulting track satisfies the quality
620 selection criteria, a high precision fit of the track parameters using the surviving hits
621 is performed. The high precision fit makes full use of all available information, and
622 uses an updated position and uncertainty estimate for each cluster obtained from
623 a Neural Network (NN) [57]. If the track has reached this stage without rejection
624 by passing various quality regiments, it is re-scored and returned to the list of track
625 candidates. If the same track is then processed again without requiring modification,
626 it is added to the final track collection. Track candidates that fall below a certain
627 quality cut are rejected. This selection does allow for the possibility of a track having
628 small number of shared hits.

list shared
hit cut?

629 Neural Network Cluster Splitting

630 As part of track cleaning, shared hits are classified by a NN to determine if they are
631 compatible with the characteristic features of a merged cluster [55, 57]. A merged
632 cluster is one made up of a combination of energy deposits from more than one
633 particle, which have become merged due to the closeness of the associated particles
634 and the limited resolution of the detector. While in general this event is rare, it
635 is common for clusters to become merged in dense environments, as discussed in
636 Section 4.1. If the cluster is predicted to be merged it is labelled as being freely
637 shareable, or *split*. Hits not compatible with the merged hypothesis can still be
638 shared by a limited number of tracks, but come with a penalty for the track which
639 may hinder its acceptance into the final track collection.

640 Pseudotracking

641 Pseudotracking uses Monte Carlo truth information to group together all the hits
642 left by each truth particle. Each collection of hits which, as a unit, satisfies basic
643 quality requirements is directly used in a full resolution track fit. If the track fit is
644 successful, a “pseudotrack” track is created and stored. If the track fit fails, or the
645 collection of hits does not pass the basic quality requirements (for example because
646 of a lack of hits) then the particle is said to be un-reconstructable. In this way,
647 pseudotracking performance represents the ideal reconstruction performance given the

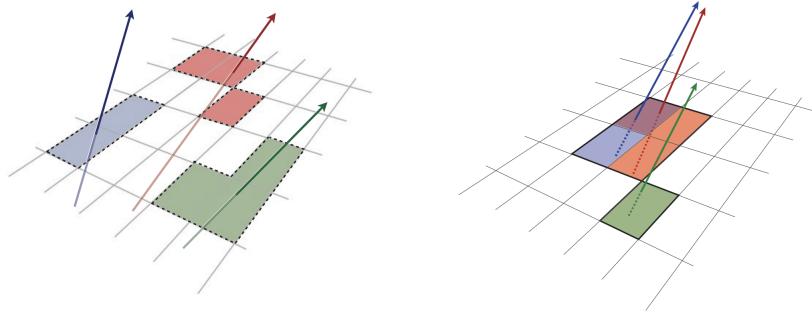


Figure 3.12: Particles (left) which have enough separation will leave charge depositions which are resolved into separate clusters. Sufficiently close particles (right) can lead to merged clusters. Their combined energy deposits are reconstructed as a single merged cluster [56].

648 ATLAS detector, with perfect hit-to-track association and and track reconstruction
 649 efficiency. The approach was introduced in Ref. [58] as a way to obtain a fast
 650 approximation of tracking reconstruction for simulated data, however the technique
 651 has become a useful tool for studying tracking performance in general [55].

652 3.4.2 Vertices

653 Groups of reconstructed tracks can be examined to determine whether the particles
 654 originated from a common spatial point of origin. This occurs when proton-proton
 655 collisions take place (primary vertices), when a particle decays or radiates, and also
 656 as a result of interaction with the detector material (secondary vertices). Vertex
 657 reconstruction is made up of two stages. First, vertex finding takes place, which
 658 is the process of grouping tracks into compatible vertices. Second, vertex fitting
 659 combines information from compatible tracks to reconstruct the physical properties
 660 of the vertex, such as mass and position.

661 Primary Vertices

662 Each proton-proton interaction happens at a *primary vertex* (PV). Primary vertices
 663 are iteratively reconstructed with tracks using the iterative vertex finder (IVF) [59].
 664 In Run 3, the IVF will be replaced with an adaptive multi-vertex finder (AMVF) [60].

665 The *hard scatter vertex* of an event is chosen as the primary vertex whose associated
666 tracks have the largest sum of transverse momentum squared, $\Sigma(p_T^2)$.

667 Secondary Vertices

668 Secondary vertices (SV) occur when a particle radiates or decays at a sufficient
669 distance from the primary vertex to be resolved from the primary vertex (see
670 Section 4.1.1). Two widely used secondary vertexing tools are used within ATLAS:
671 SV1 and JetFitter [61]. Each attempts to reconstruct secondary vertices inside a jet
672 using the tracks associated to that jet (see Section 3.4.3 for more information about
673 track association). SV1 by design attempts to reconstruct only a single inclusive
674 vertex per jet. This inclusive vertex groups all b -hadron decay products, including
675 tracks from the b -hadron decay itself and tracks from $b \rightarrow c$ decays. The second tool,
676 JetFitter attempts to resolve each displaced vertex inside the jet, such that secondary
677 vertices from b -hadron decays are reconstructed separately to tertiary vertices from
678 $b \rightarrow c$ decay chains.

679 3.4.3 Jets

680 Jets are an aggregate reconstructed object corresponding to a collection of collimated
681 stable particles which results from a decay chain of an quark or gluon progenitor. Jets
682 are built by clustering constituent objects (e.g. tracks or calorimeter clusters) using
683 a jet finding algorithm, for example the anti- k_t algorithm [62], which is implemented
684 in FASTJET [63].

685 EMTopo Jets

686 EMTopo jets are reconstructed from noise-suppressed topological clusters (topoclus-
687 ters) of calorimeter energy depositions. The clustering uses the energy significance
688 of each cell, defined as

$$S_{\text{cell}} = \frac{E_{\text{cell}}}{\sigma_{\text{noise, cell}}}, \quad (3.10)$$

689 where E_{cell} is the energy measured in a given calorimeter cell, and $\sigma_{\text{noise, cell}}$ is the
 690 expected level of noise on the cell (e.g. from pile-up interactions). Topoclusters are
 691 formed from a seed cell with a large S_{cell} , and expanded by iteratively adding neigh-
 692 bouring cells with a sufficiently large energy significance. Collections of topoclusters
 693 are then clustered into a jet using the anti- k_t algorithm with a radius parameter of
 694 0.4 (small- R jets) or 1.0 (large- R jets). More information is available in Ref. [64].

695 Particle Flow Jets

696 Particle-flow (PFlow) jets are reconstructed from particle-flow objects [65] using
 697 the anti- k_t algorithm with a radius parameter of 0.4. Particle-flow objects integrate
 698 information from both the ID and the calorimeters, improving the energy resolution
 699 at high transverse momenta and reducing pile-up contamination. The PFlow jet
 700 energy scale is calibrated according to Ref. [66].

701 Tracks are associated to jets using a ΔR association cone, the width of which
 702 decreases as a function of jet p_T , with a maximum cone size of $\Delta R \approx 0.45$ for jets
 703 with $p_T = 20 \text{ GeV}$ and minimum cone size of $\Delta R \approx 0.25$ for jets with $p_T > 200 \text{ GeV}$.
 704 If a track is within the association cones of more than one jet, it is assigned to the
 705 jet which has a smaller $\Delta R(\text{track}, \text{jet})$.

706 Jet flavour labels are assigned according to the presence of a truth hadron within
 707 $\Delta R(\text{hadron}, \text{jet}) < 0.3$ of the jet axis. If a b -hadron is found the jet is labelled a b -jet.
 708 In the absence of a b -hadron, if a c -hadron is found the jet is called a c -jet. If no b -
 709 or c -hadrons are found, but a τ is found in the jet, it is labelled as a τ -jet, else it is
 710 labelled as a light-jet.

711 PFlow jets are used to train the algorithms discussed in Chapter 5 and Chapter 6.

712 Large- R Jets

713 Large- R jets have a radius parameter $R = 1.0$ and are built by clustering topological
 714 calorimeter clusters using the anti- k_t algorithm [67]. The large radius parameter
 715 is especially useful for containing the decay products of a boosted Higgs boson, as
 716 discussed in Chapter 7. Due to their large size, large- R jets benefit from a grooming
 717 procedure called trimming which remove soft contaminants inside the jet [68, 69].

718 Trimming aims to remove jet constituents from pile-up and the underlying event,
 719 which helps to improve the jet mass resolution and its robustness to varying levels
 720 of pile-up. The jet mass is computed using a combination of information from the
 721 calorimeters and ID, and a calibration to data is applied [70].

722 Track-jets

723 Track-jets are built by clustering tracks using the anti- k_t clustering algorithm and
 724 are used in the analysis described in Chapter 7. The radius parameter is allowed
 725 to vary with transverse momentum such that a broader cone (up to $R = 0.4$) is
 726 used for low- p_T track-jets and a narrower cone (down to $R = 0.02$) for high- p_T
 727 track-jets [71, 72]. The narrower cone is better suited to clustering highly collimated
 728 jet constituents at high- p_T . Truth flavour labels for track-jets are derived using the
 729 same $\Delta R(\text{hadron}, \text{jet}) < 0.3$ matching scheme as used for PFlow jets.

730 3.4.4 Leptons

731 Electrons and muons leave characteristic signatures that are picked up in the ECal
 732 and MS respectively. The reconstruction of both types of stable lepton is briefly
 733 outlined below.

734 Electrons

735 Electrons candidates are reconstructed by matching PV-compatible³ inner detector
 736 tracks to topological calorimeter clusters. The track-cluster matching criteria takes
 737 into account the significant energy loss of the electron due to bremsstrahlung. If a
 738 match is found, a refit of the track is performed using the Gaussian Sum Filter (GSF)
 739 [73], which better handles trajectory reconstruction in the presence of bremsstrahlung.
 740 Various identification criteria are then applied to the candidates using a likelihood-
 741 based (LH) method to improve purity. These include requirements on the track
 742 quality and cluster matching, the shape of electromagnetic shower in the ECal,
 743 leakage into the HCal, and the amount of transition radiation detected in the TRT.

³The ID track associated with the electron is required to satisfy $d_0/s(d_0) < 5$ and $z_0 \sin \theta < 0.5$ mm.

- ⁷⁴⁴ Isolation criteria with respect to other nearby ID tracks and calorimeter clusters may also be applied. A full description can be obtained from Ref. [74].

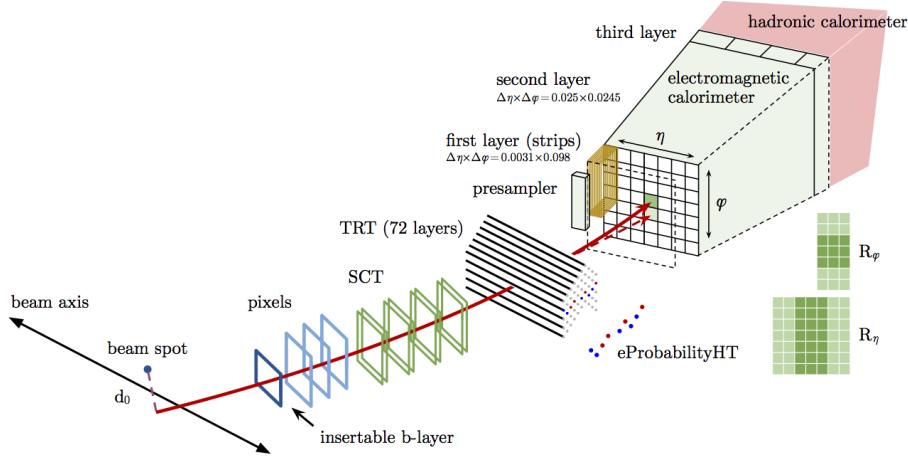


Figure 3.13: A sketch of electron reconstruction using the ATLAS detector [74]. Electron reconstruction makes use of the entire ID and the calorimeters. In particular, discriminating information comes from the TRT and ECal.

⁷⁴⁵

⁷⁴⁶ Muons

⁷⁴⁷ Muon reconstruction makes use of the dedicated MS (see Section 3.3.3), the tracks
⁷⁴⁸ from the ID, and the presence of characteristic signatures in the calorimeters. Muon
⁷⁴⁹ tracks (i.e. a track reconstructed in the MS) are reconstructed by connecting straight-
⁷⁵⁰ line track segments, which are identified via a Hough transform, and combined into
⁷⁵¹ an approximately parabolic trajectory. Finally, a global χ^2 fit is performed, taking
⁷⁵² into account possible interactions between the muon and the detector material. A
⁷⁵³ reconstructed muon is called *combined* if it completes successful matching to an
⁷⁵⁴ ID track. Combined muons undergo a further fit with the combined ID and MS
⁷⁵⁵ hits, with the energy loss due to the traversal of the calorimeters being taken into
⁷⁵⁶ account.

⁷⁵⁷ After reconstruction, candidate muons further undergo an identification processes
⁷⁵⁸ which helps to efficiently identify prompt muons whilst rejecting background sig-
⁷⁵⁹ nals (e.g. non-prompt muons from pion and kaon decays, the punch-through of a
⁷⁶⁰ hadron from the calorimeter, or the semi-leptonic decay of a heavy flavour hadron).
⁷⁶¹ Combined muon identification takes into account discrepancies in the p_T and charge

762 measurements in the MS and ID, and the χ^2 of the combined track fit. Selections
763 on the number of hits in the ID and MS are also applied. At the medium identifi-
764 cation working point, approximately 96% of muons with $20 \text{ GeV} < p_T < 100 \text{ GeV}$
765 are successfully identified. On top of the identification requirements, a number of
766 isolation requirements can also be applied to further suppress background signals. In
767 the region $|\eta| < 2.2$, the momentum resolution of reconstructed muons is 1.7%.

768 More information on muon reconstruction, identification and isolation can be found
769 in Ref. [75].

770 3.4.5 Missing Transverse Momentum

771 An imbalance in the final state transverse momentum can occur as a result of
772 incomplete measurement of the final state particles. In particular, neutrinos are
773 not measured by the detector and contribute to the missing transverse momentum
774 $\mathbf{E}_T^{\text{miss}}$. Incomplete detector acceptance and inaccuracies in the reconstruction of the
775 final state can also contribute to the missing transverse momentum of an event. In
776 order to calculate the missing transverse momentum, the negative vector sum of
777 the momentum of all photons, leptons and small- R jets with $p_T > 20 \text{ GeV}$ is taken.
778 The momenta of tracks associated to the primary vertex are also taken into account.
779 The magnitude of $\mathbf{E}_T^{\text{miss}}$ is written E_T^{miss} . More information about missing transverse
780 momentum reconstruction is provided in [76].

781

Chapter 4

782

Tracking and flavour tagging

783 Many ATLAS analyses rely on flavour tagging, which is the identification of jets
784 instantiated by heavy-flavour hadrons (b -hadrons and c -hadrons) as opposed to those
785 instantiated by light-flavour hadrons. In particular, b -tagging is the identification of
786 jets originating only from b -hadrons (i.e. b -jets). The b -jet identification algorithms
787 (also called *taggers*) work by identifying the unique signatures of b -jets, which are
788 outlined in Section 4.1. The various b -tagging algorithms ultimately take as their
789 input information about the reconstructed jet and its associated tracks. Successful
790 b -tagging relies therefore on the efficient and accurate reconstruction of tracks, and
791 especially those tracks corresponding to the products of b -hadron decays.

792 The current ATLAS flavour tagger, DL1r [77], is a deep neural network which
793 accepts as inputs the outputs of a number of independently optimised *low-level*
794 algorithms [61]. Correspondingly, DL1r is referred to as a *high-level* tagger (i.e. one
795 that uses a multivariate approach to combine the outputs of the low-level taggers).
796 Each of these low-level algorithms reconstructs a distinct feature of the experimental
797 signature of heavy flavour jets using the tracks associated to the jet. The low-level
798 algorithms are a combination of manually optimised reconstruction algorithms, for
799 example the SV1 and JetFitter algorithms that reconstruct displaced decay vertices,
800 and trained taggers such as RNNIP and DIPS that use the IP and hit information
801 from a variable number of tracks to identify the flavour of the jet [61, 78–80].

802 As the different b -tagging algorithms ultimately rely on tracks, accurate and efficient
803 track reconstruction is essential. This chapter summarises the challenges facing
804 tracking and b -tagging at high transverse momentum with an investigation into track

805 reconstruction performance in Section 4.1. Some preliminary investigations into
806 improving tracking in this regime are investigated in Section 4.2.

807 4.1 *b*-hadron Reconstruction

808 This section outlines the typical detector signature of a *b*-hadron in Section 4.1.1
809 and discusses some associated reconstruction difficulties in Section 4.1.2.

810 4.1.1 Decay Topology

811 *b*-hadrons are quasi-stable bound states of a bottom quark and one or more lighter
812 quarks. Collectively, these are the *B*-mesons (e.g. $B^+ = u\bar{b}$, $B^0 = d\bar{b}$) and baryons
813 (e.g. $\Lambda_b^0 = udb$). After a *b*-quark is produced as the result of a proton-proton collision,
814 they quickly hadronise. The hadronisation process is hard – around 70-80% of
815 the *b*-quark’s momentum is passed to the *b*-hadron, with the rest being radiated
816 as prompt hadronisation or fragmentation particles. See Ref. [81] for a more in
817 depth discussion on hadronisation and the closely related process of fragmentation.
818 Henceforth the combined hadronisation and fragmentation products will be referred
819 to collectively as fragmentation.

820 *b*-hadrons are interesting objects of study due to their relatively long proper lifetimes
821 $\tau \approx 1.5$ ps [82]. This lifetime corresponds to a proper decay length $c\tau \approx 450$ μm . In
822 the rest frame of the detector, the typical *b*-hadron travels a distance

$$d = \gamma\beta c\tau \approx \gamma c\tau \quad (4.1)$$

823 before decaying, where in the high energy limit $\gamma = E_b/m_b$ and $\beta = v/c = 1$.

824 For a 50 GeV *b*-hadron, this gives $d \approx 4.5$ mm, which is displaced enough to be
825 resolved from the primary vertex. Meanwhile for a 1 TeV *b*-hadron, $d \approx 90$ mm –
826 well beyond the radius of the first pixel layer (the IBL) which is situated at a radius
827 of approximately 33 mm from the center of the detector (the distance varies due
828 to the interleaved structure) Fig. 4.1 shows how the mean decay radius varies as a
829 function of *b*-hadron p_T . This significant displacement is characteristic of *b*-jets and
830 makes it possible to reconstruct secondary vertices at the *b*-hadron decay point.

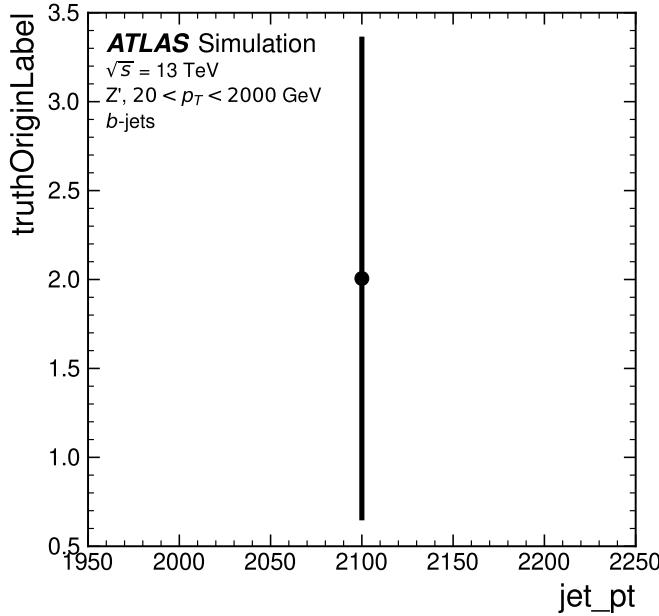


Figure 4.1: The truth b -hadron decay radius L_{xy} as a function of truth transverse momentum p_T for reconstructed b -jets in Z' events. Error bars show the standard deviation. The pixel layers are shown in dashed horizontal lines.

831 b -hadrons decay weakly to on average four or five collimated stable particles [83].
 832 These particles, along with any other fragmentation particles, are reconstructed in
 833 the detector as a jet. A b -jet has several characteristic features which differentiate
 834 it from light-jets. These features stem from the significant displacement of the
 835 b -hadron that can occur due to its lifetime. The primary feature is the presence of
 836 a high mass secondary vertex that is significantly displaced from the primary vertex.
 837 Reconstruction of these vertices from tracks with common points of spatial origin is
 838 a common approach used in the identification of b -jets.

839 Additional signatures of b -hadrons are as follows. Associated tracks and SVs can have
 840 a large transverse impact parameter d_0 as a result of the b -hadron displacement (as
 841 shown in Fig. 4.2). Since it is common for the b -hadron to decay to a c -hadron with
 842 non-negligible lifetime, tertiary vertices can be found within b -jets resulting from
 843 $b \rightarrow c$ decay chains. The b -hadron also decays semileptonically in approximately 23%
 844 of cases [15]. The presence of a reconstructed electron or muon inside a jet can also
 845 be a key indicator that the jet was instantiated by a b -hadron.

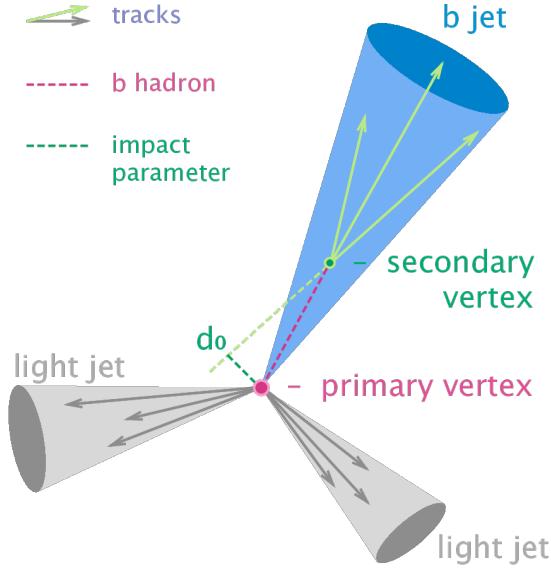


Figure 4.2: Diagram of a typical b -jet (blue) which has been produced in an event alongside two light jets (grey) [84]. The b -hadron has travelled a significant distance (pink dashed line) from the primary interaction point (pink dot) before its decay. The large transverse impact parameter d_0 is a characteristic property of the trajectories of b -hadron decay products.

846 These signatures are primarily identified using tracks associated to jets, or using re-
 847 constructed electrons or muons, which also rely on tracks as discussed in Section 3.4.4.
 848 As such, efficient and accurate track reconstruction is essential for high performance
 849 flavour tagging.

850 4.1.2 Challenges Facing b -hadron Reconstruction

851 As discussed, a necessary requirement for successful b -tagging is the efficient and
 852 accurate reconstruction of the charged particle trajectories in the jet. For high p_T jets
 853 ($p_T > 200$ GeV) this task becomes difficult due to a combination of effects. As the
 854 b -hadron energy increases, the multiplicity of the fragmentation products inside the
 855 jet increases, while the multiplicity of the products of the weak decay is unaffected.
 856 The “signal” tracks (those from the weak decay of the b -hadron) therefore become
 857 outnumbered. Both fragmentation and b -hadron weak decay products also become
 858 increasingly collimated as their inherited transverse momentum increases. At high
 859 energies, the increased decay length of b -hadrons (and c -hadrons) means that decay
 860 products have less of an opportunity to diverge before reaching the first tracking

861 layers of the detector (shown in Fig. 4.3). If the weak decay of the b -hadron takes
 862 place close enough to a detector layer, or if the particles are otherwise sufficiently
 863 collimated, charge deposits left by nearby particles may not be resolved individually,
 864 instead being reconstructed as merged clusters.

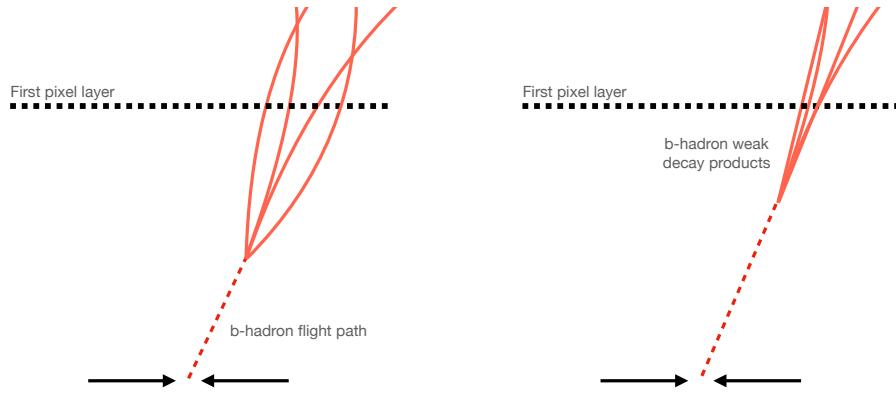


Figure 4.3: At lower p_T (left) the decay length of the b -hadron is reduced, and the resulting decay tracks are less collimated. At higher p_T (right) the b -hadron decay length increases and the resulting decay tracks are more collimated and have less distance over which to diverge before reaching detector elements. As a result, the ID may be unable to resolve charged depositions from different particles, resulting merged clusters.

865 As discussed in Section 3.4.1, merged clusters are generally rare, and so shared
 866 hits generally predict bad tracks and are correspondingly penalised during track
 867 reconstruction. However, in the core of high p_T b -jets the density of particles is high
 868 enough that the probability of cluster merging increases dramatically. Successful
 869 reconstruction of such tracks requires the presence of shared hits to be effectively
 870 dealt with but in the standard reconstruction the the presence of these can end up
 871 impairing the successfully reconstruction of the track. Furthermore, decays may also
 872 take place inside the tracking detectors themselves, which at best leads to missing
 873 measurements on the most sensitive detector layers, and at worst can lead to wrong
 874 inner layer hits being added to displaced tracks, since the reconstruction process
 875 penalises tracks without inner layer hits.

876 The above effects create two related, but distinct problems for b -tagging. The first
 877 part is a drop in track reconstruction efficiency. The presence of shared and missing
 878 hits reduces a track's score in the ambiguity solver meaning that higher ranking, but
 879 potentially worse, track candidates are processed first and take ownership of the hits.

This can make it difficult for otherwise reasonable b -hadron decay tracks to meet the ambiguity solver's stringent track quality requirements, leading to their rejection at this stage and an overall decrease in the b -hadron decay track reconstruction efficiency as shown in Fig. 4.4.

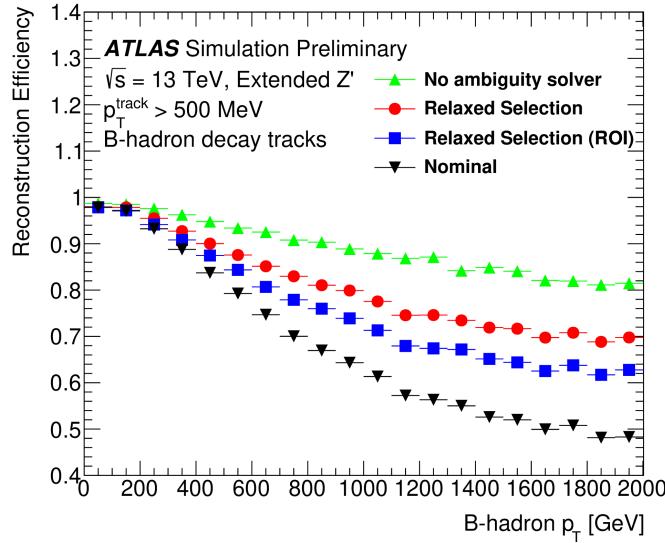


Figure 4.4: b -hadron decay track reconstruction efficiency as a function of truth b -hadron p_T [85]. Nominal track reconstruction is shown in black, while the track reconstruction efficiency for track candidates (i.e. the pre-ambiguity solver efficiency) is shown in green. For high- p_T b -hadrons, the ambiguity solver is overly aggressive in its removal of b -hadron decay tracks. Suggestions for the improvement of the track reconstruction efficiency in this regime by the loosening of cuts in the ambiguity solver are shown in blue and red.

The second part of the problem is that, due to the high multiplicity of clusters available for assignment in the vicinity of the typical high energy b -hadron decay track, and also given the strong positive bias of the ambiguity solver towards those tracks with pixel measurements in each layer (especially the innermost IBL measurement), many b -hadron decay tracks are assigned incorrect inner layer hits. This is only a problem for those decay products which were produced within the pixel detector as a result of a significantly displaced b -hadron decay, and so do not have a correct hit available for assignment. Fig. 4.5 shows the number of hits as a function of the reconstructed track p_T for fragmentation tracks and tracks from the weak decay of the b -hadron. The baseline tracks represent the standard reconstruction setup, while the pseudotrack represent the ideal tracking setup as outlined in Section 3.4.1. The incorrect hits may skew the parameters of the track, which can in turn mislead the

downstream b -tagging algorithms. In particular, b -tagging algorithms rely heavily on the transverse impact parameter significance $s(d_0)$ of the track. The quality of this measurement is expected to be adversely affected by wrong inner-layer hits on the track. Furthermore, multiple tracks sharing an incorrect hit can lead to the creation of spurious secondary vertices, which can cause further problems for the downstream b -tagging algorithms.

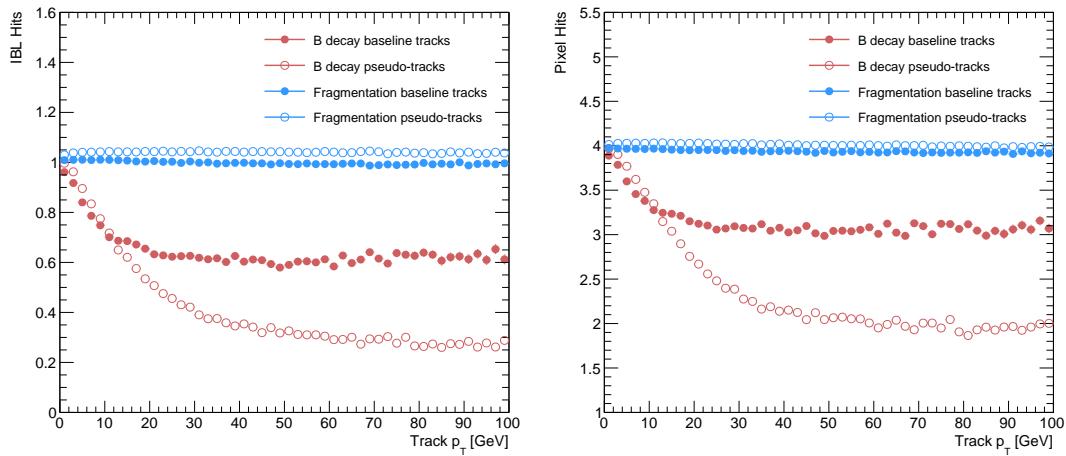


Figure 4.5: Hit multiplicities on the IBL (left) and the pixel layers (right) as a function of the p_T of the reconstructed track. Tracks from the weak decay of the b -hadron are shown in red, while fragmentation tracks (which are prompt) are in blue. Baseline tracks are those produced in the standard reconstruction described in Section 3.4.1, while pseudotrack represent the ideal performance of the ATLAS detector and are described in Section 3.4.1. Hit multiplicities on the pseudotracks decrease at high p_T due to the flight of the b -hadron before its decay. The baseline tracks have more hits than the pseudotracks, indicating that they are being incorrectly assigned additional hits on the inner layers of the detector.

The combination of the effects described makes reconstructing tracks in the core of high p_T b -jets particularly challenging. The reduced reconstruction efficiency of b -hadron decay tracks and incorrectly assigned hits is thought to be the primary cause of the observed drop in b -tagging efficiency at high energies, however further study is required to determine which effect may dominate.

4.2 Investigations into High p_T b -hadron Tracking

In Section 4.2.1 pseudotracks, a key tool for studying the ideal tracking performance of the ATLAS detector, are used to study the shared hit requirements on tracks in

include plot from sebs study showing they are approx similar impacts? or just mention result? Can do put need to remove ATLAS labels. Alternatively you can put an internal reference to his work and state what the outcome is

910 the dense cores of high- p_T b -jets. Section 4.2.2 details a study which investigated
911 modifying the global track fitter to improve reconstruction performance in this
912 regime.

913 4.2.1 Shared Hits

914 The ambiguity solver is not run for pseudotraccks. However, if the standard track
915 collection is produced alongside the pseudotraccks, then cluster splitting neural
916 networks will be run for the standard tracks, and the resulting classification of
917 clusters will be propagated to hits on pseudotraccks. This quirk allows one to study
918 the inefficiencies of the cluster splitting process, and relatedly to determine whether
919 shared hit cuts in the ambiguity solver are too loose or too tight. The fraction of hits
920 that are shared for the IBL and the B-layer is shown in Fig. 4.6. The shared hits on
921 pseudotraccks represent correctly assigned hits from merged clusters that were not
922 able to be classified as split by the cluster splitting neural networks. As such, these
923 represent the number of shared hits the ambiguity solver should aim to allow given
924 the current performance of the cluster splitting algorithm. For shared hits on the IBL
925 for particles produced before the IBL, the baseline selection appears to be successful
926 in disallowing excessive numbers of shared hits. However, the ambiguity solver fails to
927 limit shared hits for those particles produced after the IBL, reflecting the previously
928 discussed problem of displaced tracks picking up incorrect hits. Meanwhile, it is clear
929 that for the B-layer, the ambiguity solver is being overly aggressive in its rejection of
930 shared hits.

931 4.2.2 Global χ^2 Fitter Outlier Removal

932 This section documents ongoing progress into improvement of hit-to-track assignment
933 by using the Global χ^2 Fitter (GX2F) to identify and prevent incorrect hits from
934 being assigned to tracks during the track fit. This is in contrast to a previously
935 investigated approach [86] which attempted to identify and remove wrong hits after
936 the reconstruction of the track. As part of the track fit, an outlier removal procedure
937 is run, in which suspicious hits are identified and removed.

938 The GX2F code, as a relatively low-level component of track reconstruction, has
939 not undergone significant modification for several years, and was originally only

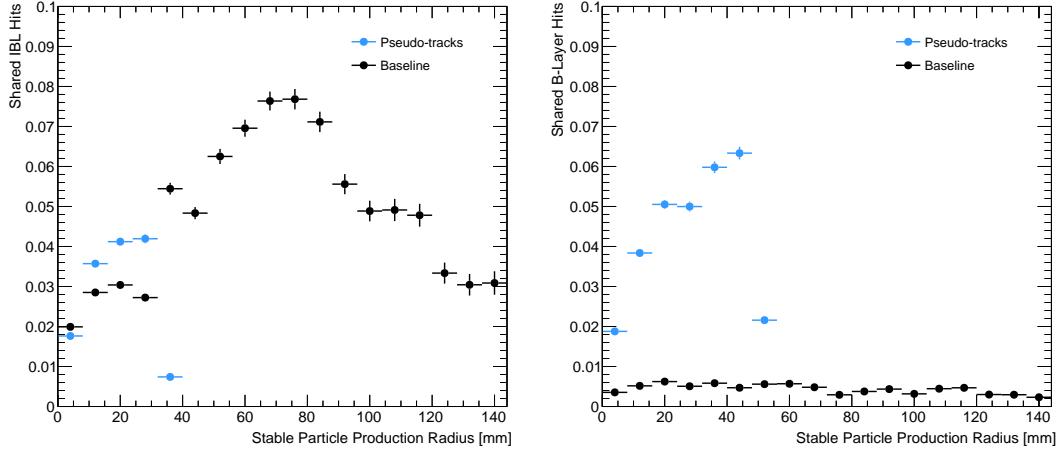


Figure 4.6: The fraction of hits which are shared on b -hadron decay tracks on the IBL (left), and the B-layer (right), as a function of the production radius of the b -hadron decay product. Pseudotrack represent the ideal performance given the ATLAS detector, see Section 3.4.1.

940 optimised in the context of prompt, isolated tracks. During this time, a new tracking
 941 sub-detector, the IBL, was installed. The motivation for looking at the GX2F is that
 942 these changes may require re-optimisation of the GX2F code, and in particular the
 943 outlier removal procedures. Further motivation for this approach comes from the low
 944 rate of labelled outliers in baseline tracking. For example, while approximately 15%
 945 of b -hadron decay tracks have a wrong IBL hit (a value which only increases with
 946 the p_T of the b -hadron), less than 1% of this tracks have had their IBL hit labelled
 947 and removed as an outlier.

948 Implementation

949 The outlier removal procedure for the pixel detector is described in this section.
 950 The hits on the track are looped over in order of increasing radial distance to the
 951 beam pipe. For each hit, errors $\sigma(m_i)$ on the measurement of the transverse and
 952 longitudinal coordinates are calculated. These errors are dependent on the sub-
 953 detector which recorded the measurement (some sub-detectors are more precise than
 954 others). Additionally, a residual displacement $r_i = m_i - x_i$ between the predicted
 955 position of the track x_i (inclusive of the current measurement), and the position of
 956 the hit itself, m_i , is calculated. The pull p_i on the track state due to the current

957 measurement is calculated according to

$$p_i = \frac{m_i - x_i}{\sqrt{\sigma(m_i)^2 - \sigma(x_i)^2}} \quad (4.2)$$

958 This pull is computed for the transverse and longitudinal coordinates of the mea-
 959 surement, and the maximum of the two is selected and checked to see if it exceeds
 960 a certain selection threshold. If it does, the hit will be removed if the track also
 961 exceeds a threshold on the total χ^2/n . The results of varying the outlier selection
 962 and χ^2/n thresholds are described below.

963 Cut Optimisation

964 A systematic variation of the outlier selection and χ^2/n thresholds has been carried
 965 out. Both thresholds were reduced in fixed step sizes of 0.25 for the outlier selection
 966 threshold and 1 for the χ^2/n threshold. The results for the best performing selections
 967 are discussed below. The value of the outlier selection threshold was reduced from 4
 968 down to 1.75, a change which affects all silicon layers (the TRT has separate outlier
 969 removal logic). Furthermore, a specific cut for the IBL was introduced, and is set
 970 to 1.25. The second threshold on the track χ^2/n was also reduced from 7 to 4.
 971 Finally, instead of taking the maximum of the pulls in the longitudinal and transverse
 972 directions, a quadrature sum is taken of these two values and used. This variation is
 973 labelled “Mod GX2F” in plots.

974 The results are shown in Fig. 4.7 and demonstrate a reduction in wrong hit assignment
 975 whilst also improving slightly the rate at which good hits are assigned to tracks. For a
 976 1 TeV track, the rate to assign good hits to the track increases by approximately
 977 10%, while the rate to assign incorrect hits decreases by approximately 16%. The
 978 improvements are also observed when looking inclusively in all tracks, which avoids
 979 the need for a specific b -jet region-of-interest selection.

980 An improvement, though modest, of all track parameter resolutions and pulls is
 981 observed. The improvement for the transverse impact parameter pull is shown in
 982 Fig. 4.8. The results demonstrate an improvement in hit assignment, unchanged
 983 reconstruction efficiency, and modest improvement in track parameter resolutions
 984 and pulls. In addition, the truth match probability of track is unchanged, suggesting

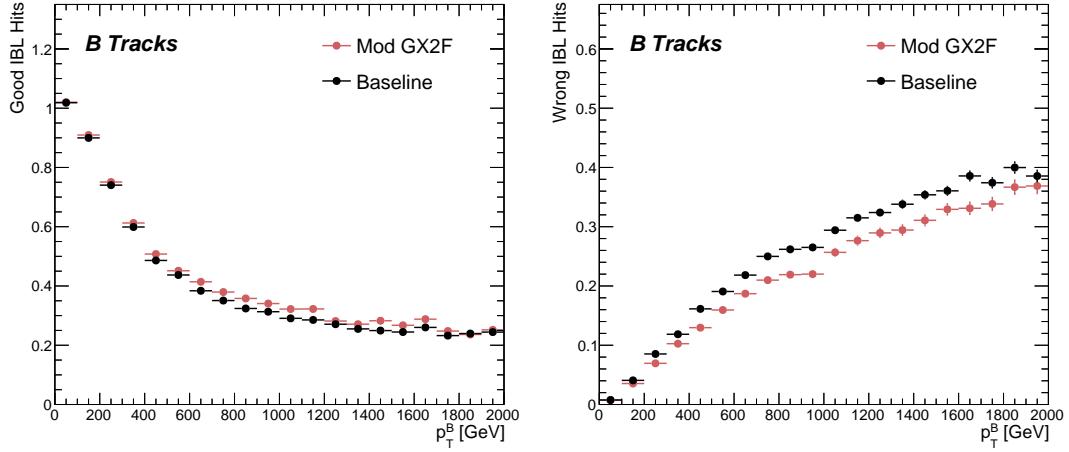


Figure 4.7: The rate to assign good (left) and wrong (right) IBL hits as a function of b -hadron p_T for tracks using baseline tracking (black) and the modified version of the outlier removal procedure (red). For each track, the corresponding p_T bin is filled with the number of good or wrong hits and this value is averaged to show the overall rate.

985 that there is no increase in fake track rates. The changes are expected to have a
 986 negligible impact on computational resources.

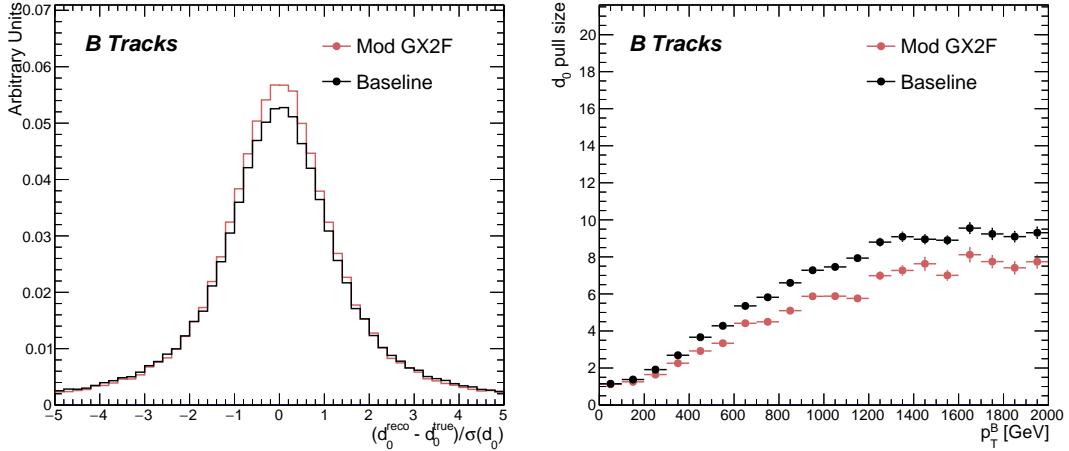


Figure 4.8: (left) b -hadron decay track d_0 pulls ($d_0/s(d_0)$) for baseline and modified GX2F tracks. (right) The absolute value of the d_0 pull as a function of b -hadron transverse momentum.

987 4.3 Conclusion

988 In this section, the difficulties facing efficient and accurate track reconstruction,
989 and hence performant b -tagging, have been outlined. The ambiguity solver, which
990 attempts to clean or reject tracks which have an excessive number of shared hits,
991 is shown to be overly aggressive in the removal of b -hadron decay product track
992 candidates. The ambiguity solving process relies on a complicated pre-defined
993 selection which has not been optimised for high transverse momentum b -hadron
994 track reconstruction. These conclusions have motivated further ongoing studies into
995 the improvement of the track reconstruction in dense environments and the high- p_T
996 regime, such as those in Ref. [85].

997 An optimisation of the outlier removal process in the global χ^2 fitter was carried
998 out. Though the results show some improvement over the baseline tracking scenario,
999 these results need to be expanded upon by looking at the impact on the downstream
1000 b -tagging algorithms before putting them into production. As there are some known
1001 data-MC discrepancies, fine tuned optimisation such as the work presented here
1002 presents an opportunity to over-optimize the tracking algorithms on MC. The studies
1003 were carried out in Release 21 of the ATLAS software, and need to be reproduced
1004 using the newer Release 22 to confirm the results against other changes in the baseline
1005 tracking configuration. Thanks to the all-in-one flavour tagging approach described
1006 in Chapter 6, it will also be easier in future to verify that the improvements to the
1007 track reconstruction have a positive impact on the flavour tagging performance.

1008 **Chapter 5**

1009 **Track Classification MVA**

1010 The chapter details work on implementing a multivariate algorithm (MVA) to predict
1011 the truth origin of reconstructed tracks. An introduction to formalisms of machine
1012 learning is given in Section 5.1. In Section 5.3, the truth origin label is defined,
1013 and in Section 5.4 these labels are used to train a machine learning model that can
1014 effectively discriminate between good and fake tracks. Several studies motivated this
1015 work by demonstrating that at high p_T , b -tagging performance was degraded by the
1016 presence of large numbers of poorly reconstructed or fake tracks. If an algorithm
1017 could be trained to detect fake tracks, these could be removed before their input to
1018 the b -tagging algorithms with the aim of improving performance.

1019 **5.1 Machine Learning Background**

1020 Over the past few decades, machine learning (ML) techniques have become increasing-
1021 ly popular in high energy physics experiments due the increased volumes of
1022 high-dimensional data and improvements in the techniques used (in particular deep
1023 learning). Machine learning is the process by which a computer program uses data
1024 to learn suitable parameters for a predictive model. This is opposed to explicitly
1025 providing instructions on how to perform a task. A subfield known as *supervised*
1026 *learning* is used in this work, and consists of exposing a model to a large number of
1027 labelled examples in order to extract relationships between the input data and their
1028 labels. These relationships are often complex, and explicitly programmed rules can
1029 fail to fully capture the relationships between inputs and outputs.

1030 In the simplest case, a set of m labelled training examples $S = \{(x_1, y_1), \dots, (x_m, y_m)\}$
 1031 is collected. Each element (x_i, y_i) consists of a input vector $x_i \in \mathbb{R}^{\text{input}}$, and the
 1032 corresponding label y_i . In classification problems, these labels are integer *class*
 1033 *labels* $y_i \in \{0, \dots, N - 1\}$, where N is the number of classes, which specify which
 1034 of a pre-determined set of categorical classes the training example belongs to. The
 1035 rest of the discussion in this chapter is limited to binary classification problems
 1036 ($N = 2$). The two classes are often referred to as signal ($y_i = 1$) and background
 1037 ($y_i = 0$), which need to be separated. Collecting sufficient and suitable data is one
 1038 of the primary challenges of machine learning, as such data is not always readily
 1039 available. Fortunately, sophisticated tools to simulate particle collisions have already
 1040 been developed by the scientific community [87, 88]. These tools play a key role in
 1041 generating a suitably large amount of labelled data which is used to train algorithms.
 1042 More detail on the input datasets is given in Section 5.4.1.

1043 After obtaining suitable training data, the next step is to define a model. Given an
 1044 input domain $\mathbb{R}^{\text{input}}$ and an output domain $(0, 1)$, the model $f_\theta : \mathbb{R}^{\text{input}} \rightarrow (0, 1)$ is a
 1045 parameterised functional mapping from input space to output space. Given an input
 1046 example x_i and a set of parameters θ , the model outputs a prediction $\hat{y}_i \in (0, 1)$ for
 1047 the true label y_i , as in

$$f_\theta(x_i) = \hat{y}_i. \quad (5.1)$$

1048 The output \hat{y}_i is in the interval $(0, 1)$ so as to be interpreted as the probability that
 1049 the input example x_i belongs to the signal class. The parameters θ of the model are
 1050 randomly initialised, and the model is designed to be expressive enough to correctly
 1051 map the inputs x_i to the outputs y_i given a reasonable optimisation of the parameters.
 1052 To perform this optimisation, the model is then trained, which amounts to showing
 1053 the model a series of labelled training examples and modifying the parameters of the
 1054 model based on its ability to correctly predict the labels.

1055 5.1.1 Neural Networks

1056 Neural networks (NNs) are a common choice for the machine learning model f since
 1057 they have the ability to approximate any function [89] and are easy to train via
 1058 backpropagation [90].

1059 **Artificial Neurons**

1060 The basic functional component of a NN is the *artificial neuron* or node, which is
1061 loosely inspired by a mathematical model of a biological neuron [91, 92]. A diagram
1062 of an artificial neuron is shown in Fig. 5.1 Each neuron is defined by its parameters
1063 or *weights* θ and a choice of activation function. Each neuron takes a fixed number
1064 of inputs and computes the dot product of the input and weight vectors $x^T \theta$ and
1065 additionally adds a constant bias term θ_0 . This term plays the role of a trainable
1066 constant value that is independent of the inputs.

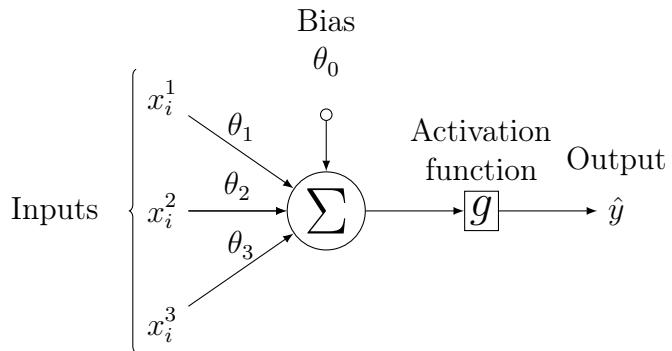


Figure 5.1: A diagram displaying the logical flow of a single neuron with three inputs x_i^j . Each input is multiplied by a weight θ_j , and the resulting values are summed. A bias term θ_0 is added, and the result z is passed to an activation function. Each neuron can be thought of as a logistic regression model.

1067 The output of the dot product and bias term z is fed into an activation function
1068 g . The activation function has several uses, most notably acting as a source of
1069 non-linearity and bounding the output of the neuron. Some common activation
1070 functions (sigmod, tanh, ReLU and SiLU) are shown in Fig. 5.2. The choice of
1071 activation function can have implications for the performance and convergence of
1072 the network, since the gradient of g is used to compute the weight updates during
1073 training. This is also why input data is typically normalised to have zero mean and
1074 unity variance [93].

1075 **Networks**

1076 Several neurons are linked together in layers to form a neural network. The inputs
1077 are propagated layer-by-layer through the network until reaching the final output

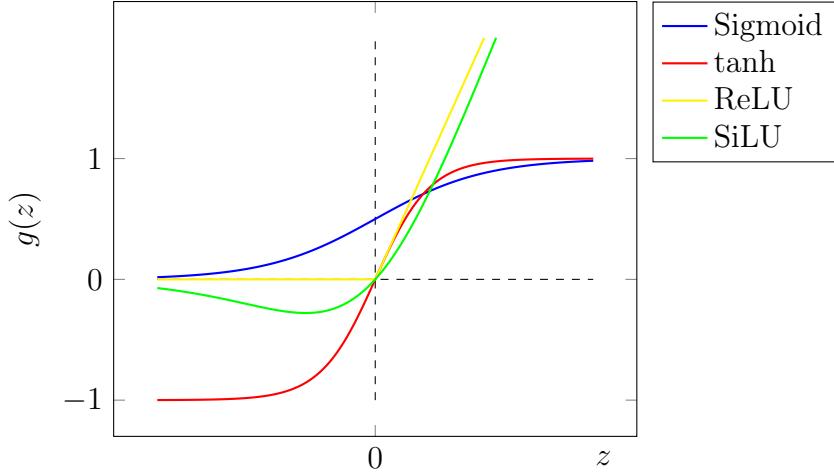


Figure 5.2: The output of several common choices for the activation function $g(z)$ of an artificial neuron. The input z is the output of the dot product between the activation and the weights, plus a bias term.

layer. The number of layers and neurons per layer are important hyperparameters (those parameters which are not optimised as part of the training process) which influence the performance of the model. In the case of binary classification, the final output layer consists of a single neuron with a sigmoid activation

$$g(z) = \frac{1}{1 + e^{-z}}, \quad (5.2)$$

where z is the output from the dot product of the inputs and the weights, plus the bias term. This value is bounded between zero and one allowing the final output to be interpreted as the probability that the input sample belongs to the signal class. NNs have the crucial property of being differentiable functions, which facilitates training process described in the next section.

5.1.2 Training with Gradient Descent

A training algorithm is used to optimise the weights of a NN after exposure to the training data. The training algorithm works by minimising a loss function L , which quantifies the error in the model's predictions. NNs are commonly trained using backpropagation in combination with a variant of the stochastic gradient descent algorithm to iteratively update the model parameters. In binary classification

1093 problems, the binary cross entropy given in Eq. (5.3) loss if often used.

$$L(x_i, \theta) = y_i \ln[f_\theta(x_i)] + (1 - y_i) \ln[1 - f_\theta(x_i)] \quad (5.3)$$

1094 Since the model f is differentiable, the error for each parameter θ_i can be computed by
1095 taking the partial derivative of L with respect to the parameter. Updated parameters
1096 θ'_i are calculated by updating the original parameter in the direction which reduces
1097 the loss.

$$\theta'_i = \theta_i - \alpha \frac{\partial L}{\partial \theta_i} \quad (5.4)$$

1098 The hyperparameter α is known as the *learning rate* and dictates the size of the
1099 step taken in the direction of the slope. The errors for each parameter are efficiently
1100 calculated using the backpropagation algorithm [90]. The process of updating weights
1101 is repeated until the weights converge, which means the network is trained. In practice,
1102 small batches of the input data are shown to the network at a time. For each batch
1103 the average loss is calculated and the network's weights are updated. There are many
1104 extensions and variations of the gradient descent algorithm. This work uses the Adam
1105 optimiser which adds momentum to the weight updates (dampening oscillations)
1106 and an adaptive per-parameter learning rate [94].

1107 5.2 Graph Neural Network Theory

1108 Graph neural networks are a more sophisticated neural network model (see Sec-
1109 tion 5.1.1) that are designed to operate on graph structured data. A brief introduction
1110 to GNNs is provided in this section following the formalism in Ref. [95].

1111 A graph \mathcal{G} consists of a set of N^n nodes $\mathcal{N} = \{h_i\}_{i=1:N^n}$, a set of N^e edges $\mathcal{E} =$
1112 $\{e_i\}_{i=1:N^e}$, and a global representation u . Each node represents an individual object,
1113 and edges are directed connections between two nodes, called the *sender* and *receiver*
1114 nodes. The connectivity of the graph therefore encodes information about the
1115 relationships between objects that exist in the graph.

1116 A single graph network layer consists of three separate update functions ϕ^e , ϕ^h and
1117 ϕ^u one for each of the nodes, edges, and global graph representation, and similarly
1118 three aggregation functions $\rho^{e \rightarrow h}$, $\rho^{e \rightarrow u}$ and $\rho^{h \rightarrow u}$. The aggregation functions combine

information across different edges or nodes for their input into the update functions, which produce new representations for the nodes, edges and global objects based on the information in the previous layer and the aggregated information. The update functions are typically each implemented as a dense feedforward neural network (as described in Section 5.1.1). The edges e_i are updated by a edge network ϕ^e as in

$$e'_i = \phi^e(e_i, h_s, h_r, u), \quad (5.5)$$

where h_s and h_r are the sender and receiver nodes respectively. The nodes are updated with a node network ϕ^h as in

$$h'_i = \phi^h(\bar{e}'_i, h_i, u), \quad (5.6)$$

where $\bar{e}'_i = \rho^{e \rightarrow h}(E'_i)$, and E'_i is the set of sender nodes for receiver node h_i . $\rho^{e \rightarrow h}$ is referred to as the edge aggregation function. The global representation is updated using the global network ϕ^u as in

$$u' = \phi^u(\bar{e}', \bar{h}', u), \quad (5.7)$$

where \bar{e}' is the aggregation $\rho^{e \rightarrow u}$ over all updated edges e'_i and \bar{h}' is the aggregation $\rho^{h \rightarrow u}$ over all updated nodes h'_i .

The graph network layer performs a graph convolution, in an analogous way to a convolutional neural network operating on a grid of pixels. The above description is general, and not all concrete implementations of GNNs need implement every aspect. For example, the global graph representation need not be present, and it is also possible that no dedicated edge features are present. In such cases the corresponding update and aggregation functions are not needed. Fig. 5.3 shows two possible graph network update layers. The layer used in the GN1 model is specified in more detail in Section 6.3.3.

5.3 Track Truth Origin Labelling

Crucial to supervised learning techniques are the ground truth class labels which the machine learning model is trained to predict. A set of track truth labels which a

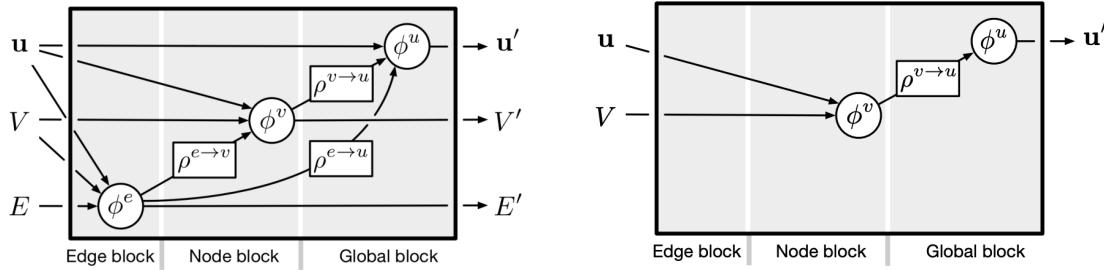


Figure 5.3: The flow of information through a graph neural network layer for (left) a full implementation of the layer and (right) a deep sets model [96]. Reproduced from Ref. [95].

high degree of granularity have been implemented in the ATLAS software stack, and are listed in Table 5.1. The labelling scheme has been designed to be useful beyond the classification of good and fake tracks. The origins are determined by analysing the simulated record to determine the physical process that led to the creation of the truth (i.e. simulated) particle which is associated with each reconstructed track. Tracks are associated with truth particles by selecting the particle with the highest *truth-matching probability* (TMP), defined in Eq. (5.8). This is a weighted sum of the number of hits on a reconstructed track which are from the same truth particle, versus the total number of hits on the track. The weights are subdetector-dependent and are designed to account for the varying importance of the different subdetectors (based upon their precision) in the reconstruction of a track.

$$\text{TMP} = \frac{10N_{\text{Pix}}^{\text{good}} + 5N_{\text{SCT}}^{\text{good}} + N_{\text{TRT}}^{\text{good}}}{10N_{\text{Pix}}^{\text{all}} + 5N_{\text{SCT}}^{\text{all}} + N_{\text{TRT}}^{\text{all}}} \quad (5.8)$$

For the fake track classification tool, the track truth origins in Table 5.1 are used to construct a binary label by assigning all fake tracks to the background category, and all other tracks as signal. The fake track classifier is then trained to distinguish between these two categories of tracks. Fake tracks are defined using the TMP, with a $\text{TMP} < 0.75$ ¹ giving a track the label of fake. Fake tracks are made up of combinatorial fakes, which are tracks which do not correspond to the trajectory of any truth particle, and poorly reconstructed tracks, which may somewhat resemble the trajectory of a truth particle due to the presence of some wrong hits on the track, will not accurately reproduce a true trajectory.

¹An alternative definition of a fake track as one with $\text{TMP} < 0.5$ is also in use within ATLAS. Both values were investigated, but 0.75 was used for this study.

Truth Origin	Description
Pileup	From a pp collision other than the primary interaction
Fake	Created from the hits of multiple particles
Primary	Does not originate from any secondary decay
fromB	From the decay of a b -hadron
fromBC	From a c -hadron decay which itself is from the decay of a b -hadron
fromC	From the decay of a c -hadron which is not from the decay of a b -hadron
OtherSecondary	From other secondary interactions and decays

Table 5.1: Truth origins which are used to categorise the physics process that led to the production of a track. Tracks are matched to charged particles using the truth-matching probability [56]. A truth-matching probability of less than 0.5 indicates that reconstructed track parameters are likely to be mismeasured and may not correspond to the trajectory of a single charged particle. The “OtherSecondary” origin includes tracks from photon conversions, K_S^0 and Λ^0 decays, and hadronic interactions.

5.4 Fake Track Identification Tool

The rate of fake tracks increases at high transverse momentum as shown in Fig. 5.4 due to the difficulties in track reconstruction outlined in Section 4.1.2. The performance of b -tagging algorithms is reduced as a direct result of the presence of these tracks as shown for SV1 (see Section 3.4.2) in Fig. 5.5, where the light-jet efficiency decreases by up to 35% at a b -jet efficiency of 35%.

To identify and remove fake tracks, a NN classification tool was trained with all non-fake tracks as the signal class and fake tracks as the background class. Inputs to the model are described in Section 5.4.2, while fake track removal performance is given in Section 5.4.4.

5.4.1 Datasets

To train and evaluate the model, simulated SM $t\bar{t}$ and BSM Z' events initiated by proton-proton collisions at a center of mass energy $\sqrt{s} = 13$ TeV are used. The Z' sample is constructed in such a manner that it has a relatively flat jet p_T spectrum up to 5 TeV and decays democratically to equal numbers of b -, c - and light-jets. The generation of the simulated event samples includes the effect of multiple pp

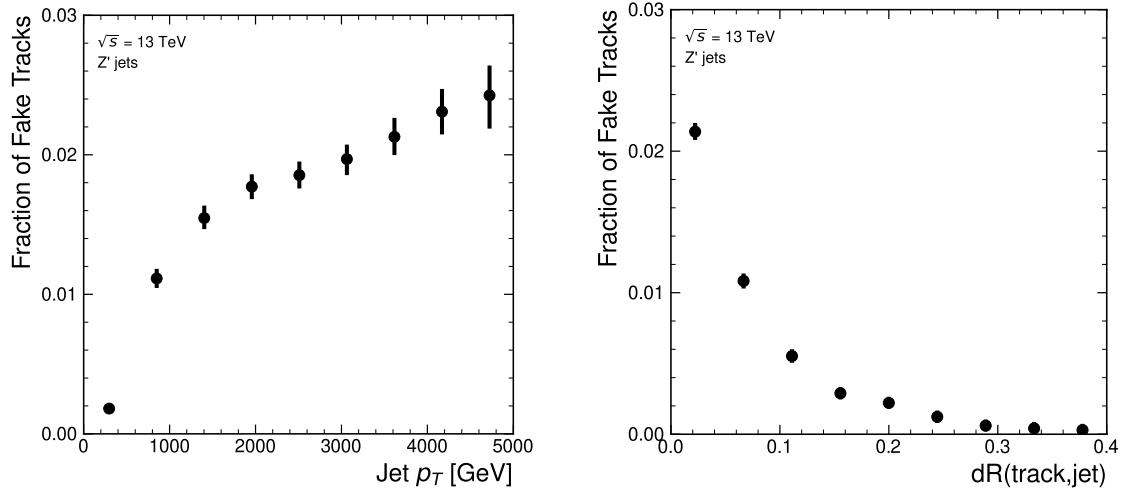


Figure 5.4: Rate of fake tracks as a function of jet transverse momentum (left) and $\Delta R(\text{track},\text{jet})$ (right). The rate of fake tracks increases significantly as a function of p_T , and also increases as the distance to the jet axis decreases.

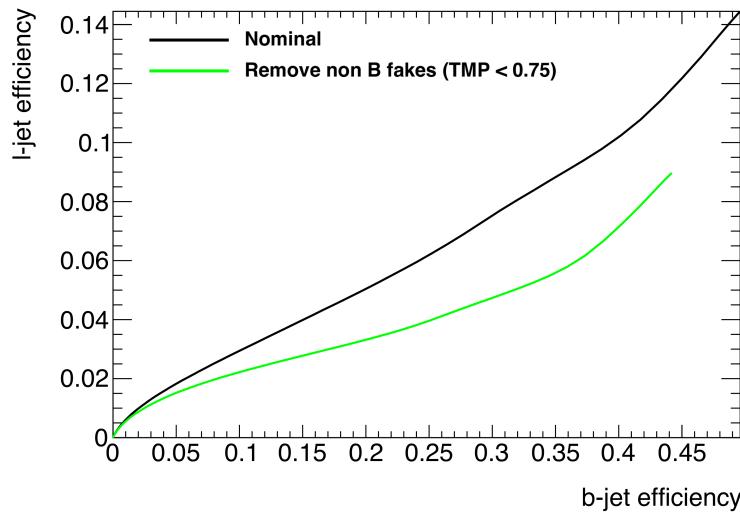


Figure 5.5: The light-jet efficiency of the low level tagger SV1 for jets in the Z' sample with $250 < p_T < 5000 \text{ GeV}$, as a function of b -jet efficiency. The nominal tracking setup (black) is shown alongside the case where fake tracks which are not from the decay of a b -hadron are removed. The light-jet efficiency is decreased, demonstrating that the presence of fake tracks is detrimental to the algorithm performance.

1178 interactions per bunch crossing with an average pileup of $\langle \mu \rangle = 40$, which includes
1179 the effect on the detector response due to interactions from bunch crossings before
1180 or after the one containing the hard interaction.

1181 The $t\bar{t}$ events are generated using the POWHEGBox [97–100] v2 generator at next-
1182 to-leading order with the NNPDF3.0NLO [101] set of parton distribution func-
1183 tions (PDFs). The h_{damp} parameter² is set to 1.5 times the mass of the top-quark
1184 (m_{top}) [102], with $m_{\text{top}} = 172.5$ GeV. The events are interfaced to PYTHIA 8.230 [103]
1185 to model the parton shower, hadronisation, and underlying event, with parameters
1186 set according to the A14 tune [104] and using the NNPDF2.3LO set of PDFs [105].
1187 Z' events are generated with PYTHIA 8.2.12 with the same tune and PDF set. The
1188 decays of b - and c -hadrons are performed by EVTGEN v1.6.0 [106]. Particles are
1189 passed through the ATLAS detector simulation [107] based on GEANT4 [108].

1190 Jets are required to have a pseudorapidity $|\eta| < 2.5$ and $p_{\text{T}} > 20$ GeV. Additionally, a
1191 standard selection using the Jet Vertex Tagger (JVT) algorithm at the tight working
1192 point is applied to jets with $p_{\text{T}} < 60$ GeV and $|\eta| < 2.4$ in order to suppress pile-up
1193 contamination [109].

1194 5.4.2 Model Inputs

1195 The fake track MVA is given two jet variables and 20 tracking related variables
1196 for each track fed into the network. The jet transverse momentum and signed
1197 pseudorapidity constitute the jet-level inputs, with the track-level inputs listed in
1198 Table 5.2. The track parameters and hit pattern are key indicators of whether or
1199 not a track is fake. The FracRank variable is the ordered index of the tracks that
1200 pass the ambiguity solver’s selection divided by the total number of successfully
1201 reconstructed tracks in the event. The ambiguity solver processes track candidates
1202 iteratively in order of an internal score (see Section 3.4.1), and the order in which
1203 tracks are accepted is preserved. Since tracks with shared hits have lower scores,
1204 tracks which do not require the removal of shared hits are likely to be processed
1205 and accepted earlier on, whereas tracks with shared hits will be processed later and

²The h_{damp} parameter is a resummation damping factor and one of the parameters that controls the matching of POWHEG matrix elements to the parton shower and thus effectively regulates the high- p_{T} radiation against which the $t\bar{t}$ system recoils.

1206 potentially have their shared hits removed. Hence the FracRank variable gives an
1207 indication of the of how easy it was for the track to be reconstructed.

Jet Input	Description
p_T	Jet transverse momentum
η	Signed jet pseudorapidity
Track Input	Description
p_T	Track transverse momentum
ΔR	Angular distance between the track and jet
d_0	Closest distance from the track to the PV in the longitudinal plane
z_0	Closest distance from the track to the PV in the transverse plane
nIBLHits	Number of IBL hits
nPixHits	Number of pixel hits
nSCTHits	Number of SCT hits
nTRTHits	Number of TRT hits
nBLHits	Number of B-layer hits
nIBLShared	Number of shared IBL hits
nIBLSplit	Number of split IBL hits
nPixShared	Number of shared pixel hits
nPixSplit	Number of split pixel hits
nSCTShared	Number of shared SCT hits
r_{first}	Radius of first hit
nDOF	Number of degrees of freedom on the track
FracRank	Ambiguity solver ordering variable

Table 5.2: Input features to the fake track classification NN. Basic jet kinematics, along with information about the reconstructed track parameters and constituent hits are used. Shared hits, are hits used on multiple tracks which have not been classified as split by the cluster-splitting neural networks [56], while split hits are hits used by multiple tracks which have been identified as merged, and therefore split.

1208 Track selection follows the loose selection described in Ref. [80] and outlined in
1209 Table 5.3, which was found to improve the performance compared to previous tighter
1210 selections, whilst ensuring good resolution of tracks and a low fake rate [56]. Inputs
1211 are scaled to have a central value of zero and a variance of unity before training and
1212 evaluation.

Parameter	Selection
p_T	$> 500 \text{ MeV}$
$ d_0 $	$< 3.5 \text{ mm}$
$ z_0 \sin \theta $	$< 5 \text{ mm}$
Silicon hits	≥ 8
Shared silicon hits	< 2
Silicon holes	< 3
Pixel holes	< 2

Table 5.3: Quality selections applied to tracks, where d_0 is the transverse IP of the track, z_0 is the longitudinal IP with respect to the PV and θ is the track polar angle (see Section 3.2.2 for the IP definitions). Shared hits are hits used on multiple tracks which have not been classified as split by the cluster-splitting neural networks [56]. A hole is a missing hit, where one is expected, on a layer between two other hits on a track.

5.4.3 Model Hyperparameters

Due to the imbalance between the two classes (with fake tracks being relatively uncommon), a weight was added to the loss function for the background class to account for this. The NN was made up of two hidden layers with 220 nodes per layer. The ReLU activation function was used in conjunction with the Adam optimiser with a learning rate of $1\text{e}{-}3$. Optimisation of the networks architecture was carried out to ensure optimal performance with a relatively small number of learnable parameters – 54 thousand. The model was trained using 40 million tracks with a further 1 million tracks each used for validation and testing. A full list of the model hyperparameters is given in Table 5.4.

5.4.4 Results

In order to evaluate the fake track classification tool, a orthogonal test sample of 1 million tracks in jets in the combined $t\bar{t}$ and Z' samples is used. The continuous scalar output from the NN model is interpreted as the probability that a given track is a signal track (i.e. not fake). Fig. 5.6 shows the performance of the fake track classification MVA. The signal and background classes are well separated in the output of the tool. Also shown is a receiver operating characteristic (ROC) curve,

Hyperparameter	Value
Batch size	2048
Activation	ReLU
Optimiser	Adam
Initial learning rate	$1e-3$
Training epochs	20
Training tracks	40m
Validation tracks	4m
Testing tracks	4m

Table 5.4: Hyperparameter for the track classification model

which plots the rate of true positives against the rate of false positives over a scan of cut points on the NN output ranging from zero to one. The area under the curve (AUC) gives a summary of the aggregate classification power of the model. The fake track classification tool achieves an AUC of 0.935 for all tracks, which is indicative of a well-performing model. Considering only tracks from b -hadron decays, this value drops slightly to 0.928.

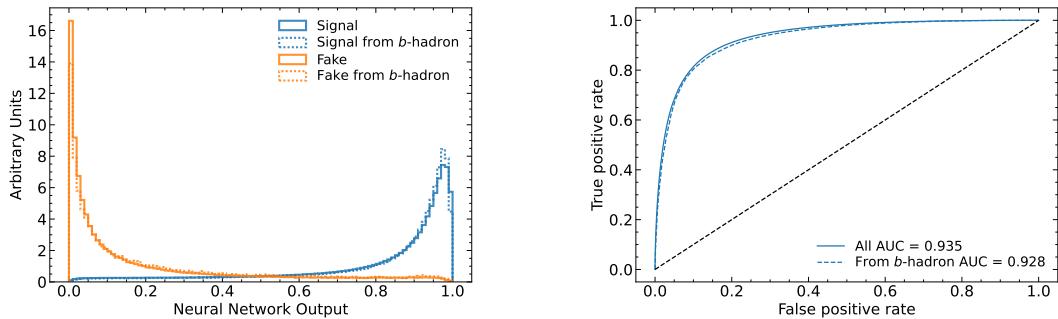


Figure 5.6: (left) Normalised histogram of the model output separated for signal and fake tracks, and further separated by those tracks which are from the decay of a b -hadron. (right) The ROC curve for all tracks (solid line) and tracks from the decay of a b -hadron (dashed line). The model is able to successfully discriminate between signal and fake tracks, and shows a very similar performance when looking specifically at tracks from the decay of a b -hadron.

Signal and fake track efficiencies at two different NN output cut points are shown in Table 5.5. The results demonstrate that the tool is effective in retaining 98.8% of signal tracks, while correctly identifying (and therefore enabling the removal of)

1239 45.6% of fake tracks. Table 5.5 also shows that a significant amount of tracks which
1240 are labelled as both fake and from the decay of a b -hadron are also removed. This can
1241 happen because fake tracks with $\text{TMP} < 0.75$ are still matched to a truth particle,
1242 which can be the decay product of a b -hadron.

MVA Output Cut	Signal Track Efficiency		Fake Track Efficiency	
	All	From b	All	From b
0.06	98.8%	98.9%	45.6%	39.8%
0.12	97.3%	97.5%	59.4%	53.6%

Table 5.5: Good and fake track selection efficiencies for the combined $t\bar{t}$ and Z' samples. Two working points are defined, cutting on the NN output at 0.06 and 0.12. The continuous output of the model allows for the tuning of good and fake track identification efficiencies.

1243 5.5 b -hadron Track Identification

1244 After initial tests and investigation, it was found that fake tracks which were the
1245 result of b -hadron decays actually aided b -tagging performance. The application of
1246 a single tool which removed all fake tracks was therefore not optimal. A second
1247 tool was therefore trained in the same manner as the first, this one was designed to
1248 distinguish between those tracks which were from the decay of a b -hadron (FromB
1249 and FromBC in Table 5.1) and those which were not (all other truth origins). The
1250 b -hadron decay track MVA was trained using the same setup as described above,
1251 with the same tracks, input variables, and training procedure. The performance of
1252 the model to separate b -hadron decay tracks from other tracks is shown in Fig. 5.7.
1253 Using a selection WP of 0.1, the model can retain 98.5% of b -hadron tracks and
1254 reject 46.2% of tracks not from the decay of a b -hadron. In Section 5.6, this model is
1255 used in conjunction with the fake track identification MVA described in Section 5.4.4
1256 to identify and remove fake tracks which are not from the decay of a b -hadron.

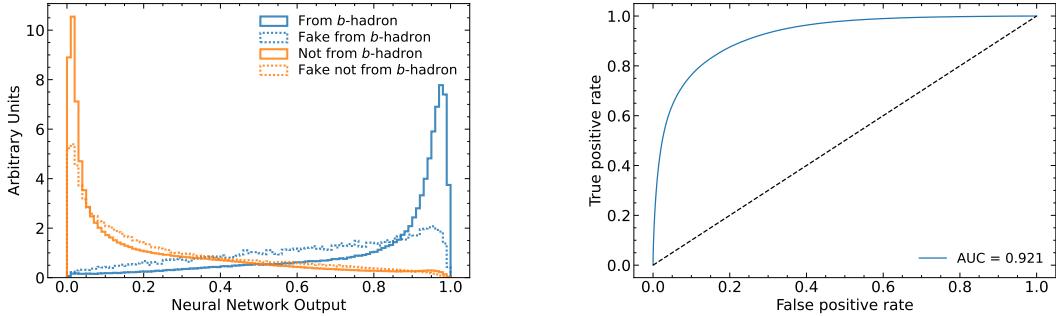


Figure 5.7: (left) Normalised histogram of the model output separated for tracks from the decay of a b -hadron and tracks from other sources. The two groups are further separated into those tracks which are fake. (right) The ROC curve for all tracks (solid line).

1257 5.6 Combined Approach

1258 A 2-dimensional cut was then used to only reject those tracks that had a high
 1259 probability of being fake, and also a low probability of being a b -hadron decay track.

WP	Fake Cut	MVA	b -hadron Decay MVA Cut	Retained Tracks	b -hadron	Fake & Non b -hadron Tracks Rejected
A	0.5		0.4	98.6%		50.7%
B	0.6		0.5	97.5%		62.0%

Table 5.6: Cut values for the fake and b -hadron decay track MVAs for the two defined working points. Working point “B” cuts more aggressively on the MVA outputs than WP “A”, removing more fake tracks but resulting in an increased loss of signal tracks (which here are all b -hadron decay tracks).

1260 The light-jet efficiency of SV1 is successfully reduced when using the combined tools
 1261 to remove fake tracks that are not from a b -hadron decay, as shown in Fig. 5.8. At a
 1262 b -jet efficiency of 70%, the light-jet mistag rate for jets with $250 < p_T < 400$ GeV
 1263 is reduced from 0.054 to 0.044, a relative improvement of approximately 20%. For
 1264 jets with $400 < p_T < 1000$ GeV the mistage rate drops from 0.1 to 0.08 for a similar
 1265 relative improvement of 20%. The performance of the fake track removal approach
 1266 was also tested for the other low level vertexing algorithm: JetFitter. A similar level
 1267 of improvement in the light-jet mistag rate was observed of up to a 20% reduction

for both low- and high- p_T jets in the Z' sample. Together, these results demonstrate that by identifying and removing fake tracks which are not the result of the weak decay of a b -hadron, the performance of the low level tagging algorithms can be improved.

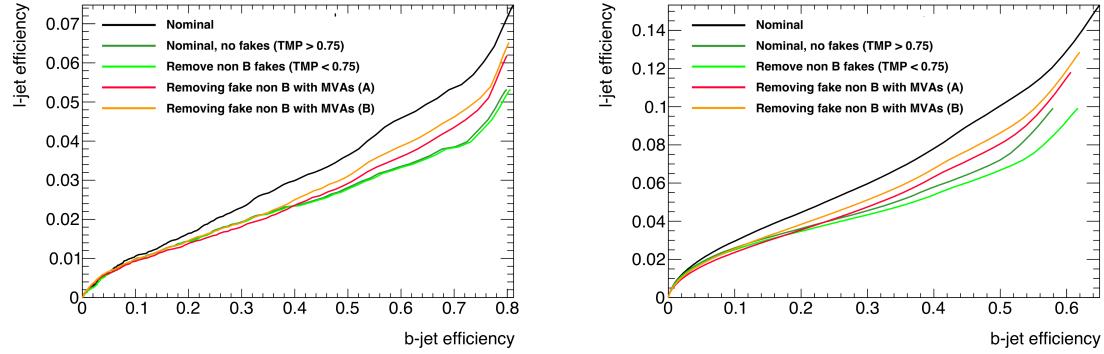


Figure 5.8: The effect of applying the fake track identification algorithm together with the b -hadron decay track identification on the jet tagging performance of SV1 for jets in the Z' sample with $250 \text{ GeV} < p_T < 400 \text{ GeV}$ (left) and $400 \text{ GeV} < p_T < 1 \text{ TeV}$ (right). The nominal SV1 light-jet rejection (black) is compared to two working points of fake track removal, labelled “A” (red) and “B” (orange), which represent two different 2D working points of the track classification tools. Removal of fake tracks based on truth information is shown by the green curves.

5.7 Conclusion

Fake tracks, which are prevalent in the core of high p_T jets, have an adverse impact on b -tagging performance. A ML tool to identify fake tracks has been developed, which can be used to limit the number of fake tracks being input to the b -tagging algorithms. Since it was found that b -hadron decay tracks can also be poorly reconstructed and thus marked as fake, it was deemed necessary also to train a second algorithm to detect b -hadron decay tracks so that the removal of these tracks could be avoided. Removing fake and non- b decay tracks in this way was found to improve the light-jet mistagging rate of SV1 and JetFitter by up to 20% at high transverse momentum. The improvement achieved using the classification tools was in general comparable with the improvement achieved when using the truth information to remove the fake tracks not from the decay of a b -hadron.

1284 Future Work

1285 While removing tracks prior to their input to the low level tagging algorithms is
1286 shown here to be beneficial, a more performant alternative might be to keep these
1287 tracks but label them as being fake (for example using the output of the classification
1288 tool), and allow the tagging algorithms to take this into consideration, potentially
1289 making use of this information. This is not straightforward with manually optimised
1290 taggers such as SV1 and JetFitter, but is possible with more advanced taggers as
1291 described in Chapter 6.

1292 Tools which identify the origin of a given track have other potential uses. One
1293 application is to isolate a relatively pure sample of fake tracks which can be used
1294 to estimate the fake track rate in data, which would be useful for estimating the
1295 uncertainty on fake track modelling. Another application would be to use the
1296 b -hadron track identification tool to improve the track-to-jet association. Both
1297 applications are currently under investigation.

1298 The approach here works on a track-by-track basis, but a more sophisticated approach
1299 would consider the correlations between the tracks inside a jet, as shown in Chapter 6.

1300 Also left for future work is to simultaneously train a single tool which discriminates
1301 between all the truth origins listed in Table 5.1. Such a tool would be useful as a
1302 general purpose multiclass classifier.

₁₃₀₃ **Chapter 6**

₁₃₀₄ **Graph Neural Network Flavour
Tagger**

₁₃₀₆ As discussed in Chapter 4, flavour tagging is the identification of jets instantiated
₁₃₀₇ from b - and c -hadrons. Flavour tagging is a critical component of the physics
₁₃₀₈ programme of the ATLAS experiment. It is of crucial importance for the study of the
₁₃₀₉ Standard Model (SM) Higgs boson and the top quark, which decay preferentially to
₁₃₁₀ b -quarks [110, 111], and additionally for several Beyond the Standard Model (BSM)
₁₃₁₁ resonances that readily decay to heavy flavour quarks [112].

₁₃₁₂ This chapter introduces GN1, a novel ML-based flavour tagging algorithm based
₁₃₁₃ on graph neural networks (GNNs). In Section 6.1, an overview of the approach
₁₃₁₄ used for GN1 is provided. An introduction to the theory of GNNs is provided in
₁₃₁₅ Section 5.2. Details of the experimental setup are provided in Section 6.2, while
₁₃₁₆ the architecture of GN1 is specified in Section 6.3.3. In Section 6.3.4, the training
₁₃₁₇ procedure is described, and in Section 6.4 the results are shown.

₁₃₁₈ **6.1 Motivation**

₁₃₁₉ GN1 is a monolithic approach to flavour tagging as illustrated in Fig. 6.1. As opposed
₁₃₂₀ to the existing approach to flavour tagging described in Chapter 4, which relies
₁₃₂₁ on a two tiered approach requiring the use of both low- and high-level algorithms,
₁₃₂₂ GN1 takes as inputs information directly from an unordered variable number of
₁₃₂₃ tracks as input, and predicts the jet flavour without requiring outputs from the

intermediate low-level algorithms. In addition to predicting the flavour of the jet, the model predicts which physical processes produced the various tracks, and groups the tracks into vertices. These auxiliary training objectives provide valuable additional information about the contents of the jet and enhance the performance of the primary flavour prediction task. The use of GNNs offers a natural way to classify jets with variable numbers of unordered associated tracks (see Section 5.2), while allowing for the inclusion of auxiliary training objectives [113, 114].

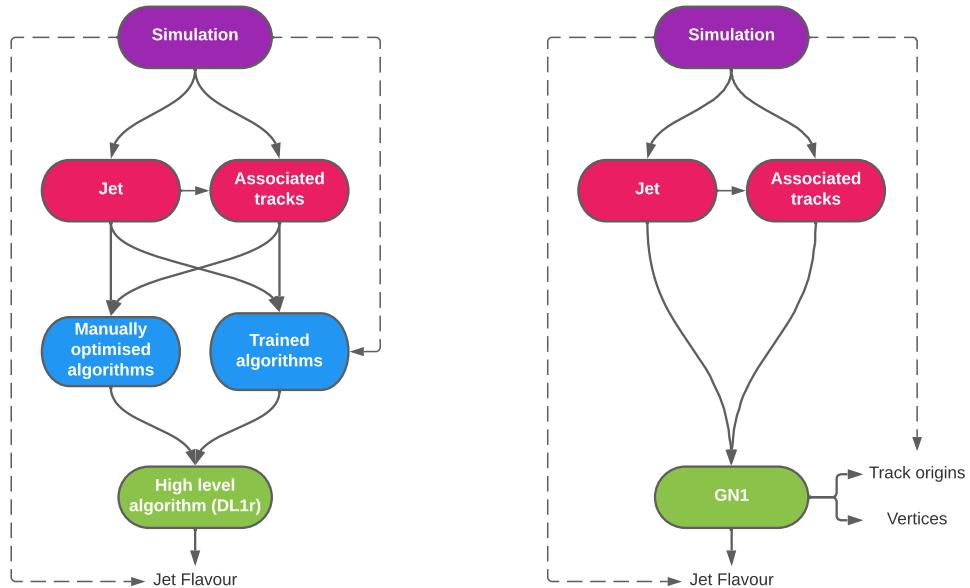


Figure 6.1: Comparison of the existing flavour tagging scheme (left) and GN1 (right) [2]. The existing approach utilises low-level algorithms (shown in blue), the outputs of which are fed into a high-level algorithm (DL1r). Instead of being used to guide the design of the manually optimised algorithms, additional truth information from the simulation is now being used as auxiliary training targets for GN1. The solid lines represent reconstructed information, whereas the dashed lines represent truth information.

As described in Chapter 4, current flavour tagging algorithms utilise a two-tiered approach. The high-level tagger DL1r outputs variables which provides good discrimination between the different jet flavours. In contrast GN1 consists of only a single neural network, which takes tracks as inputs along with some kinematic information about the jet. As a result, it does not depend on the outputs of any other flavour tagging algorithm. A simple training of the model fully optimises its parameters, representing a significant simplification with respect to the optimisation procedure for

1338 DL1r. This is particularly important when optimising the tagger for new regions of
1339 phase space (e.g. c -tagging or high- p_T b -tagging), or when the detector is upgraded
1340 or the charged particle reconstruction or selection algorithms are re-optimised.

1341 GN1 is trained to learn about the internal structure of the jet through the use of two
1342 auxiliary training objectives: the prediction of the underlying physics process from
1343 which each track originated, and the grouping of tracks originating from a common
1344 spatial position (i.e. a common vertex). These auxiliary objectives are meant to
1345 guide the neural network towards a more complete understanding of the underlying
1346 physics inside the jet, thereby removing the need for the low-level algorithms, which
1347 previously contained information about the underlying physics in their design. The
1348 training targets for the primary and auxiliary objectives are extracted from truth
1349 information, i.e. information that is only available in simulation, as opposed to
1350 reconstructed quantities available in both collision data and simulation.

1351 In this chapter, the following advantages of the GN1 approach will be demonstrated:

- 1352 1. GN1 boasts improved performance with respect to the current ATLAS flavour
1353 tagging algorithms, with significantly larger background rejection rates for a
1354 given signal efficiency. Alternatively the rejection rates can be kept fixed for a
1355 substantial increase in signal efficiency, in particular at high- p_T .
- 1356 2. The same network architecture can be easily optimised for a wider variety of
1357 use cases (e.g. c -jet tagging and high- p_T jet tagging) since there are no low-level
1358 algorithms to retune.
- 1359 3. There are fewer algorithms to maintain.
- 1360 4. Alongside the network’s prediction of the jet flavour, the auxiliary vertex and
1361 track origin predictions provide more information on why a jet was (mis)tagged
1362 or not. This information can also have uses in other applications, for instance
1363 to explicitly reconstruct displaced decay vertices or to remove fake tracks.¹

¹A fake track is defined as a track with a truth-matching probability less than 0.5, where the truth-matching probability is defined in Ref. [56].

1364 6.2 Experimental Setup

1365 6.2.1 Datasets

1366 The datasets used to train the GN1 tagger are the same as described in Section 5.4.1.
1367 The training dataset contains 30 million jets, 60% of which are $t\bar{t}$ jets and 40%
1368 of which are Z' jets. In order to evaluate the performance of the model during, a
1369 statistically independent set of 500k testing jets from both the $t\bar{t}$ and Z' samples are
1370 used. For the final testing of the model and the creation of the performance plots,
1371 a further 1 million independent testing jets from each of the $t\bar{t}$ and Z' samples are
1372 used. Before being fed into the model, the track- and jet-level inputs are normalised
1373 to have a mean of zero and a variance of unity. The jet flavour labels are assigned
1374 as described in Section 3.4.3. Truth labelled b -, c - and light-jets are kinematically
1375 re-sampled in p_T and η to ensure identical distributions in these variables.

1376 6.3 Model Architecture

1377 6.3.1 Model Inputs

1378 As inputs, GN1 is fed two kinematic jet variables and an unordered set of up to 40
1379 tracks which have been associated to the jet. Each track consists of 21 variables. The
1380 kinematic jet variables are the jet transverse momentum and signed pseudorapidity.
1381 The input variables which are provided for each track are listed in Table 6.1. For
1382 each track, variables containing the track parameters and uncertainties, and detailed
1383 information on the hit content are provided as inputs to the model.
1384 In cores of high- p_T jets, track density is high due to the increased multiplicity and
1385 collimation of tracks (see Chapter 4). As a result, the separation between tracks
1386 can be of the same order as the active sensor dimensions, resulting in an increase
1387 in merged clusters and tracks which share hits [56]. Due to the relatively long
1388 lifetimes of b -hadrons and c -hadrons, which can traverse several layers of the ID
1389 before decaying and have highly collimated decay products, the presence of shared
1390 or missing hits is a critical signature of heavy flavour jets.

1391 Dependence of the model on the absolute value of the azimuthal jet angle ϕ is
1392 explicitly removed by providing only the azimuthal angle of tracks relative to the jet
1393 axis. The track pseudorapidity is also provided relative to the jet axis.

1394 Since heavy flavour hadrons can decay semileptonically approximately 20% of the time,
1395 the presence of a reconstructed lepton in the jet carries discriminating information
1396 about the jet flavour. To exploit this, a variant of GN1 called GN1Lep is trained in
1397 addition to the baseline model. The GN1Lep variant is identical to the baseline model,
1398 except for the inclusion an additional track-level input, leptonID, which indicates
1399 if the track was used in the reconstruction of an electron, a muon or neither. The
1400 variable is signed by the charge of the reconstructed lepton. The leptons used in the
1401 definition of the leptonID variable are required to satisfy basic quality requirements.
1402 The muons are required to be combined [115], and the electrons are required to pass
1403 the *VeryLoose* likelihood-based identification working point [116].

1404 The selections applied to the tracks is the same as that used for the fake track
1405 classification MVA described in Chapter 5. The full set of track selections is listed
1406 in Table 5.3. This selection was found to improve the flavour tagging performance
1407 compared to previous tighter selections, whilst ensuring good resolution of tracks
1408 and a low fake rate [56]. However, Section 6.4.8 demonstrates that further relaxation
1409 of the track selection requirements may be warranted.

1410 If more than 40 tracks are associated to a given jet, only the first 40 tracks with the
1411 largest transverse IP significance² $s(d_0)$ are fed into the model as inputs.

1412 6.3.2 Auxiliary Training Objectives

1413 In addition to the jet flavour classification, two auxiliary training objectives are
1414 defined. The first auxiliary objective is the prediction of the physical process that
1415 gave rise to each track within the jet (i.e. the track origin), while the second is the
1416 prediction of track-pair vertex compatibility. Each auxiliary training objective comes
1417 with a training target which, similar to the jet flavour label, is a truth labels derived

²Impact parameter significances are defined as the IP divided by its corresponding uncertainty, $s(d_0) = d_0/\sigma(d_0)$ and $s(z_0) = z_0/\sigma(z_0)$. Track IP significances are lifetime signed according to the track's direction with respect to the jet axis and the primary vertex [38].

Jet Input	Description
p_T	Jet transverse momentum
η	Signed jet pseudorapidity
Track Input	Description
q/p	Track charge divided by momentum
$d\eta$	Pseudorapidity of the track, relative to the jet η
$d\phi$	Azimuthal angle of the track, relative to the jet ϕ
d_0	Closest distance from the track to the PV in the longitudinal plane
$z_0 \sin \theta$	Closest distance from the track to the PV in the transverse plane
$\sigma(q/p)$	Uncertainty on q/p
$\sigma(\theta)$	Uncertainty on track polar angle θ
$\sigma(\phi)$	Uncertainty on track azimuthal angle ϕ
$s(d_0)$	Lifetime signed transverse IP significance
$s(z_0)$	Lifetime signed longitudinal IP significance
nPixHits	Number of pixel hits
nSCTHits	Number of SCT hits
nIBLHits	Number of IBL hits
nBLHits	Number of B-layer hits
nIBLShared	Number of shared IBL hits
nIBLSplit	Number of split IBL hits
nPixShared	Number of shared pixel hits
nPixSplit	Number of split pixel hits
nSCTShared	Number of shared SCT hits
nPixHoles	Number of pixel holes
nSCTHoles	Number of SCT holes
leptonID	Indicates if track was used to reconstruct an electron or muon

Table 6.1: Input features to the GN1 model [2]. Basic jet kinematics, along with information about the reconstructed track parameters and constituent hits are used. Shared hits, are hits used on multiple tracks which have not been classified as split by the cluster-splitting neural networks [56], while split hits are hits used on multiple tracks which have been identified as merged. A hole is a missing hit, where one is expected, on a layer between two other hits on a track. The track leptonID is an additional input to the GN1Lep model.

1418 from the simulation. The presence of the auxiliary training objectives improves the
1419 jet classification performance as demonstrated in Section 6.4.3.

1420 For the track origin prediction objective, each track is labelled with one of the
1421 exclusive categories defined in Table 5.1 of Section 5.3 after analysing the particle
1422 interaction (or lack thereof) which led to its formation. Since the presence of different
1423 track origins is strongly related to the flavour of the jet, training GN1 to recognise
1424 the origin of the tracks provides an additional handle on the classification of the
1425 jet flavour. This task may also aid the jet flavour prediction by acting as a form of
1426 supervised attention [117] - in detecting tracks from heavy flavour decays the model
1427 may learn to pay more attention to these tracks.

1428 The vertexing auxiliary objective makes use of the fact that displaced decays of b -
1429 and c -hadrons lead to secondary and tertiary vertices inside the jet, as described in
1430 Section 4.1.1. The presence of displaced secondary vertices is not a completely clean
1431 signal of a heavy flavour jet, as displaced secondary vertices can also occur in light-jets
1432 as a result of material interactions, conversions, and long-lived particle decays (e.g.
1433 K_S^0 and Λ^0). For the auxiliary object, GN1 predicts a binary label for each pair of
1434 tracks in the jet. The label has a value of 1 if the truth particles associated with the
1435 two tracks in the pair originated from the same spatial point, and 0 otherwise. To
1436 derive the corresponding truth labels for training, truth production vertices within 0.1
1437 mm are merged. Track-pairs where one or both of the tracks in the pair have an origin
1438 label of either Pileup or Fake are given a label of 0. Using the pairwise predictions
1439 from the model, groups of tracks that have common compatibility can be formed,
1440 resulting in the finding of vertices. Two existing low-level tagging algorithms, SV1
1441 and JetFitter (introduced in Section 3.4.2), are currently used to find and reconstruct
1442 vertices inside jets and are used as inputs to the existing jet flavour tagger DL1r.
1443 The addition of this auxiliary training objective removes the need for inputs from a
1444 dedicated secondary vertexing algorithm.

1445 Both of the auxiliary training objectives described here can be considered as “stepping
1446 stones” on the way to classifying the flavour of the jet. By requiring the model to
1447 predict the truth origin of each track and the vertex compatibility of each track-pair,
1448 the model is guided to learn representations of the jet which are connected to the
1449 underlying physics and therefore relevant for classifying the jet flavour.

1450 6.3.3 Architecture

1451 As discussed in the previous sections, GN1 is a graph neural network which makes
1452 use of auxiliary training objectives in order to determine the jet flavour. A coarse
1453 optimisation of the network architecture hyperparameters (for example number of
1454 layers and number of neurons per layer) has been carried out in order to maximise
1455 the flavour tagging performance, but it is likely that further dedicated optimisation
1456 studies could lead to further performance improvements.

1457 The model architecture builds on a previous implementation of a GNN-based jet
1458 tagger [114]. The previous approach was comprised of two separate graph neural
1459 networks with the auxiliary tasks being performed at an intermediate stage after the
1460 first and before the second. This two stage approach was found to be unnecessary and
1461 as such GN1 simplifies the architecture into a single graph neural network with the
1462 auxiliary tasks being performed at the end, alongside the primary jet classification
1463 task. GN1 makes use of a more sophisticated graph neural network layer [118],
1464 which is described in more detail below. The changes significantly improved tagging
1465 performance and also led to a significant reduction in training time.

1466 As inputs, the model takes information about the jet and a number of associated
1467 tracks, as detailed in Section 6.3.1. The jet variables are concatenated with the
1468 variables for each track as shown in Fig. 6.2. The combined jet-track input vectors
1469 are then fed into a per-track initialisation network with three hidden layers, each
1470 containing 64 neurons, and an output layer with a size of 64, as shown in Fig. 6.3. The
1471 track initialisation network is similar to a deep sets model [96], but does not include
1472 a reduction operation (mean or summation) over the output track representations.
1473 The initialisation network allows for initial per-track input processing without the
1474 associated parameter count cost of the graph convolutional layers described below.

1475 The outputs of the track initialisation network are used to populate the nodes of a
1476 fully connected graph, such that each node in the graph neighbours every other node.
1477 Each node h_i in the graph corresponds to a single track in the jet, and is characterised
1478 by a feature vector, also called a representation. The per-track output representations
1479 from the initialisation networks are used as the initial feature vectors of each node
1480 in the graph. In each layer of the graph network, output node representations h'_i
1481 are computed by aggregating the features of h_i and neighbouring nodes \mathcal{N}_i using
1482 a multi-head attention mechanism ($n = 2$) as described in Ref. [118, 119]. First,

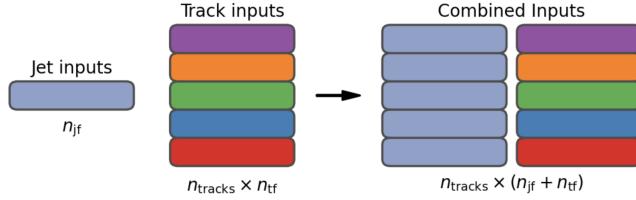


Figure 6.2: The inputs to GN1 are the two jet features ($n_{jf} = 2$), and an array of n_{tracks} , where each track is described by 21 track features ($n_{tf} = 21$) [2]. The jet features are copied for each of the tracks, and the combined jet-track vectors of length 23 form the inputs of GN1.

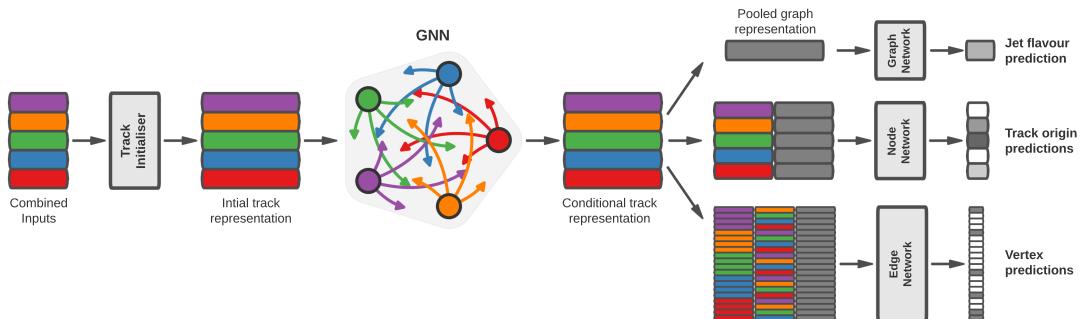


Figure 6.3: The network architecture of GN1. Inputs are fed into a per-track initialisation network, which outputs an initial latent representation of each track. These representations are then used to populate the node features of a fully connected graph network. After the graph network, the resulting node representations are used to predict the jet flavour, the track origins, and the track-pair vertex compatibility.

1483 the feature vectors of receiver and sender nodes are fed into two fully connected
 1484 linear layers \mathbf{W}_r and \mathbf{W}_s , to produce an updated representation for each sender and
 1485 receiver node $\mathbf{W}_r h_i$ and $\mathbf{W}_s h_j$. These updated feature vectors are used to compute
 1486 edge scores $e(h_i, h_j)$ for each node pair, as in

$$e(h_i, h_j) = \mathbf{a} \cdot \theta [\mathbf{W}_r h_i + \mathbf{W}_s h_j], \quad (6.1)$$

1487 where, θ is a non-linear activation function, and \mathbf{a} is a learned vector. These edge
 1488 scores are then used to calculate attention weights a_{ij} for each pair of nodes using
 1489 the softmax function over the edge scores

$$a_{ij} = \text{softmax}_j [e(h_i, h_j)]. \quad (6.2)$$

1490 Finally, the updated representations for the receiver nodes h'_i are computed by taking
 1491 the weighted sum over each updated node representation $\mathbf{W}_r h_i$, with weights a_{ij}

$$h'_i = \sigma \left[\sum_{j \in \mathcal{N}_i} a_{ij} \cdot \mathbf{W}_r h_j \right]. \quad (6.3)$$

1492 The set of operations described above constitute a single graph network layer. Three
 1493 such layers are stacked to construct the graph network, representing a balance
 1494 between achieving good performance in a reasonable time and avoiding overtraining
 1495 due to inflation of the parameter count of the model. The final output from the graph
 1496 neural network is a set of per-node (i.e. per-track) feature vectors that are conditional
 1497 representations of each track given the other tracks in the jet. In order to perform
 1498 the jet flavour prediction, a flattened global representation of the jet is needed. To
 1499 produce this, the output track representations are combined using a weighted sum,
 1500 where the weights are learned during training and therefore act as a form of attention
 1501 over the different tracks. The flattened outputs from the sum are then fed into a
 1502 fully connected feedforward neural network with four layers and three outputs, one

for each jet flavour. Two other separate fully connected feedforward neural networks are then also used to independently perform the auxiliary classification objectives of GN1. Both of the auxiliary classification tasks also take in the global representation of the jet as inputs. A summary of the different classification networks used for the various training objectives is shown in Table 6.2.

Network	Hidden layers	Output size	Label
Node classification network	128, 64, 32	7	Track origin
Edge classification network	128, 64, 32	1	Track-pair compatibility
Graph classification network	128, 64, 32, 16	3	Jet flavour

Table 6.2: A summary of GN1’s different classification networks used for the various training objectives, adapted from Ref. [2]. The hidden layers column contains a list specifying the number of neurons in each layer.

The node classification network predicts the track truth origin as defined in Table 5.1. This network takes as inputs the features from a single output node from the graph network and the global representation of the jet. The node network has three hidden layers containing 128, 64 and 32 neurons respectively, and an output size of seven, corresponding to the seven different truth origins defined in Table 5.1.

The edge classification network is used to predict whether the tracks in the track-pair belong to a common vertex. This network takes as inputs the concatenated representations from each pair of tracks and the global jet representation. Similar to the node network, the edge network has three hidden layers containing 128, 64 and 32 neurons respectively, and a single output, which is used to perform binary classification of the track-pair compatibility. The output predictions for the two auxiliary networks are used for the auxiliary training objectives discussed in Section 6.3.2.

Finally, the graph classification network is used to predict the jet flavour. This network takes only the global jet representation as input. The graph classification network is comprised of four fully connected hidden layers with 128, 64, 32 and 16 neurons respectively, and has three outputs corresponding to the b -, c - and light-jet classes.

1526 6.3.4 Training

1527 The full GN1 training procedure minimises the total loss function L_{total} , defined
 1528 in Eq. (6.4). This loss is composed of three terms: L_{jet} , the categorical cross
 1529 entropy loss over the different jet flavours; L_{vertex} , the binary track-pair compatibility
 1530 cross entropy loss; and L_{track} , the categorical cross entropy loss for the track origin
 1531 prediction. L_{vertex} is computed via a weighted average over all intra-jet track-pairs in
 1532 the batch, and L_{track} is computed by a weighted average over all tracks in the batch,
 1533 where the weights are described below.

$$L_{\text{total}} = L_{\text{jet}} + \alpha L_{\text{vertex}} + \beta L_{\text{track}} \quad (6.4)$$

1534 The different losses converge to different values during training, reflecting differences
 1535 in the relative difficulty of the various training objectives. The values of L_{vertex} and
 1536 L_{track} are weighted by $\alpha = 1.5$ and $\beta = 0.5$ respectively to ensure they converge to
 1537 similar values, giving them an equal weighting towards L_{total} . The values of α and β
 1538 are chosen to ensure that L_{jet} converges to a larger value than either L_{vertex} and L_{track} ,
 1539 which reflects the primary importance of the jet classification objective. It was found
 1540 that in practice the overall performance of the model was not sensitive to modest
 1541 changes in the loss weights α and β . Pre-training using L_{total} (i.e. on all tasks) and
 1542 fine tuning on only the jet classification task also did not improve performance versus
 1543 the described standard setup, indicating that the auxiliary tasks are not in direct
 1544 competition with the jet classification task. As there was a large variation in the
 1545 relative abundance of tracks of the different origins, the contribution of each origin to
 1546 L_{track} was weighted by the inverse of the frequency of their occurrence. In vertexing
 1547 loss L_{vertex} , the class weight for track-pairs where both tracks are from either a b - or
 1548 c -hadron was increased by a factor of two as compared with other track-pairs, to
 1549 encourage the network to focus on correctly classifying heavy flavour vertices.

1550 GN1 can be trained with either the node or edge networks (and their corresponding
 1551 auxiliary tasks), or both, removed, as discussed in Section 6.4.3. In such cases,
 1552 the corresponding losses L_{vertex} and L_{track} are also removed from the calculation
 1553 of the overall loss L_{total} . The performance of the resulting models provides a

1554 useful indication of the benefit of including the auxiliary tasks to the primary jet
1555 classification objective.

1556 GN1 was trained for 100 epochs on 4 NVIDIA V100 GPUs. Each epoch takes
1557 approximately 25 mins to complete over the training sample of 30 million jets
1558 described in Section 6.2.1. The Adam optimiser [120] with an initial learning rate of
1559 $1e-3$, and a batch size of 4000 jets (spread across the 4 GPUs) was used. Typically
1560 the validation loss, calculated on 500k jets, became stable after around 60 epochs.
1561 The epoch that minimized the validation loss was used for evaluation. GN1 has
1562 been integrated into the ATLAS software [53] using ONNX [121]. The test sample
1563 jet flavour predictions scores are computed using the ATLAS software stack as a
1564 verification of this process.

1565 6.4 Results

1566 The GN1 tagger is evaluated both as a b -tagging and c -tagging algorithm in Sec-
1567 tion 6.4.1 and Section 6.4.2 respectively. Evaluation is performed separately on
1568 both jets in the $t\bar{t}$ sample with $20 < p_T < 250$ GeV and jets in the Z' sample with
1569 $250 < p_T < 5000$ GeV. The performance of the model is compared to the DL1r
1570 tagger [77, 122], which has been retrained on 75 million jets from the same samples
1571 as GN1. The input RNNIP tagger [79] to DL1r has not been retrained. As discussed,
1572 each tagger predicts the probability that a jet belongs to the b -, c - and light-classes.
1573 To use the model for b -tagging, these probabilities are combined into a single score
1574 D_b , which is defined as

$$D_b = \log \frac{p_b}{(1 - f_c)p_l + f_c p_c}, \quad (6.5)$$

1575 where f_c is a free parameter that determines the relative weight of p_c to p_l in the
1576 score D_b , controlling the trade-off between c - and light-jet rejection performance.
1577 The choice of f_c is arbitrary, and is optimised based upon the desired light- vs c -jet
1578 rejection performance. This parameter is set to a value of $f_c = 0.018$ for the DL1r
1579 model, obtained through an optimisation procedure described in Ref. [77]. Based on
1580 a similar optimisation procedure, a value of $f_c = 0.05$ is used for the GN1 models.

1581 A fixed-cut working point (WP) defines the corresponding selection applied to the
 1582 tagging discriminant D_b in order to achieve a given efficiency on the inclusive $t\bar{t}$
 1583 sample.

1584 A comparison of the b -tagging discriminant D_b between DL1r and GN1 is shown in
 1585 Fig. 6.4. The shapes of the D_b distributions are generally similar for b -, c - and light-
 1586 jets between both models, however, GN1 shifts the b -jet distribution to higher values
 1587 of D_b in the regions with the greatest discrimination. The GN1 c -jet distribution is
 1588 also shifted to lower values of D_b when compared with DL1r, enhancing the separation
 1589 and indicating that GN1 is improving c -jet rejection when compared with DL1r.

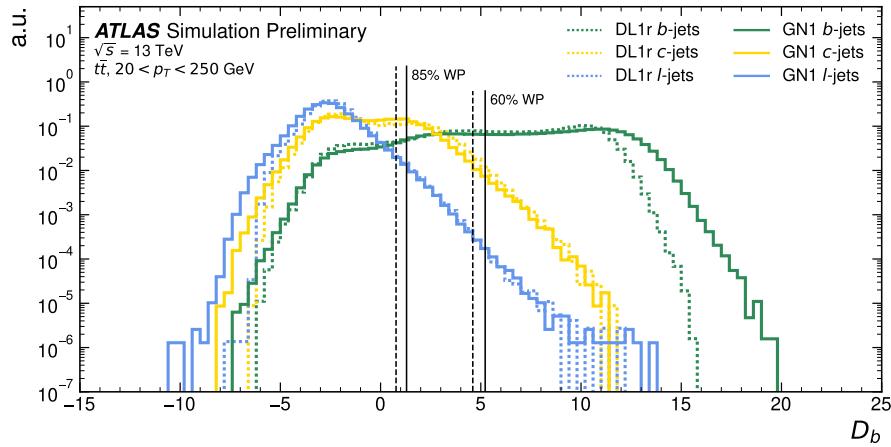


Figure 6.4: Comparison between the DL1r and GN1 b -tagging discriminant D_b for jets in the $t\bar{t}$ sample [2]. The 85% WP and the 60% WP are marked by the solid (dashed) lines for GN1 (DL1r), representing respectively the loosest and tightest WPs typically used by analyses. A value of $f_c = 0.018$ is used in the calculation of D_b for DL1r and $f_c = 0.05$ is used for GN1. The distributions of the different jet flavours have been normalised to unity area.

1590 6.4.1 b -tagging Performance

1591 The performance of b -tagging algorithms is quantified by their ability to reject c - and
 1592 light-jets for a given b -jet selection efficiency WP. In order to compare the b -tagging
 1593 performance of the different taggers for the b -jet tagging efficiencies in the range
 1594 typically used by analyses, the corresponding c - and light-jet rejection rates are
 1595 displayed in Figs. 6.5 and 6.6 for jets in the $t\bar{t}$ and Z' samples respectively. Four
 1596 standard WPs are defined with b -jet tagging efficiencies of 60%, 70%, 77% and 85%

1597 respectively. These WPs are commonly used by physics analyses depending on their
1598 specific signal and background requirements. The WPs are defined based on jets
1599 in the $t\bar{t}$ sample only. Due to the much higher jet p_T range in the Z' sample, and
1600 the increased difficulty in tagging jets at high- p_T (see Chapter 4), the b -jet tagging
1601 efficiencies for jets in the Z' sample are lower than the corresponding WPs calculated
1602 in the $t\bar{t}$ sample. For instance the WP cut value computed to provide a 70% b -jet
1603 tagging efficiency on the $t\bar{t}$ sample results in a b -jet tagging efficiency of just \sim 30%
1604 on the Z' sample. In order to account for this, the range of b -jet tagging efficiencies
1605 displayed for plots showing the performance for jets in the Z' sample (for example
1606 Fig. 6.6) is chosen to span the lower efficiencies achieved in the Z' sample at high- p_T .

1607 For jets in the $t\bar{t}$ sample with $20 < p_T < 250$ GeV, GN1 demonstrates considerably
1608 better c - and light-jet rejection when compared with DL1r across the full range of
1609 b -jet tagging efficiencies studied. The relative improvement is strongly dependent
1610 on the b -jet tagging efficiency under study. The largest improvements are found at
1611 lower b -jet tagging efficiencies. At a b -jet tagging efficiency of 70%, the c -jet rejection
1612 improves by a factor of \sim 2.1 while the light-jet rejection improves by a factor of \sim 1.8
1613 with respect to DL1r. For high- p_T jets in the Z' sample with $250 < p_T < 5000$ GeV,
1614 GN1 also brings a significant performance improvement with respect to DL1r across
1615 the range of b -jet tagging efficiencies studied. Again, the largest relative improvement
1616 in performance comes at the lower b -jet tagging efficiencies. At a b -jet efficiency of
1617 30%, GN1 improves the c -jet rejection with respect to DL1r by a factor of \sim 2.8 and
1618 the light-jet rejection by a factor of \sim 6. The performance comparison at lower b -jet
1619 tagging efficiencies is made more difficult due to the increased statistical uncertainties
1620 which result from the high rejection of background. Given that GN1 exploits the
1621 low-level detector information in a more complete and sophisticated way than DL1r,
1622 further studies are needed to confirm that the performance gain observed in these
1623 simulated samples is also observed in experimental data.

1624 The GN1Lep variant of GN1 demonstrates further improved performance with respect
1625 to the baseline model. This demonstrates the additional jet flavour discrimination
1626 power provided by the leptonID track input. For jets in the $t\bar{t}$ sample, the relative c -
1627 jet rejection improvement with respect to GN1 at the 70% b -jet WP is approximately
1628 30%. The improvement in light-jet rejection also increases by 40% at the same WP.
1629 For jets in the Z' sample, the relative c -jet rejection (light-jet rejection) performance

1630 with respect to GN1 improves by approximately 10% (25%) at a b -jet tagging
1631 efficiency of 30%.

1632 In general, the performance of all the taggers is strongly dependent on the jet p_T .
1633 This is due to the increased multiplicity and collimation of tracks, and the displaced
1634 decays that result from within the heavy flavour jets (see Chapter 4). Together,
1635 they contribute to a reduced reconstruction efficiency for heavy flavour tracks, and a
1636 general degradation in quality of tracks inside the core of a jet, which in turn reduces
1637 the jet tagging performance.

1638 In order to study how the tagging performance changes as a function of the jet p_T ,
1639 the b -jet tagging efficiency as a function of p_T for a fixed light-jet rejection of 100 in
1640 each bin is shown in Fig. 6.7. For jets in the $t\bar{t}$ sample, at a fixed light-jet rejection
1641 of 100, GN1 improves the b -jet tagging efficiency by approximately 4% across all the
1642 jet p_T bins. Meanwhile, GN1Lep again demonstrates improved performance with
1643 respect to GN1, in particular at lower p_T . The relative increase in the b -jet tagging
1644 efficiency increases from 4% to 8% with respect to DL1r. For jets in the Z' sample,
1645 GN1 again outperforms DL1r across the entire jet p_T range studied. The largest
1646 relative improvement in performance is found at the highest transverse momenta
1647 of jet $p_T > 2 \text{ TeV}$, and corresponds to an approximate factor of 2 improvement in
1648 efficiency with respect to DL1r.

1649 The performance of the model was also evaluated as a function of the average
1650 number of pileup interactions in the event. No significant dependence of the tagging
1651 performance was observed.

1652 6.4.2 c -tagging Performance

1653 As discussed previously, GN1 does not rely on any inputs from manually optimised
1654 low-level tagging algorithms. Since these algorithms were originally designed and
1655 tuned with the aim of b -tagging, and not c -tagging, the low level tagging algorithms
1656 may perform suboptimally for c -tagging purposes. The tagging of c -jets therefore
1657 presents a compelling use case for GN1. As each of the the models is trained with
1658 three output classes, using it as a c -tagging algorithm is trivially analogous to the
1659 approach used for b -tagging. The model output probabilities are combined into a
1660 single score D_c , which is defined similarly to Eq. (6.5) as

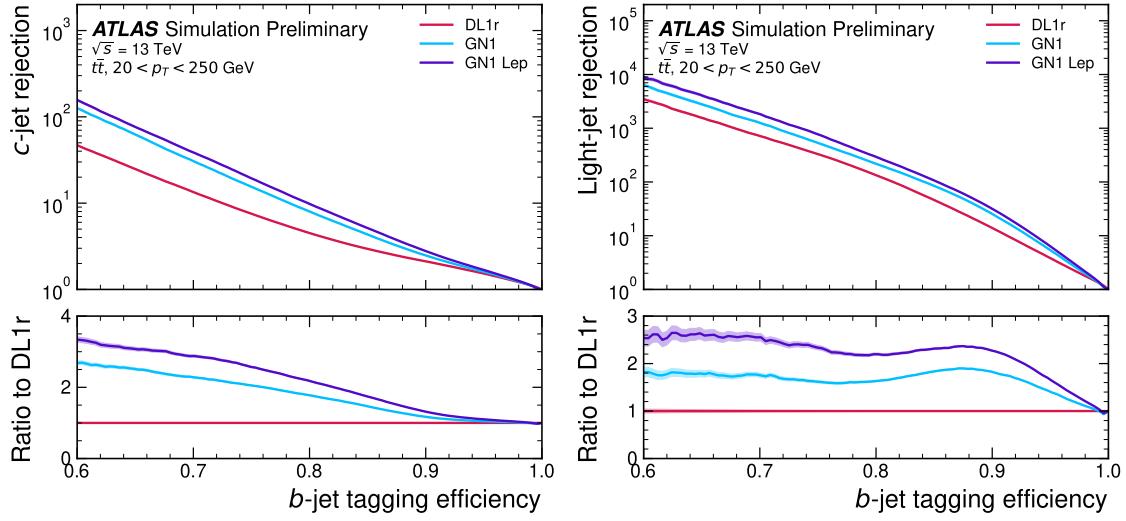


Figure 6.5: The c -jet (left) and light-jet (right) rejections as a function of the b -jet tagging efficiency for jets in the $t\bar{t}$ sample with $20 < p_T < 250 \text{ GeV}$ [2]. The ratio with respect to the performance of the DL1r algorithm is shown in the bottom panels. A value of $f_c = 0.018$ is used in the calculation of D_b for DL1r and $f_c = 0.05$ is used for GN1 and GN1Lep. Binomial error bands are denoted by the shaded regions. The x -axis range is chosen to display the b -jet tagging efficiencies usually probed in these regions of phase space.

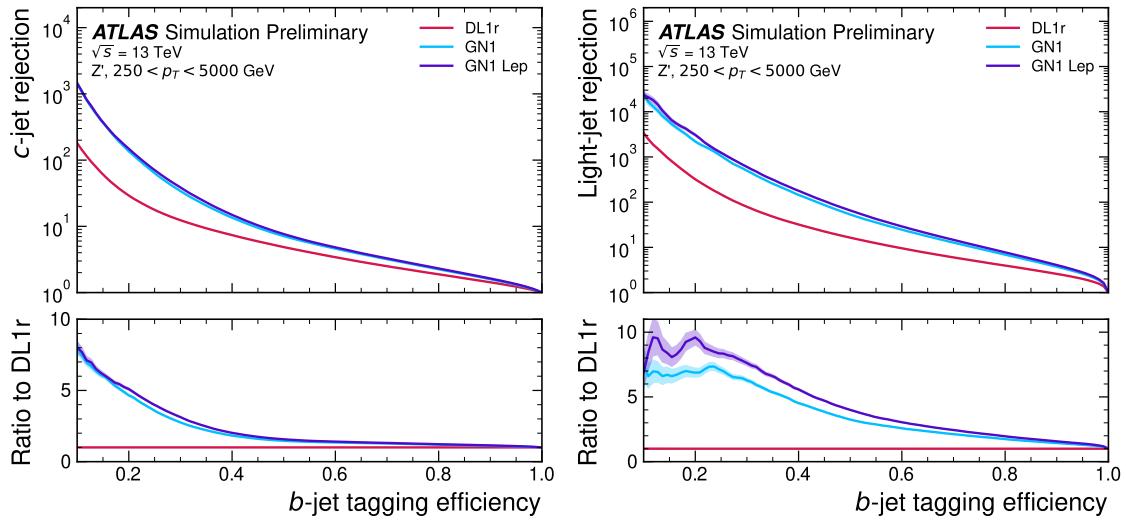


Figure 6.6: The c -jet (left) and light-jet (right) rejections as a function of the b -jet tagging efficiency for jets in the Z' sample with $250 < p_T < 5000 \text{ GeV}$ [2]. The ratio with respect to the performance of the DL1r algorithm is shown in the bottom panels. A value of $f_c = 0.018$ is used in the calculation of D_b for DL1r and $f_c = 0.05$ is used for GN1 and GN1Lep. Binomial error bands are denoted by the shaded regions. The x -axis range is chosen to display the b -jet tagging efficiencies usually probed in these regions of phase space.

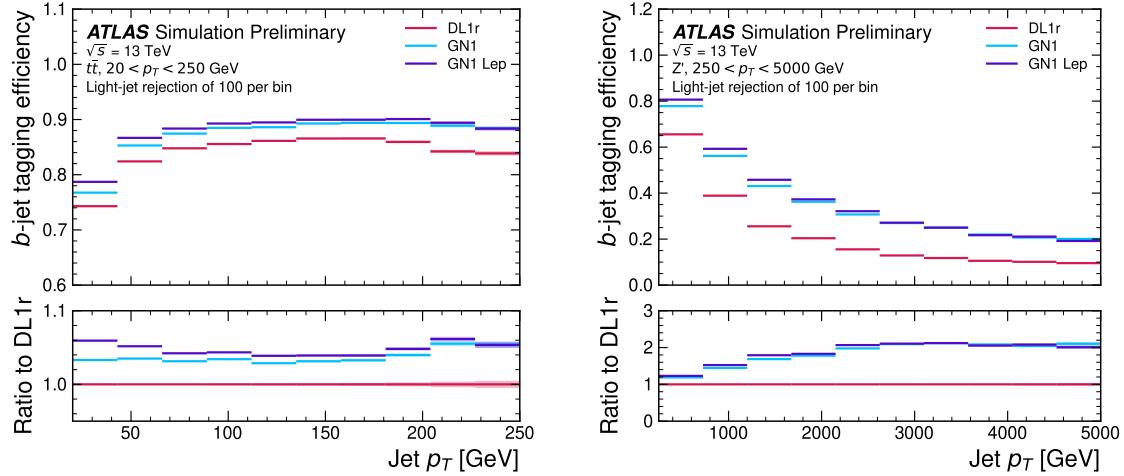


Figure 6.7: The *b*-jet tagging efficiency for jets in the $t\bar{t}$ sample (left) and jets in the Z' sample (right) as a function of jet p_T with a fixed light-jet rejection of 100 in each bin [2]. A value of $f_c = 0.018$ is used in the calculation of D_b for DL1r and $f_c = 0.05$ is used for GN1 and GN1Lep. GN1 demonstrates improved performance with respect to DL1r across the p_T range shown. Binomial error bands are denoted by the shaded regions.

$$D_c = \log \frac{p_c}{(1 - f_b)p_l + f_b p_b}. \quad (6.6)$$

1661 A value of $f_b = 0.2$ is used for all models, based on the same optimisation procedure
 1662 that was used for the *b*-tagging use case. Similar to Section 6.4.1, the different taggers
 1663 are compared to one another by scanning through a range of *c*-jet tagging efficiencies
 1664 and plotting the corresponding *b*- and light-jet rejection rates. As in Section 6.4.1,
 1665 the WPs are defined using jets in the $t\bar{t}$ sample. Standard *c*-jet tagging efficiency
 1666 WPs used by physics analyses are significantly lower than the *b*-tagging WPs in order
 1667 to maintain reasonable *b*- and light-jet rejection rates. This is reflected in the range
 1668 of *c*-jet tagging efficiencies used in *c*-tagging plots such as Figs. 6.8 and 6.9. Fig. 6.8
 1669 displays the *c*-tagging performance of the models on the jets in the $t\bar{t}$ sample. GN1
 1670 is shown to perform significantly better than DL1r. Similar to the *b*-tagging case,
 1671 the *b*- and light-jet rejection improve most at lower *c*-jet tagging efficiencies, with
 1672 the *c*-jet rejection (light-jet rejection) improving by a factor 2 (1.6) with respect to
 1673 DL1r at a *c*-jet tagging efficiency of 25%. GN1Lep again outperforms GN1, though
 1674 the improvements are more modest than observed for the *b*-tagging use case, with

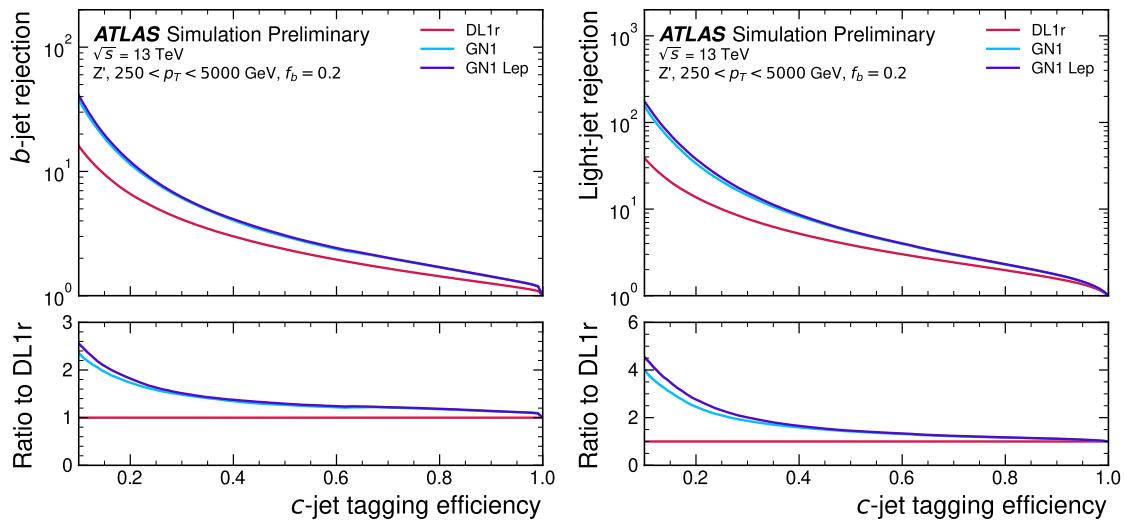
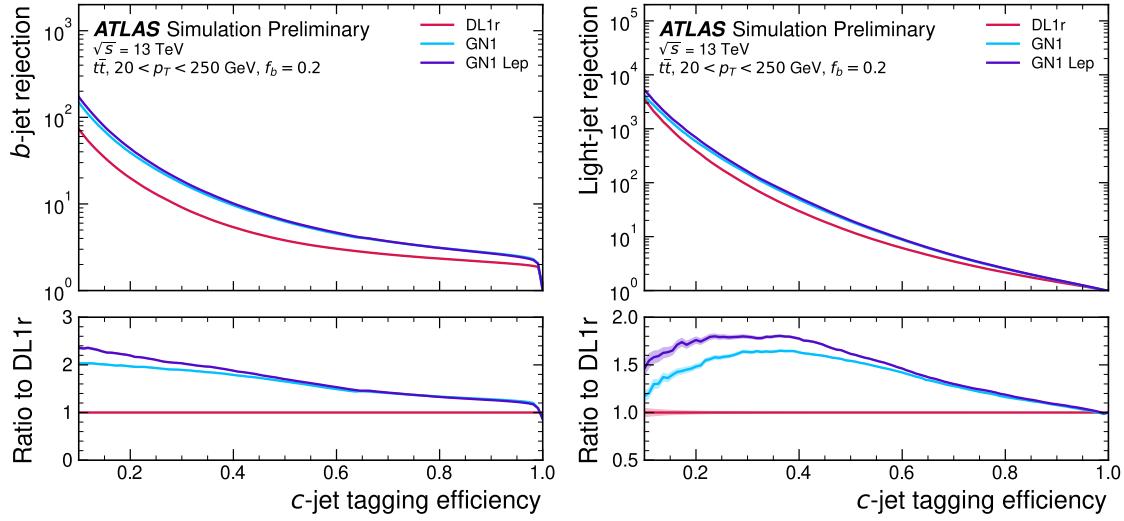
the both the b -jet rejection and light-jet rejection improving with respect to GN1 by approximately 10% at the 25% c -jet WP. Fig. 6.9 shows the c -tagging performance on the jets in the Z' sample with $250 < p_T < 5000$ GeV. Both GN1 and GN1Lep perform similarly, improving the b -jet rejection by 60% and the light-jet rejection by a factor of 2 at the 25% c -jet WP.

6.4.3 Ablations

Ablation studies (the removal of certain components of a given model in order to study the impact of that component) are carried out to determine the importance of the auxiliary training objectives of GN1 to the overall performance. The “GN1 No Aux” variant retains the primary jet classification objective, but removes both track classification and vertexing auxiliary objectives (see Section 6.3.2) and correspondingly only minimises the jet classification loss. The “GN1 TC” variant includes track classification objective but not the vertexing objective. Finally, the “GN1 Vert” includes the vertexing objective, but not the track classification objective.

For jets in both the $t\bar{t}$ and Z' samples, a general trend is observed that the models trained without one or both of the auxiliary objectives results in significantly reduced c - and light-jet rejection when compared with the baseline GN1 model. This result is shown clearly in Figs. 6.10 and 6.11. For jets in the $t\bar{t}$ sample, the performance of GN1 No Aux is similar to DL1r, while GN1 TC and GN1 Vert perform similarly to each other. For jets in the Z' sample meanwhile, the GN1 No Aux model already shows a clear improvement in c - and light-jet rejection when compared with DL1r at lower b -jet tagging efficiencies. Similar to jets in the $t\bar{t}$ sample, GN1 TC and GN1 Vert perform similarly, and bring large gains in background rejection when compared with GN1 No Aux, but the combination of both auxiliary objectives yields the best performance.

It is notable that the GN1 No Aux model matches or exceeds the performance of DL1r without the need for inputs from the low-level algorithms. This indicates that the performance improvements enabled by the improved neural network architecture used in GN1 appear to be able to compensate for the removal of the low-level algorithm inputs. The GN1 TC and GN1 Vert variants each similarly outperform DL1r, demonstrating that both contribute to the overall high performance of the baseline model. The overall best performing model is the full version of GN1 trained



1707 with both auxiliary objective, demonstrating that the two auxiliary objectives are
1708 complementary.

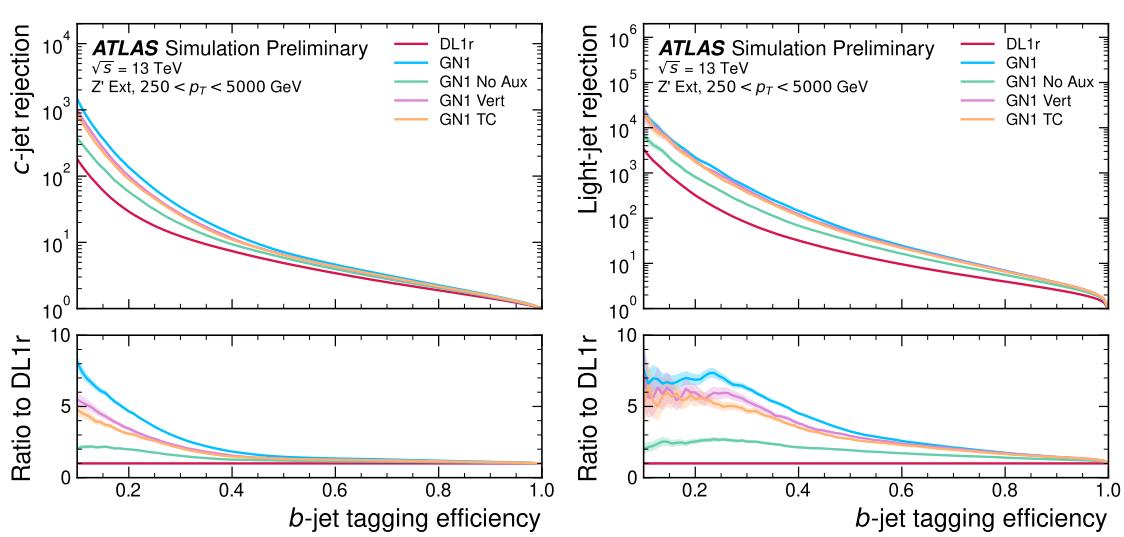
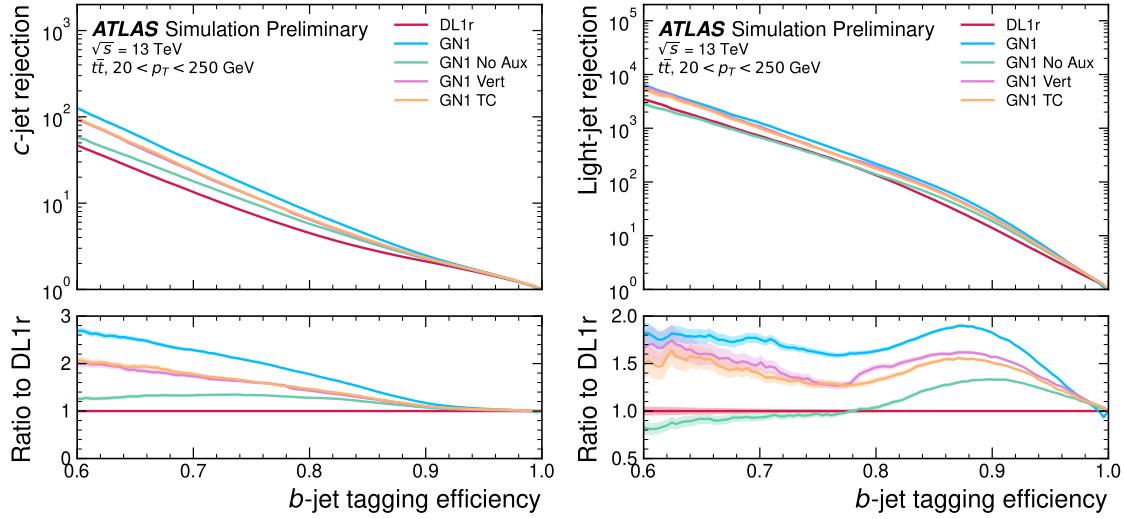
1709 6.4.4 Inclusion of Low-Level Vertexing Algorithms

1710 As already mentioned, GN1 does not include any inputs from the low-level tagging
1711 algorithms, including the vertexing algorithms SV1 and JetFitter [61]. Since these
1712 algorithms are known to play a key role in contributing to the performance of DL1r, it
1713 was necessary to study whether their inclusion in GN1 resulted in further performance
1714 improvements. In a dedicated training of GN1 the SV1 and JetFitter tagger outputs
1715 were added to the GN1 jet classification network as an input, similar to how they
1716 are used in DL1r. These outputs include information on the reconstructed vertices,
1717 including the number of vertices, and the properties of the highest ranking recon-
1718 structed vertex (in the case of JetFitter). In addition, the index of the reconstructed
1719 SV1 or JetFitter vertices were included as two track-level inputs to GN1. These
1720 indices were also used to construct an input feature for the edge classification
1721 network used to identify vertices, which was given a value of one if the track-pair
1722 were from a common reconstructed SV1 or JetFitter vertex, and zero otherwise. The
1723 jet classification performance of this GN1 model was not significantly different to the
1724 baseline model, and in some cases the performance was slightly reduced. GN1 does
1725 not benefit from the inclusion of information from SV1 and JetFitter, indicating
1726 that the model is able to reconstruct the relevant information provided by these
1727 low-level algorithms. The study also demonstrates that the model can function as a
1728 highly performant standalone tagger that does not require (beyond retraining) any
1729 manual optimisation to achieve good performance in a wide range of phase spaces.
1730 A dedicated look at the vertexing performance of GN1 with some comparisons to
1731 SV1 and JetFitter is found in Section 6.4.6

determine ranking

1732 6.4.5 Jet Display Diagrams

1733 The auxiliary training objectives of GN1 allow for improved model interpretability,
1734 which is especially important for a monolithic approach as the low level taggers,
1735 which provide useful physical insight, are no longer present. Figs. 6.12 and 6.13
1736 provide example comparisons of the true origin and vertexing information compared



1737 with the predicted values from GN1, SV1 and JetFitter. Such comparisons can be
1738 used to provide an indication that GN1 reconstructs the correct representation of the
1739 jet structure, and may also help to identify limitations of the model. In the figures,
1740 the tracks in the jet are indexed twice on each of the x - and y -axes, and tracks are
1741 grouped into vertices along with other tracks as indicated by common markings in
1742 the relevant rows and columns.

1743 In Fig. 6.12, GN1 correctly groups the three primary tracks as having come from the
1744 primary vertex. The b -hadron and $b \rightarrow c$ -hadron decay vertices are also correctly
1745 predicted, and the origin of the tracks in each is correct. There is a single OtherSec-
1746 ondary track which GN1 incorrectly predicts as having come pileup. Meanwhile SV1
1747 (by design) merges the two heavy flavour decay vertices, but incorrectly includes a
1748 track from the primary vertex. JetFitter reconstructs two vertices, one which is a
1749 combination of two tracks from different truth vertices and two other single track
1750 vertices in each of the heavy flavour vertices. GN1 also predicts the flavour of the jet
1751 with a high degree of certainty.

1752 Similarly, Fig. 6.12 shows that GN1 is able to relatively accurately predict the origin
1753 and vertex information of tracks inside a jet. The pileup tracks and primary vertex
1754 tracks are correctly identified, and the heavy flavour decay tracks are also correctly
1755 identified with the exception of one of the b -hadron decay tracks. Again, SV1 merges
1756 the two heavy flavour decay vertices along with a track from pileup, while JetFitter
1757 shows signs of being underconstrained by reconstructing two single track vertices,
1758 one with a pileup track and one with a track from a $b \rightarrow c$ -hadron decay.

1759 6.4.6 Vertexing Performance

1760 From the track-pair vertex prediction described in Section 6.3.2, tracks can be
1761 partitioned into compatible groups representing vertices (see [114]). As such, GN1
1762 can perform vertex “finding”, but not vertex “fitting”, i.e. the reconstruction of
1763 a vertex’s properties, which currently still requires the use of a dedicated vertex
1764 fitter. In order to study the performance of the different vertexing tools, the truth
1765 vertex label of the tracks, discussed in Section 6.3.2, are used. To estimate the
1766 efficiency with which GN1 manages to find vertices inclusively, vertices containing
1767 tracks identified as coming from a b -hadron are merged together and compared to the
1768 inclusive truth decay vertices that result from a b -hadron decay (where if there are

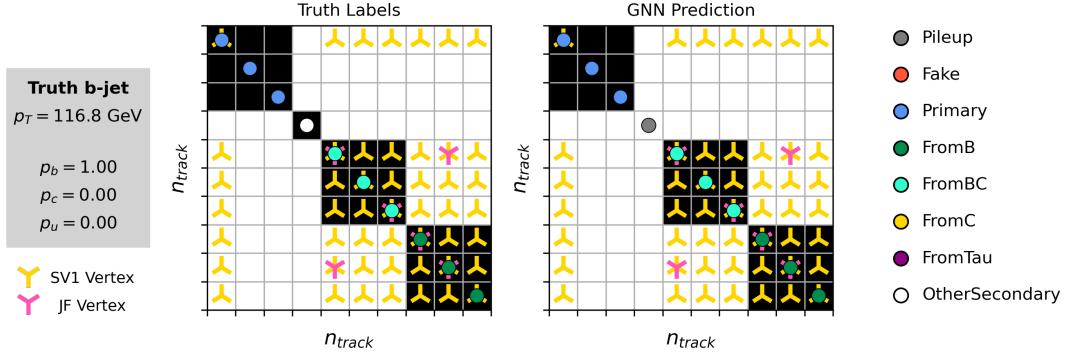


Figure 6.12: A schematic showing the truth track origin and vertex information (left) compared with the predictions from GN1 (right). The diagrams show the truth (left) and predicted (right) structure of a b -jet. The shaded black boxes show the groupings of tracks into different vertices. Vertices reconstructed by SV1 and JetFitter are also marked. Class probabilities p_b , p_c and p_u are rounded to three significant figures. GN1 improves over SV1 and JetFitter by successfully determining the origins and vertex compatibility of all the tracks in the jet with the exception of the truth OtherSecondary track, which is misidentified as pileup.

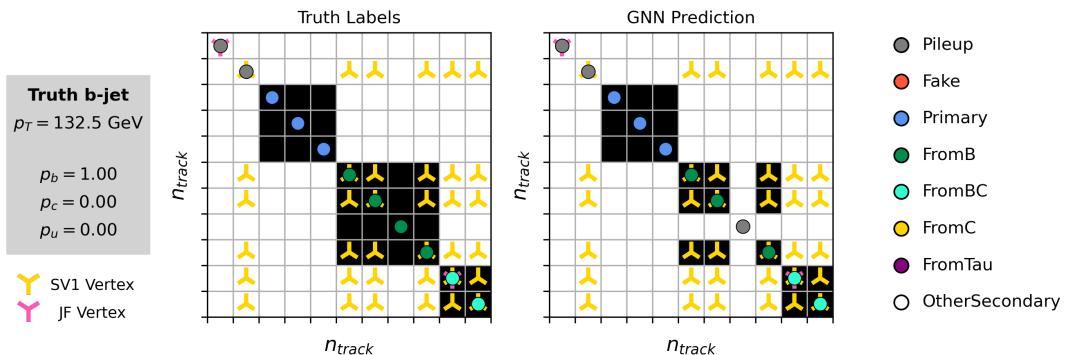


Figure 6.13: A schematic showing the truth track origin and vertex information (left) compared with the predictions from GN1 (right). The diagrams show the truth (left) and predicted (right) structure of a b -jet. The shaded black boxes show the groupings of tracks into different vertices. Vertices reconstructed by SV1 and JetFitter are also marked. Class probabilities p_b , p_c and p_u are rounded to three significant figures. GN1 improves over SV1 and JetFitter by successfully determining the origins and vertex compatibility of all but one tracks in the jet.

multiple distinct truth vertices from a b -hadron decay they are also merged together). Vertices are compared with the target truth vertex and the number of correctly and incorrectly assigned tracks is computed. Since secondary vertex information is only recovered for reconstructed tracks, a vertex finding efficiency of 100% denotes that all possible secondary vertices are found given the limits set by the track reconstruction efficiency. A vertex is considered matched if it contains at least 65% of the tracks in the corresponding truth vertex, and has a purity of at least 50%. GN1 manages to achieve an inclusive reconstruction efficiency in b -jets of $\sim 80\%$, demonstrating that it effectively manages to identify the displaced vertices from b -hadron decays.

There are several caveats to a comparison of the vertexing tools which are a result of the different approaches they take to vertexing. SV1 and JetFitter are designed to only find secondary vertices in the jet, whereas GN1 is also trained to determine which tracks in the jet belong to the primary vertex (the vertex of the hard scatter pp interaction). To account for this the GN1 vertex with the largest number of predicted primary tracks is excluded from the vertex finding efficiency calculation. While JetFitter and GN1 aim to resolve each displaced vertex inside the jet, such that secondary vertices from b -hadron decays are found separately to tertiary vertices from $b \rightarrow c$ decay chains, SV1 by design attempts to find a single inclusive vertex per jet. This inclusive vertex groups tracks from the b -hadron decay itself (FromB) and tracks from $b \rightarrow c$ decays (FromBC). In order to fairly compare the performance of the different tools, both the exclusive and inclusive vertex finding efficiency is studied. For the exclusive vertex finding case JetFitter and GN1 can be directly compared, while a comparison with SV1 is not possible due to the aforementioned design constraints. The inclusive vertex finding performance of all three tools can be compared using the procedure outlined below.

The starting point for the secondary vertex finding efficiency in both the exclusive and inclusive cases is to select truth secondary vertices, defined as those containing only inclusive b -hadron decays. For exclusive vertex finding, these truth secondary vertices can be used directly as the denominator for the efficiency calculation. Meanwhile for the inclusive efficiency all such truth secondary vertices in the jet are merged into a single inclusive target vertex. Correspondingly, for the inclusive vertex finding case, the vertices found by JetFitter are merged into a single vertex, and the vertices found by GN1, which contain at least one predicted b -hadron decay track, are also

merged similarly. SV1 does not require any vertex merging. Only jets containing a single b -hadron at truth level are considered.

Next, vertices in the jet found by the different vertexing tools are compared with the target truth vertices. The number of correctly and incorrectly assigned tracks is computed. In order to call a vertex efficient, it is required to contain at least 65% of the tracks in the corresponding truth vertex, and to have a purity of at least 50%. Single track vertices are required to have a purity of 100%. Additionally, for GN1 only, at least one track in the vertex is required to have a predicted heavy flavour origin.

Vertex finding efficiencies for b -jets in the $t\bar{t}$ sample are displayed as a function of p_T separately for the inclusive and exclusive approaches in Fig. 6.14. For b -jets in the $t\bar{t}$ sample with $20 < p_T < 250$ GeV, the exclusive vertex finding efficiency of JetFitter and GN1 is relatively flat as a function of p_T . For the truth secondary vertices in this p_T region, JetFitter efficiently finds approximately 40% and GN1 finds approximately 55%. When finding vertices inclusively the vertex finding efficiency is generally higher. An increased dependence on p_T is also visible for JetFitter and SV1. As the jet p_T increases from 20 GeV to 100 GeV, the efficiency of JetFitter increases from 60% to 65%. In the same range, the efficiency of SV1 increases from 60% to 75%. GN1 displays less dependence on p_T than JetFitter and SV1, efficiently finding upwards of 80% of vertices in b -jets in this p_T region. For b -jets with $p_T > 100$ GeV, JetFitter finds approximately 65% of vertices, SV1 finds approximately 75% of vertices, and GN1 finds approximately 80% of vertices.

Fig. 6.15 compares the exclusive vertex finding efficiencies of JetFitter and GN1 for multitrack vertices. For b -jets in the Z' sample, the vertex finding efficiency drops steeply with increasing p_T up until $p_T = 3$ TeV. GN1 outperforms SV1 and JetFitter across the p_T spectrum. In the first bin, the efficiency of GN1 is 75%, while the efficiencies of SV1 and JetFitter are around 60%. The efficiency of SV1 drops rapidly to almost zero above 3 TeV, while JetFitter and GN1 retain approximately 25% and 30% efficiency respectively. JetFitter finds 45-50% of vertices in b -jets in the $t\bar{t}$ sample, while GN1 finds 60-65%. For b -jets in the Z' sample, JetFitter finds 35% of vertices in the first bin, dropping to 20% of vertices above 2 TeV. GN1 finds 55% of vertices in the first bin, dropping to 30% above 2 TeV.

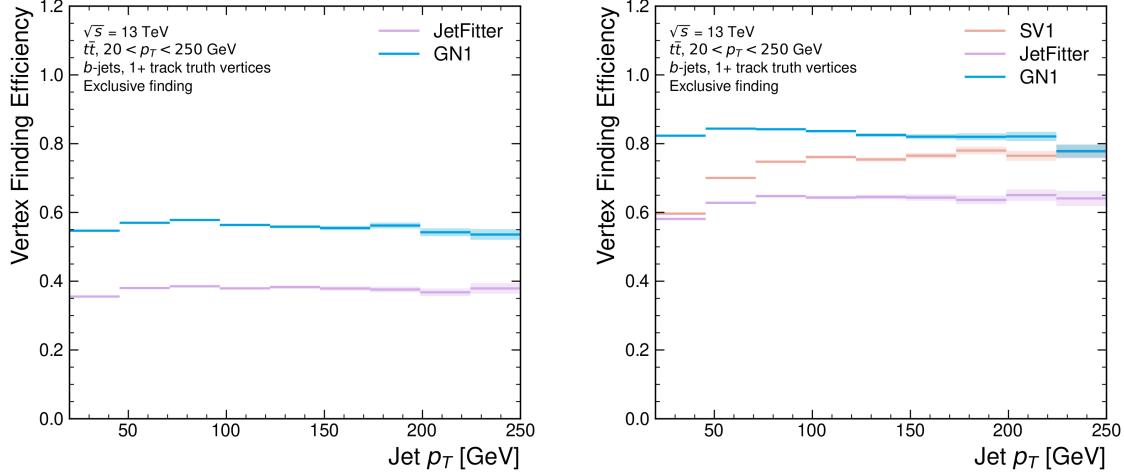


Figure 6.14: Vertex finding efficiency as a function of jet p_T for b -jets in the $t\bar{t}$ sample using the exclusive (left) and inclusive (right) vertex finding approaches. The exclusive vertexing approach includes single track vertices while the inclusive approach requires vertices to contain at least two tracks. Efficient vertex finding requires the recall of at least 65% of the tracks in the truth vertex, and allows no more than 50% of the tracks to be included incorrectly. Binomial error bands are denoted by the shaded regions.

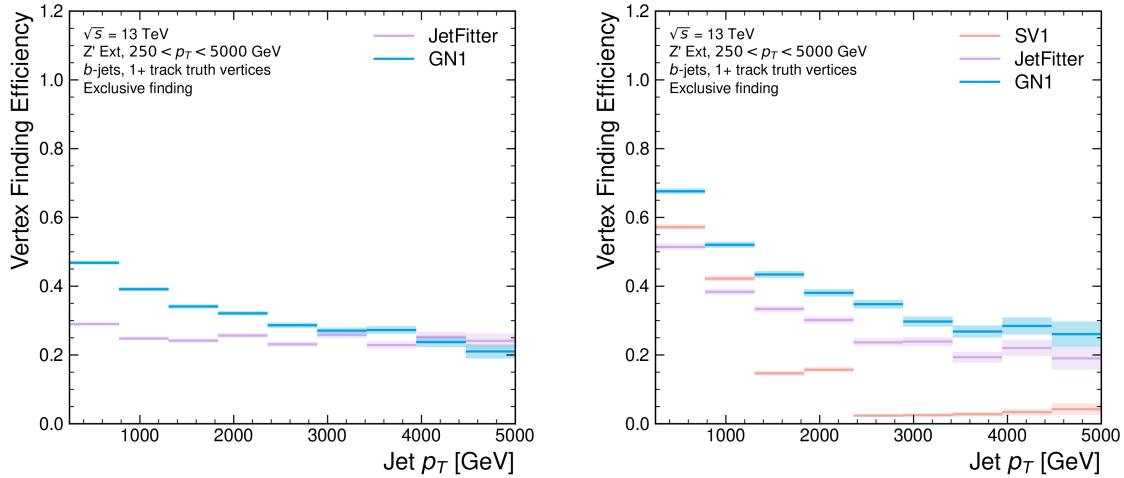


Figure 6.15: Inclusive vertex finding efficiency for multitrack truth vertices in b -jets in the $t\bar{t}$ sample (left) and jets in the Z' sample (right) as a function of jet p_T . The exclusive vertexing approach includes single track vertices while the inclusive approach requires vertices to contain at least two tracks. Efficient vertex finding requires the recall of at least 65% of the tracks in the truth vertex, and allows no more than 50% of the tracks to be included incorrectly.

6.4.7 Track Classification Performance

One of the two auxiliary training objectives used by GN1 is to predict the truth origin of each track associated to the jet, as discussed in Section 6.3.2. Since the equivalent information is not provided by any of the existing flavour tagging tools, a benchmark model used to predict the truth origin of each track is trained based on a standard multi-class feed-forward classification network. The benchmark model is trained on the same tracks used for the baseline GN1 training. The model uses precisely the same concatenated track-and-jet inputs as used by GN1 (see Section 6.3.1), but processes only a single track at a time, meaning it cannot take into account the correlations between tracks when determining the track origin. The model is made up of five densely connected linear layers with 200 neurons in each layer. The performance of the model was found to be unsensitive to changes in the network structure.

To measure the track classification performance, the area under the curve (AUC) of the receiver operating characteristic (ROC) curve is computed for each origin class, using a one-versus-all classification approach. The AUCs for the different truth origins are averaged using both an unweighted and a weighted mean. The unweighted mean treats the performance of each class equally, while the weighted mean uses as a weight the relative abundance of tracks of each class. Table 6.3 demonstrates clearly that GN1 outperforms the MLP both at $20 < p_T < 250 \text{ GeV}$ for jets in the $t\bar{t}$ sample and at $250 < p_T < 5000 \text{ GeV}$ for jets in the Z' sample. For example, GN1 can reject 65% of fake tracks in jets in the $t\bar{t}$ sample, while retaining more than 99% of good tracks (i.e. those tracks which are not fake). The GN1 model has two advantages over the MLP which can explain the performance improvement. Firstly, the graph neural network architecture enables the sharing of information between tracks as discussed in Section 6.3.3. This is likely to be beneficial since the origins of different tracks within a jet are correlated. Secondly, the jet classification and vertexing objectives may be complementary to the track classification objective, and so the track classification performance is improved by the combined training of complementary objectives.

Fig. 6.16 shows the track origin classification ROC curves for the different track origins for jets in both the $t\bar{t}$ and Z' samples. In order to improve visual readability of the plot, the curves for the heavy flavour truth origins (FromB, FromBC and

		AUC		Precision		Recall		F1	
		Mean	Weighted	Mean	Weighted	Mean	Weighted	Mean	Weighted
$t\bar{t}$	MLP	0.87	0.89	0.39	0.71	0.51	0.56	0.36	0.62
	GN1	0.92	0.95	0.51	0.82	0.64	0.70	0.51	0.74
Z'	MLP	0.90	0.94	0.36	0.84	0.47	0.72	0.31	0.76
	GN1	0.94	0.96	0.48	0.88	0.60	0.79	0.48	0.82

Table 6.3: The area under the ROC curves (AUC) for the track classification from GN1, compared to a standard multilayer perceptron (MLP) trained on a per-track basis. The unweighted mean AUC over the origin classes and weighted mean AUC (using as a weight the fraction of tracks from the given origin) is provided. GN1, which uses an architecture that allows track origins to be classified in a conditional manner as discussed in Section 6.3.3, outperforms the MLP model for both $t\bar{t}$ and Z' jets.

FromC) have been combined (weighted by their relative abundance), as have the Primary and OtherSecondary origins. In jets in both the $t\bar{t}$ and Z' samples, the AUC of all the different origin groups exceeds 0.9, representing strong overall classification performance. In both samples fake tracks are the easiest to classify, followed by pileup tracks. The FromC tracks which are c -hadron decay products, are the hardest to classify, possibly due to their similarity to both fragmentation tracks and b -hadron decay tracks, depending on the c -hadron species in question.

6.4.8 Looser Track Selection

The track selections used to produce the main results are listed in Table 5.3. This selection includes a cut on the number of shared silicon modules used to reconstruct the track $N_{\text{shared}}^{\text{Si}}$. This value is calculated as

$$N_{\text{shared}}^{\text{Si}} = \frac{N_{\text{shared}}^{\text{Pix}} + N_{\text{shared}}^{\text{SCT}}}{2} \quad (6.7)$$

where $N_{\text{shared}}^{\text{Pix}}$ is the number of shared pixel hits and $N_{\text{shared}}^{\text{SCT}}$ is the number of shared SCT modules on a track. The nominal cut used elsewhere in this thesis is $N_{\text{shared}}^{\text{Si}} < 2$. As the rate of shared hits is significantly higher for b -hadron decay tracks than for other tracks, especially at high- p_T , this cut rejects a significant proportion of these tracks.

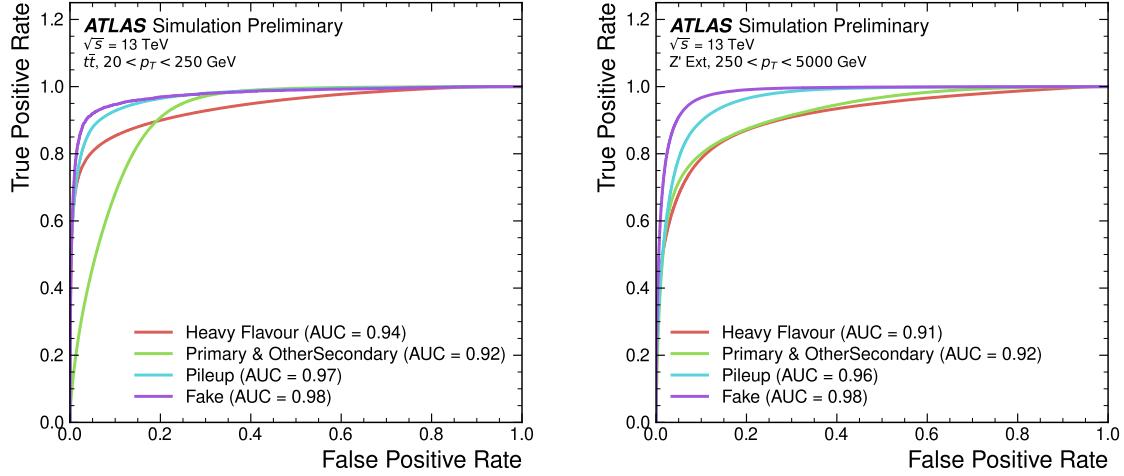


Figure 6.16: ROC curves for the different groups of truth origin labels defined in Table 5.1 for jets in the $t\bar{t}$ sample (left) and jets in the Z' sample [2]. The FromB, FromBC and FromC labels have been combined, weighted by their relative abundance, into the Heavy Flavour category, and the Primary and OtherSecondary labels have similarly been combined into a single category. The mean weighted area under the ROC curves (AUC) is similar for both samples.

1883 Figs. 6.17 and 6.18 show the result of training the GN1 tagger with the full relaxation
1884 of this cut, i.e. allowing tracks with any number of shared hits. The shared hit
1885 requirements applied by the ambiguity solver as part of track reconstruction (see
1886 Section 3.4.1) are still applied. In addition, the maximum allowed value of d_0 is
1887 increased from 3.5 mm to 5.0 mm. The results show that optimisation of the input
1888 track selection can lead to significant improvements in performance over the default
1889 selection. For the jets in the $t\bar{t}$ sample shown in Fig. 6.17, the effect of loosening
1890 the track selection is limited. This is expected due to the lower prevalence of shared
1891 hits at highly displaced tracks at lower transverse momenta. However for jets in the
1892 Z' sample as shown in Fig. 6.18, the light-jet rejection improves with respect to the
1893 baseline GN1 model by 30%, while the light-jet rejection improves by 70% at the
1894 50% b -jet WP.

1895 Although the results demonstrate a significant performance improvement at high- p_T ,
1896 it is also possible that additional studies on further loosening the selection could yield
1897 further improved results. For example the selections on the number of number of
1898 holes and the longitudinal impact parameter could be further relaxed. The maximum
1899 number of tracks provided as input to the model could also be increased from the

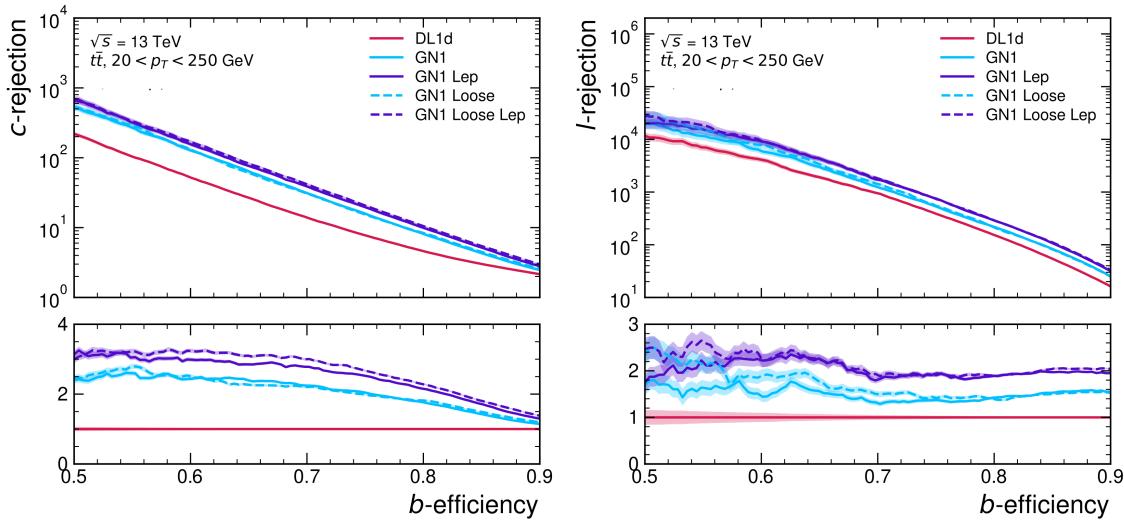


Figure 6.17: The c -jet (left) and light-jet (right) rejections as a function of the b -jet tagging efficiency for $t\bar{t}$ jets with $20 < p_T < 250$ GeV, for the looser track selection trainings of GN1. The ratio to the performance of the DL1d algorithm [122] is shown in the bottom panels. A value of $f_c = 0.018$ is used in the calculation of D_b for DL1d and $f_c = 0.05$ is used for GN1. Binomial error bands are denoted by the shaded regions.

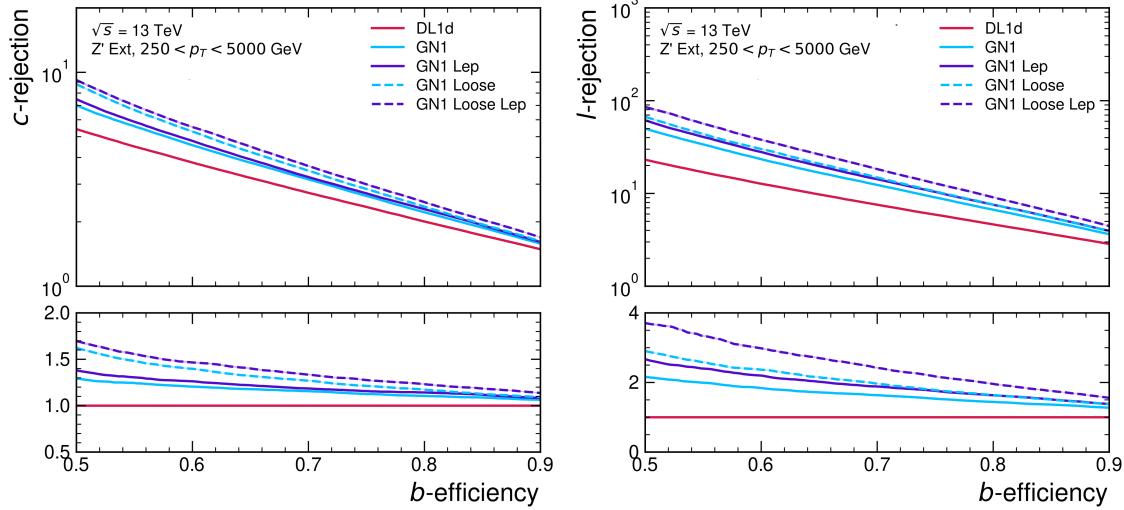


Figure 6.18: The c -jet (left) and light-jet (right) rejections as a function of the b -jet tagging efficiency for Z' jets with $250 < p_T < 5000$ GeV, for the looser track selection trainings of GN1. The ratio to the performance of the DL1d algorithm [122] is shown in the bottom panels. A value of $f_c = 0.018$ is used in the calculation of D_b for DL1d and $f_c = 0.05$ is used for GN1. Binomial error bands are denoted by the shaded regions.

1900 default value of 40. In order to change the default tracking setup, studies investigating
1901 the modelling uncertainties of the additional tracks need to be carried out.

1902 6.5 Other Implementations of GN1

1903 The implementation of GN1 described in this chapter has been re-used in several
1904 other contexts, demonstrating its flexibility to easily provide good jet flavour tagging
1905 performance with minimal overhead. The model has been implemented as a b -jet
1906 tagger in the High Level Trigger (HLT) (see Section 3.3.4). The inputs to the
1907 model are the running on precision tracks and jet level quantities reconstructed after
1908 primary vertexing. Fig. 6.19 shows the performance of GN1 versus a comparable
1909 DL1d model [122], and two versions of DIPS [80], with EMTopo and PFlow jets (see
1910 Section 3.4.3) based on a low-precision region-of-interest based tracking pass. The
1911 trigger implementation of GN1 improves upon the light-jet rejection of DL1d by 50%
1912 at the 60% b -jet WP for jets in the $t\bar{t}$ sample with $20 < p_T < 250$ GeV.

1913 The model also demonstrates strong performance for the High Luminosity LHC
1914 (HL-LHC), as documented in Ref. [124]. Figs. 6.20 and 6.21 are reproduced from
1915 Ref. [124]. The results show that GN1 outperforms other existing flavour tagging
1916 algorithms when trained on an entirely different detector geometry. When compared
1917 with DL1d [122], GN1 improves on the c -jet rejection (light-jet rejection) by a factor
1918 of ~ 2 (~ 2.5) for jets in the $t\bar{t}$ sample at the 60% b -jet WP. Significant improvements
1919 in rejections are also observed for jets in the Z' sample.

1920 6.6 Conclusion

1921 In this chapter a novel jet tagger, GN1, is presented. The model has a graph neural
1922 network architecture and is trained with auxiliary training objectives, which are
1923 shown to improve the performance of the basic model. GN1 significantly improves
1924 flavour tagging performance with respect to DL1r, the current default ATLAS flavour
1925 tagging algorithm, when compared in simulated collisions. GN1 improves c - and
1926 light-jet rejection for jets in the $t\bar{t}$ sample with $20 < p_T < 250$ GeV by factors of
1927 ~ 2.1 and ~ 1.8 respectively at a b -jet tagging efficiency of 70% when compared with

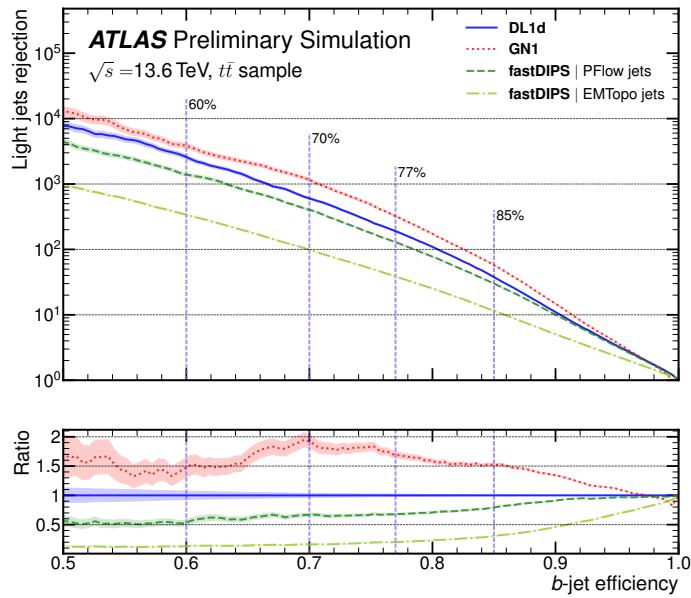


Figure 6.19: The light-jet rejection as a function of the b -jet efficiency jets in the $t\bar{t}$ sample with $20 < p_T < 250 \text{ GeV}$ for events with a centre of mass energy $\sqrt{s} = 13.6 \text{ TeV}$ [123]. The ratio to the performance of the DL1d algorithm [122] is shown in the bottom panels. Binomial error bands are denoted by the shaded regions. The purple vertical dashed lines represent the most common working points used for b-tagging.

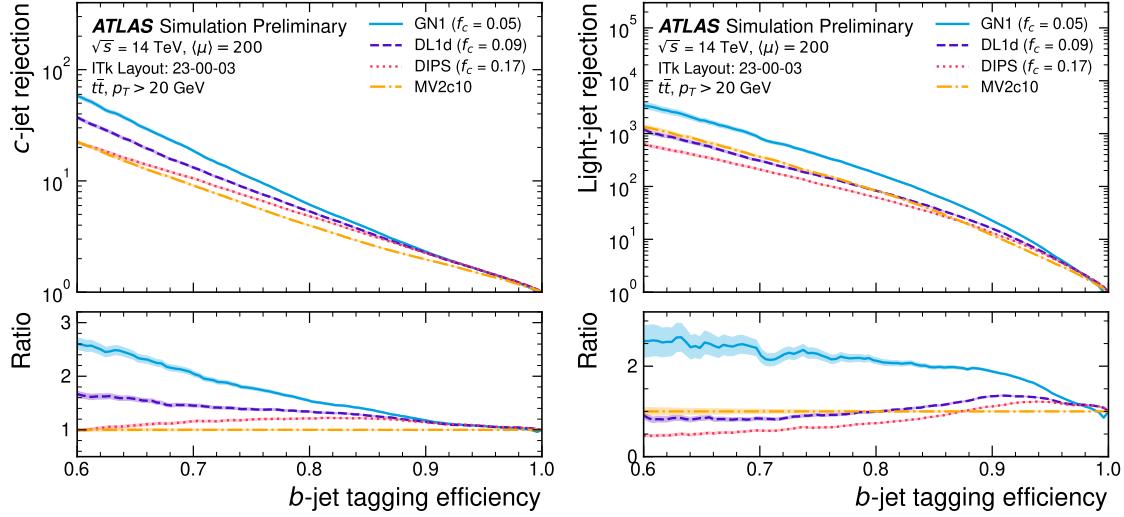


Figure 6.20: The c -jet rejection (left) and light-jet rejection (right) as a function of the b -jet efficiency for jets in the $t\bar{t}$ sample with $20 < p_T < 250 \text{ GeV}$ for events with a centre of mass energy $\sqrt{s} = 14 \text{ TeV}$ [124]. The ratio to the performance of the DL1d algorithm is shown in the bottom panels. Binomial error bands are denoted by the shaded regions. The purple vertical dashed lines represent the most common working points used for b -tagging.

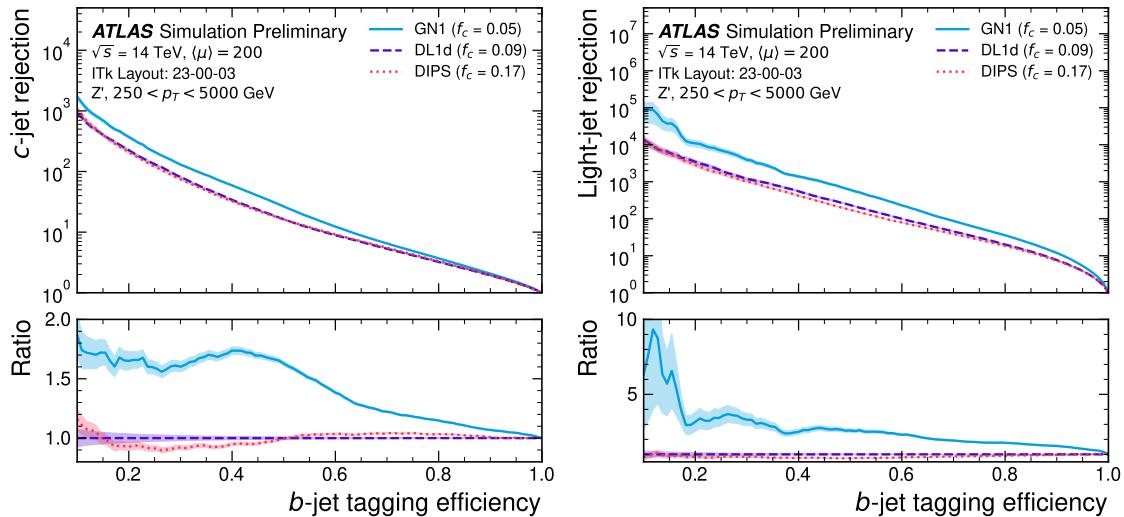


Figure 6.21: The c -jet rejection (left) and light-jet rejection (right) as a function of the b -jet efficiency for jets in the Z' sample with $250 < p_T < 5000 \text{ GeV}$ for events with a centre of mass energy $\sqrt{s} = 14 \text{ TeV}$ [124]. The ratio to the performance of the DL1d algorithm is shown in the bottom panels. Binomial error bands are denoted by the shaded regions.

1928 DL1r. For jets in the Z' sample with $250 < p_T < 5000 \text{ GeV}$, GN1 improves the
1929 c -jet rejection by a factor of ~ 2.8 and light-jet rejection by a factor of ~ 6 for a
1930 comparative b -jet efficiency of 30%.

1931 Previous multivariate flavour tagging algorithms relied on inputs from low-level
1932 tagging algorithms, whereas GN1 needs no such inputs, making it more flexible.
1933 It can be easily fully optimised via a retraining for specific flavour tagging use
1934 cases, as demonstrated with c -tagging and high- p_T b -tagging, without the need for
1935 time-consuming retuning of the low-level tagging algorithms. The model is also
1936 simpler to maintain and study due to the reduction of constituent components.

1937 GN1 demonstrates improved track classification performance when compared with
1938 a simple per-track MLP and an efficiency of $\sim 80\%$ for inclusive vertex finding in
1939 b -jets. The model is also able to perform vertex finding, and preliminary studies
1940 suggest it outperforms previous manually optimised approaches. The auxiliary track
1941 classification and vertex finding objectives are shown to significantly contribute to
1942 the performance in the jet classification objective, and, along with the more advanced
1943 graph neural network architecture, are directly responsible for the improvement over
1944 DL1r.

1945 Further improvements in the b - and c -tagging performance are likely possible with
1946 a more thorough optimisation of the model architecture, and the integration of
1947 additional information from other parts of the ATLAS detector. The addition of
1948 other auxiliary training objectives, such as the truth b -hadron decay radius and
1949 transverse momentum, may also yield additional performance gains on top of the
1950 gains achieved by loosening the input track selection (demonstrated in Section 6.4.8).

1951 Additional future work includes the verification of the performance of GN1 on collision
1952 data, and the full calibration of the model so it can be used by analyses. The flexible
1953 nature of the model means it can also be readily applied to other related problems
1954 outside of standard b - and c -tagging applications, for example $X \rightarrow bb$ and $X \rightarrow cc$
1955 tagging. The model could also be repurposed as a pileup jet tagger, or general
1956 primary and secondary vertexing tool.

1957 And flavour tagging in the trigger and for the High Luminosity LHC as described in
1958 Section 6.5.

₁₉₅₉ **Chapter 7**

₁₉₆₀ **Boosted VHbb Analysis**

₁₉₆₁ The Higgs boson, first observed by ATLAS and CMS at the LHC in 2012 [13, 14],
₁₉₆₂ is predicted by the standard model to decay primarily to a pair of b -quarks, with a
₁₉₆₃ branching factor of 0.582 ± 0.007 for $m_H = 125$ GeV [25]. Observation of this decay
₁₉₆₄ mode was reported by ATLAS [110] and CMS [27] in 2018, establishing the first
₁₉₆₅ direct evidence for the Yukawa coupling of the Higgs boson to down-type quarks
₁₉₆₆ (see Section 2.2.2). The $H \rightarrow b\bar{b}$ process is also important for constraining the total
₁₉₆₇ decay width of the Higgs [125].

₁₉₆₈ Whilst the dominant Higgs production mechanism at the LHC is gluon-gluon fusion
₁₉₆₉ as outlined in Section 2.2.3, this mechanism has an overwhelming QCD multijet
₁₉₇₀ background and so overall sensitivity to the Higgs is low. The QCD multijet
₁₉₇₁ background refers to events containing one or more strongly produced jets which are
₁₉₇₂ not the decay product of heavy resonances, for example $g \rightarrow q\bar{q}$. The gluon-gluon
₁₉₇₃ fusion channel contains to leading order only jets in the final state, and therefore
₁₉₇₄ it is extremely difficult to distinguish signal events from the overwhelming multijet
₁₉₇₅ background. The $H \rightarrow b\bar{b}$ observation therefore searched for Higgs bosons produced
₁₉₇₆ in association with a vector boson V (where V can be a W or Z boson) which
₁₉₇₇ subsequently decays leptonically. The leptonic final states from the decay of the
₁₉₇₈ vector boson allow for leptonic triggering whilst at the same time significantly
₁₉₇₉ reducing the multijet background.

₁₉₈₀ A closely related analysis [126] has more recently measured the associated production
₁₉₈₁ of a Higgs boson decaying to b -quarks in events where the vector and Higgs bosons are
₁₉₈₂ highly boosted. The analysis is outlined in Section 7.1. Modelling studies performed
₁₉₈₃ by the author are detailed in Section 7.2, and the results of the analysis are presented

1984 in Section 7.4. The author contributed to various signal and background modelling
1985 studies, fit studies, and to the diboson unblinding effort. This analysis has been
1986 published in Ref. [126]. Figures and tables from Ref. [126] are reproduced here.

1987 7.1 Analysis Overview

1988 The boosted VH , $H \rightarrow b\bar{b}$ analysis is focused on the high transverse momentum
1989 regime, which has the benefit of being more sensitive to physics beyond the Standard
1990 Model [127], but the disadvantage of being more challenging due to the increased dif-
1991 ficulty in the accurate reconstruction of highly energy events (discussed in Chapter 4).
1992 In order to focus on the high- p_T regime, the reconstructed vector boson is required to
1993 have $p_T^V > 250$ GeV (see Section 7.1.2). Events are also split into two p_T^V bins with the
1994 first bin covering $250 \text{ GeV} < p_T^V < 400 \text{ GeV}$ and the second covering $p_T^V > 400 \text{ GeV}$,
1995 which allows the analysis to account for the improved signal-to-background in the
1996 high- p_T regime.

1997 The previous ATLAS analysis in Ref. [110] was primarily sensitive to vector bosons
1998 with a more modest p_T^V boost in the region of 100–300 GeV. In this regime, the Higgs
1999 candidate was reconstructed using a pair of jets with radius parameter of $R = 0.4$,
2000 called small- R jets. However in the high- p_T regime, the decay products of the Higgs
2001 boson become increasingly collimated and the small- R jets may overlap. In order to
2002 avoid the associated problems and to aid in the reconstruction of the Higgs boson
2003 candidate, the present analysis uses instead a large- R jet with radius parameter
2004 $R = 1.0$ to reconstruct the Higgs boson candidate in all channels (see Section 3.4.3).
2005 The Higgs candidate is required to have exactly two ghost-associated and b -tagged
2006 variable-radius track-jets. The candidate large- R jet is reconstructed using jet
2007 substructure techniques, for example it is trimmed by removing soft and wide-angle
2008 components, which helps to remove particles from the underlying event and pileup
2009 collisions [128]. Refer to Section 3.4.3 for more details on jet reconstruction.

2010 On top of the binning in p_T^V , selected events are further categorised into 0-, 1- and
2011 2-lepton channels depending on the number of selected charged leptons (electrons
2012 and muons) are present in the reconstructed final state (also referred to as 0L, 1L,
2013 and 2L respectively). The 0-lepton channel targets the $ZH \rightarrow \nu\nu b\bar{b}$ process, the
2014 1-lepton channel targets $WH \rightarrow \ell\nu b\bar{b}$, and the 2-lepton channel targets $ZH \rightarrow \ell\ell b\bar{b}$,

where ℓ is an electron or muon and ν is a neutrino. Each channel has a dedicated set of selections which are listed in more detail in Section 7.1.3. Events in the 0- and 1-lepton channels are further split depending on the number of additional small- R jets not matched to the Higgs-jet candidate. The high-purity signal region (HP SR) has zero such jets, while the low-purity signal region (LP SR) has one or more. The 0- and 1-lepton channels also make use of a dedicated $t\bar{t}$ control region, described in Section 7.1.4. A complete overview of the different analysis regions is given in Table 7.1.

Channel	Analysis Regions					
	$250 < p_T^V < 400 \text{ GeV}$		$p_T^V \geq 400 \text{ GeV}$			
	0 add. b -track-jets		≥ 1 add. b -track-jets	0 add. b -track-jets		≥ 1 add. b -track-jets
	0 add. small- R jets	≥ 1 add. small- R jets		0 add. small- R jets	≥ 1 add. small- R jets	
0-lepton	HP SR	LP SR	CR	HP SR	LP SR	CR
1-lepton	HP SR	LP SR	CR	HP SR	LP SR	CR
2-lepton	SR			SR		

Table 7.1: Summary of the definitions of the different analysis regions [126]. Signal enriched regions are marked with the label SR. There are regions with relatively large signal purity (HP SR) and with low purity (LP SR). Background enriched regions are marked with the label CR. The shorthand “add” stands for additional small- R jets, i.e. number of small- R jets not matched to the Higgs-jet candidate.

7.1.1 Data & Simulated Samples

The analysis uses pp collision data recorded between 2015 and 2018 by the ATLAS detector [32] during Run 2 at the LHC. This dataset corresponds to an integrated luminosity of 139 fb^{-1} .

Data from centre-of-mass energy $\sqrt{s} = 13 \text{ TeV}$ proton-proton collisions at the LHC recorded over the course of Run 2 were used for the analysis. The resulting dataset corresponds to a total integrated luminosity of 139 fb^{-1} (see Fig. 3.4).

An overview of the MC simulated samples used in the analysis is given in Table 7.2. These samples are used to model the signal and background processes relevant to the

2032 analysis, with the exception of the multijet background which is modelled using a
2033 data-driven technique. Data and simulated events are reconstructed using the same
2034 algorithms, and a reweighting is applied to the simulated events in order to match
2035 the pile-up distribution observed in the data.

2036 **7.1.2 Object Reconstruction**

2037 The presence of neutrinos in the $WH \rightarrow \ell\nu b\bar{b}$ and $ZH \rightarrow \ell\ell b\bar{b}$ signatures can be
2038 inferred from a momentum imbalance in the transverse plane Section 3.4.5. The
2039 vector boson transverse momentum p_T^V is reconstructed as the missing transverse
2040 energy E_T^{miss} in the 0-lepton channel, as the magnitude of the summed $\mathbf{E}_T^{\text{miss}}$ and
2041 charged-lepton momentum in the 1-lepton channel, and as the transverse momentum
2042 of the 2-lepton system in the 2-lepton channel (see Section 3.4.5).

2043 Leptons are used for the channel classification and to select relevant events as outlined
2044 in Section 7.1.3. Electrons and muons are reconstructed as outlined in Section 3.4.4.
2045 Electron identification follows the approach outlined in Ref. [110]. In addition to the
2046 likelihood-based method described in Section 3.4.4, *baseline* electrons are required to
2047 satisfy $p_T > 7 \text{ GeV}$, $|\eta| < 2.47$, $s(d_0) < 5$, and $|z_0 \sin(\theta)| < 0.5 \text{ mm}$. *Signal* electron
2048 additionally are required to satisfy a tighter likelihood identification selection. Muons
2049 are required to satisfy $p_T > 7 \text{ GeV}$, $|\eta| < 2.7$, $s(d_0) < 3$, and $|z_0 \sin(\theta)| < 0.5 \text{ mm}$.
2050 *Baseline* muons are required to pass the ‘loose’ identification described in Ref. [75],
2051 while *signal* muons are required to pass the ‘medium’ identification working point.
2052 All signal leptons are required to additionally satisfy a $p_T > 27 \text{ GeV}$ selection criteria,
2053 except for muons in the 1-lepton channel where a cut of 25 GeV is used. The number
2054 of baseline leptons is used to categorise the event into the 0-, 1- or 2-lepton channels.
2055 The 1- and 2-lepton channels additionally require one signal lepton to be present.

2056 The track-jets matched to the Higgs candidate are b -tagged using the MV2c10 b -
2057 tagging algorithm [61, 77, 163]. MV2c10 is a machine learning algorithm using a
2058 Boosted Decision Tree (BDT) which is tuned to achieve an average b -jet efficiency of
2059 70% on simulated $t\bar{t}$ events. At this efficiency working point, rejection factors for
2060 c -jets and light-jets are approximately 9 and 304 respectively. The MV2 algorithm
2061 takes inputs from the outputs of a number of low-level algorithms (IPxD, SV1 and
2062 JetFitter). The outputs of the low-level algorithms are provided as inputs to the
2063 boosted decision tree. The efficiency of the tagging algorithm is calibrated to events

Process	ME generator	ME PDF	PS and Hadronisation	UE model tune	Cross-section order
Signal ($m_H = 125$ GeV and $b\bar{b}$ branching fraction set to 58%)					
$gg \rightarrow WH \rightarrow \ell\nu b\bar{b}$	Powheg-Box v2 [129] + GoSAM [131] + MiNLO [132, 133]	NNPDF3.0NLO (*) [101]	Pythia 8.212 [103]	AZNLO [130]	NNLO(QCD) + NLO(EW) [134–140]
$qq \rightarrow ZH \rightarrow \nu\nu b\bar{b}/\ell\ell b\bar{b}$	Powheg-Box v2 + GoSAM + MiNLO	NNPDF3.0NLO (*)	Pythia 8.212	AZNLO	NNLO(QCD) ^(†) + NLO(EW)
$gg \rightarrow ZH \rightarrow \nu\nu b\bar{b}/\ell\ell b\bar{b}$	Powheg-Box v2	NNPDF3.0NLO (*)	Pythia 8.212	AZNLO	NLO + NLL [141–145]
Top quark ($m_t = 172.5$ GeV)					
$t\bar{t}$	Powheg-Box v2 [129, 146]	NNPDF3.0NLO	Pythia 8.230	A14 [104]	NNLO+NNLL [147]
s-channel	Powheg-Box v2 [129, 148]	NNPDF3.0NLO	Pythia 8.230	A14	NLO [149]
t-channel	Powheg-Box v2 [129, 148]	NNPDF3.0NLO	Pythia 8.230	A14	NLO [150]
Wt	Powheg-Box v2 [129, 151]	NNPDF3.0NLO	Pythia 8.230	A14	Approximate NNLO [152]
Vector boson + jets					
$W \rightarrow \ell\nu$	SHERPA 2.2.1 [153–156]	NNPDF3.0NNLO	SHERPA 2.2.1 [157, 158]	Default	NNLO [159]
$Z/\gamma^* \rightarrow \ell\ell$	SHERPA 2.2.1	NNPDF3.0NNLO	SHERPA 2.2.1	Default	NNLO
$Z \rightarrow \nu\nu$	SHERPA 2.2.1	NNPDF3.0NNLO	SHERPA 2.2.1	Default	NNLO
Diboson					
$qq \rightarrow WW$	SHERPA 2.2.1	NNPDF3.0NNLO	SHERPA 2.2.1	Default	NLO
$qq \rightarrow WZ$	SHERPA 2.2.1	NNPDF3.0NNLO	SHERPA 2.2.1	Default	NLO
$qq \rightarrow ZZ$	SHERPA 2.2.1	NNPDF3.0NNLO	SHERPA 2.2.1	Default	NLO
$gg \rightarrow VV$	SHERPA 2.2.2	NNPDF3.0NNLO	SHERPA 2.2.2	Default	NLO

Table 7.2: Signal and background processes with the corresponding generators used for the nominal samples [126]. If not specified, the order of the cross-section calculation refers to the expansion in the strong coupling constant (α_s). (*) The events were generated using the first PDF in the NNPDF3.0NLO set and subsequently reweighted to the PDF4LHC15NLO set [160] using the internal algorithm in POWHEG-BOX v2. (†) The NNLO(QCD)+NLO(EW) cross-section calculation for the $pp \rightarrow ZH$ process already includes the $gg \rightarrow ZH$ contribution. The $gg \rightarrow ZH$ process is normalised using the cross-section for the $pp \rightarrow ZH$ process, after subtracting the $gg \rightarrow ZH$ contribution. An additional scale factor is applied to the $gg \rightarrow VH$ processes as a function of the transverse momentum of the vector boson, to account for electroweak (EW) corrections at NLO. This makes use of the VH differential cross-section computed with HAWK [161, 162].

2064 in data [164–166]. The jet tagging strategy relies on extensive studies into track-jet
2065 b -tagging in boosted topologies [167, 168].

2066 The jet flavour labelling scheme is described in Section 3.4.3.

2067 7.1.3 Selection Criteria

2068 An extensive list of selection cuts are applied to each event in order to reject
2069 background events whilst retaining as many signal events as possible. A full list of
2070 selection cuts applied to the different analysis regions is given in Table 7.3, while
2071 some key selections are listed below.

2072 All channels are require events with at least one large- R jet with $p_T > 250 \text{ GeV}$
2073 and $|\eta| < 2.0$. The vector boson transverse momentum is also required to satisfy
2074 $p_T^V > 250 \text{ GeV}$. The Higgs candidate is chosen as the highest p_T large- R jet satisfying
2075 these requirements. As mentioned, the candidate large- R jet is required to have
2076 two ghost-assciated and b -tagged variable-radius track-jets. These track-jets are
2077 required to have at least two constituent tracks with $p_T > 500 \text{ MeV}$ and $|\eta| < 2.5$.
2078 The track-jets themselves must satisfy $p_T > 10 \text{ GeV}$ and $|\eta| < 2.5$.

2079 In the 0-lepton channel, trigger selections are applied using an E_T^{miss} trigger with a
2080 luminosity-dependent threshold between 70–110 GeV. In the 1-lepton electron sub-
2081 channel a combination of single electron triggers is used with minimum p_T thresholds
2082 between 24–26 GeV. In the muon sub-channel the same E_T^{miss} trigger as the 0-lepton
2083 channel is used. Since muons are not used for the E_T^{miss} trigger calculations, this
2084 is in effect a p_T requirement on the muon-neutrino system, which in the analysis
2085 phase space is more efficient than a single-muon trigger. The 2-lepton channel uses
2086 the same triggering strategy as the 1-lepton channel. In all channels, the trigger
2087 selections applied are fully efficient for events selected using the full requirements in
2088 Table 7.3.

2089 The combined selections in Table 7.3 result in a signal efficiency ranging from 6–16%
2090 for the WH and ZH processes depending on the channel and p_T^V bin.

Selection	0 lepton channel	1 lepton channel	2 leptons channel
Trigger	E_T^{miss}	e sub-channel Single electron	μ sub-channel E_T^{miss}
Leptons	0 <i>baseline</i> leptons	$p_T > 27 \text{ GeV}$ 1 <i>signal</i> lepton no second <i>baseline</i> lepton	$p_T > 25 \text{ GeV}$ both leptons of the same flavour - opposite sign muons
E_T^{miss}	$> 250 \text{ GeV}$	$> 50 \text{ GeV}$	-
p_T^V			$p_T^V > 250 \text{ GeV}$
Large- R jets		at least one large- R jet, $p_T > 250 \text{ GeV}, \eta < 2.0$	
Track-jets		at least two track-jets, $p_T > 10 \text{ GeV}, \eta < 2.5$, matched to the leading large- R jet	
b -tagged jets		leading two track-jets matched to the leading large- R must be b -tagged (MV2c10, 70%)	
m_1			$> 50 \text{ GeV}$
$\min[\Delta\phi(E_T^{\text{miss}}, \text{small-}R \text{ jets})]$	$> 30^\circ$		-
$\Delta\phi(E_T^{\text{miss}}, H_{\text{cand}})$	$> 120^\circ$		-
$\Delta\phi(E_T^{\text{miss}}, E_{T, \text{trk}}^{\text{miss}})$	$< 90^\circ$		-
$\Delta y(V, H_{\text{cand}})$	-		$ \Delta y(V, H_{\text{cand}}) < 1.4$
$m_{\ell\ell}$	-		$66 \text{ GeV} < m_{\ell\ell} < 116 \text{ GeV}$
Lepton p_T imbalance	-		$(p_T^{\ell_1} - p_T^{\ell_2})/p_T^Z < 0.8$

Table 7.3: Event selection requirements for the boosted VH , $H \rightarrow b\bar{b}$ analysis channels and sub-channels [126]. Various channel dependent selections are used to maximise the signal efficiency and reduce the number of background events in each analysis region.

2091 7.1.4 Control Regions

2092 The $t\bar{t}$ process presents a major background in the 0- and 1-lepton channels. In these
 2093 events, the Higgs candidate is often reconstructed from a correctly tagged b -jet from
 2094 the top decay $t \rightarrow Wb$, and an incorrectly tagged c - or light-jet from the subsequent
 2095 decay of the W , as shown in Fig. 7.1.

not sure
where the
0L ttbar
ETmiss
comes from

2096 The only known decay mode of the top quark is via the weak force to a W and
 2097 a down-type quark. (it is the only quark heavy enough to decay into an on-shell
 2098 W). Overwhelmingly (96% of the time) the down-type quark is a b -quark Hence, the
 2099 second top quark is also likely to result in a second tagged b -tagged track-jet outside
 2100 of the large- R Higgs candidate. To ensure sufficient $t\bar{t}$ rejections, 0- and 1-lepton
 2101 channel signal regions are defined using a veto on events with b -tagged track-jets
 2102 outside the Higgs-jet candidate. These events are used to construct a control region
 2103 (CR) which is enriched in $t\bar{t}$ events. The CR is used to constrain the normalisation
 2104 of the $t\bar{t}$ background in the fit.

2105 7.1.5 Background Composition

2106 After the selections described in Section 7.1.3 the number of background events
 2107 mimicking the VH , $H \rightarrow b\bar{b}$ signal is greatly reduced. However, the number of
 2108 background events still greatly outnumbers that of signal events. The background
 2109 processes are channel dependent. In the 0-lepton channel the dominant sources of
 2110 backgrounds are $Z+jets$ ($Z \rightarrow \nu\nu$) and $t\bar{t}$, with $W+jets$ and diboson events being
 2111 subdominant. In the event of $W \rightarrow \tau\nu$, and subsequent hadronic decay of the τ or
 2112 lack of successful reconstruction/selection of the leptonic decay products, $W+jets$
 2113 can also contribute to the 0-lepton channel. $t\bar{t}$ and $W+jets$ (with a leptonic decay
 2114 of the W as in $W \rightarrow \ell\nu$) are dominant in the 1-lepton channel, while single-top is
 2115 subdominant. In the 2-lepton channel, $Z+jets$ ($Z \rightarrow \ell\ell$) is again dominant followed
 2116 by $Z Z$ diboson events.

2117 The diboson background VV consists primarily of WZ and ZZ events in which the
 2118 Z decays to a pair of b -quarks. This process very closely matches the signal, with
 2119 a resonant peak occurring at $m_Z = 91$ GeV and so is considered as an irreducible
 2120 background ($V+b$ -jets is also irreducible).

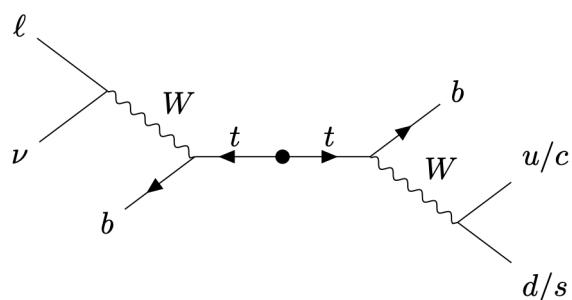
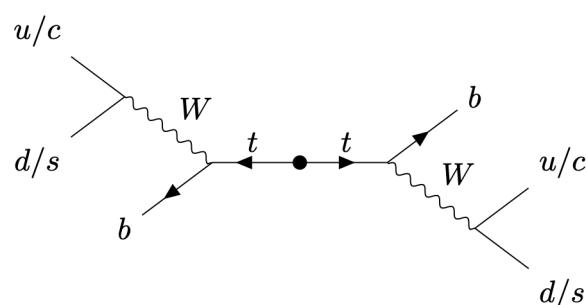
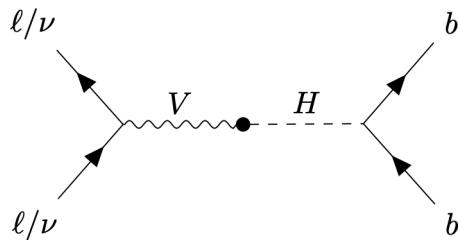


Figure 7.1: Diagrams of the signal process (top) and the 0-lepton and 1-lepton $t\bar{t}$ backgrounds (middle, bottom). Objects to the right of centre are reconstructed within the large- R jet. For the backgrounds, the large- R jet contains a mis-tagged c - or light-jet.

2121 The $t\bar{t}V$, $t\bar{t}H$ and multijet backgrounds are negligible in the analysis phase space
2122 after the selections have been applied, with the exception of the 1-lepton electron
2123 sub-channel, in which multijet background is not ignored. The multijet background
2124 is made up of jets with semileptonic heavy-flavour-hadron decays (e.g. $b \rightarrow c\ell\nu$) and
2125 jets which are mis-tagged by the flavour tagging algorithm MV2c10.

2126 The contributions from the different backgrounds are modelled using Monte Carlo
2127 event generators and the impacts on the analysis are studied in Section 7.2. The
2128 multijet background is not modelled but instead estimated using a data-driven
2129 technique.

2130 7.2 Systematic Uncertainties & Background 2131 Modelling

2132 Systemic uncertainties are extensively employed to give the fit model described in
2133 Section 7.3 enough flexibility to account for inaccuracies in the various inputs to the fit.
2134 Two main types of systematic uncertainty are considered: experimental and modelling.
2135 Experimental uncertainties arise due to the limited due to limited detector precision,
2136 imperfect reconstruction algorithms (in particular the b -tagging algorithms), and
2137 due to the imperfect measurement of pile-up and integrated luminosity. Modelling
2138 is the simulation processes relevant to the analysis using Monte-Carlo (MC) event
2139 generators, and is used to predict the outcome of the analysis. Modelling uncertainties
2140 arise due to the imperfections in the simulation of signal and background events, for
2141 example differences between event generators, or use of different model parameters
2142 when producing simulated events. In order to observe a certain process, for example
2143 VH , $H \rightarrow b\bar{b}$, an increase in the number of observed events with respect to the
2144 background-only hypothesis is looked for. The excess is often relatively small against
2145 the total number of background events, and hence accurate modelling of the expected
2146 number of background and signal events is crucial for successfully performing the
2147 analysis. Particular care is paid to the uncertainties on the modelling predictions as
2148 discussed in this section.

2149 Modelling uncertainties are described in detail in the following sections. Modelling
2150 uncertainties: *Nominal* samples are used as a reference to which different vari-

2151 ations can be compared. The nominal samples are chosen as the best possible
2152 representation of the underlying physical process. *Alternative* samples are used to
2153 understand inaccuracies that may be present in the nominal samples. Some aspect
2154 of the nominal model is varied, and the discrepancy with respect to the nominal
2155 model is quantified. The discrepancy is used to systematic uncertainty associated
2156 with the model parameter which was changed.

2157 Modelling studies involving c - and light-jets is hampered by the low available statistics
2158 of jets pass the analysis selections, due to the high rejection rates of the b -tagging
2159 algorithm MV2c10. For modelling studies therefore, truth tagging (TT) is employed
2160 to ensure sufficient numbers of jets are available to calculate uncertainties. TT works
2161 by computing a 2-dimensional efficiency map using the jet p_T and jet η . The two
2162 leading track-jets associated to the large- R jet automatically passes the b -tagging
2163 requirement, and are weighted based on their p_T and η using the pre-calculated
2164 efficiency map.

2165 7.2.1 Sources of Systematic Uncertainties

2166 This section briefly describes the different sources of uncertainty in the predictive
2167 model used in the analysis, and how each source of uncertainty is implemented within
2168 the analysis framework. Considered sources of systematic uncertainty are listed in
2169 Table 7.4. For each source of uncertainty, acceptance and shape uncertainties are
2170 derived.

2171 QCD Scales

2172 The $V+jets$ matrix element calculations contains infrared and ultraviolet divergences.
2173 These are handled by introducing spurious parameters corresponding to the renormalisation scale (μ_R) and factorisation scale (μ_F). Physical observables are not
2174 dependent on these parameters when using the infinite perturbation series expansion,
2175 however at some fixed order in QCD a limited dependence is present. To assess the
2176 impact of this, both μ_R and μ_F are independently varied from their nominal values
2177 by factors of 0.5 and 2 to account for higher order corrections to the calculation of
2178 the matrix element used to simulate the process.

2180 PDF Sets

2181 Parton distribution functions (PDFs) specify the probability of finding a parton
2182 with a given momentum inside a hadron (in this case, inside colliding protons).
2183 PDFs have to be derived from data and are a significant source of uncertainty in
2184 analyses of hadronic collision data. There are three sources of PDF uncertainties:
2185 the statistical and systematic errors on the underlying data used to derive the PDFs,
2186 the theory which is used to describe them (which is based on some fixed order
2187 perturbative QCD expansion), and finally the procedure which is used to extract the
2188 PDFs from the data. PDF-related uncertainties were derived following Ref. [160].
2189 This involves considering 100 PDF replicas which, when combined, form a central
2190 value and associated uncertainty, and also in parallel direct changes to the central
2191 values of PDFs using the MMHT2014 [169] and CT14NLO [170] PDF sets.

2192 Event Generator

2193 The choice of parton shower (PS) and underlying event (UE) generators can affect
2194 the analysis outcome. Changing these models modifies several aspects of the event
2195 generation at the same time, such as the accuracy of matrix element predictions and
2196 different approaches to parton showering. This change tends to lead to the largest
2197 discrepancy with respect to the nominal samples.

2198 Resummation and Merging Scales

2199 Resummation is a technique used in QCD to help cope with calculations involving
2200 disparate energy scales, and involves the introduction of an associated resummation
2201 scale, the choice of which introduces some systematic uncertainty into the model.
2202 Parton showering models are accurate when simulating low- p_T radiation, however
2203 inaccuracies start to arrive when simulating hard emissions. To combat this, par-
2204 ton showering models utilise more precise matrix element calculations above some
2205 momentum threshold. The choice of threshold, or *merging scale* introduces some
2206 uncertainty into the final result. Resummation (QSF) and merging (CKKW) scale
2207 variations are available for a subset of the SHERPA samples. The number of available
2208 events is significantly lower than the number of events in the nominal sample, and no

- 2209 statistically significant discrepancy with respect to the nominal samples is observed.
2210 The corresponding uncertainties and therefore neglected.

2211 7.2.2 Implementation of Variations

- 2212 Modelling variations are implemented in different ways, depending on the associated
2213 uncertainty. Table 7.4 lists the different sources of uncertainty described in Section 7.2.1
and for each lists the implementation. As production of high-stastic MC samples

Source of Uncertainty	Implementation
Renormalisation scale (μ_R)	Internal weights
Factorisation scale (μ_F)	Internal weights
PDF set	Internal weights
Parton Shower (PS) models	Alternative samples
Underlying Event (UE) models	Alternative samples
Resummation scale (QSF)	Parameterisation
Merging scale (CKKW)	Parameterisation

Table 7.4: Different sources of uncertainty (i.e. variations in the model) considered for the $V + \text{jets}$ background, and the corresponding implementation. For each uncertainty, acceptance and shape uncertainties are derived.

- 2214
- 2215 is computationally expensive, a technique in state of the art simulation packages
2216 is to store some sources of variation as internal weights, which can be generated
2217 alongside the nominal samples, saving computation time. The nominal sample then
2218 effectively contains information about an ensemble of different samples, corresponding
2219 to different model parameters, which are accessible via reweightings. When filling
2220 histograms for the variations, bins are incremented by the internal weight of the
2221 event associated with the variation in question.

- 2222 While the inclusion of internal weight variation in MC event generators has decreased
2223 simulation times and increased available statistics, there are in SHERPA 2.2.1 currently
2224 some sources of systematic uncertainty that are unable to be stored as internal weight
2225 variations due to technical limitations. Two examples are the choice of resummation
2226 and merging scales. A method to parameterise the systematic variation using
2227 one sample, and to then apply this parameterisation to another sample, has been

2228 developed by ATLAS [171]. This method was used to derive resummation and
2229 merging uncertainties for the nominal SHERPA 2.2.1 sample, using a previous (lower
2230 statistic) SHERPA 2.1 alternative sample. The resulting uncertainties were studied
2231 and found to be negligible in comparison with systematics from other sources.

2232 **7.2.3 Vector Boson + Jets Modelling**

2233 After event selection, the $V+jets$ background is a dominant background in all three
2234 analysis channels as described in Section 7.1.5. The $V+jets$ samples are split into
2235 categories depending on the truth flavour of the track-jets which are ghost-associated
2236 to the large- R jet Higgs candidate. The categories are $V+bb$, $V+bc$, $V+bl$, $V+cc$,
2237 $V+cl$, $V+ll$, and $V+hf$ refers collectively to the categories containing at least one
2238 b - or c -jet. $V+bb$ is dominant generally accounting for 80% of the jets, while $V+hf$
2239 accounts for around 90% of jets. The full flavour composition breakdown for each
2240 channel and analysis region are given in Tables 7.5, 7.7 and 7.8.

2241 In order to access uncertainties associated with the use of MC generators, varia-
2242 tions of the data are produced using alternative generators or variation of nominal
2243 generator parameters as described in Section 7.2.2. As described in Section 7.1.1,
2244 the nominal MC event generator used for $V+jets$ events is SHERPA 2.2.1, while
2245 MADGRAPH5_AMC@NLO+PYTHIA8 (which uses a different parton showering
2246 model) is used as an alternative generator.

2247 Modelling systematics can have several impacts, including affecting the overall
2248 normalisation for different processes, and the relative acceptances between different
2249 analysis regions (i.e. migrations between HP and LP SRs, between the SR and CR,
2250 and between p_T^V bins), and the shapes of the m_J distributions. Since the fit model
2251 fits only the large- R jet mass m_J to data, all shape uncertainties are estimated with
2252 respect to this observable. Several sources of uncertainty, summarised in Section 7.2.1,
2253 have been assessed.

Sample	$M_{p_T}^V$ HP SR	$H_{p_T}^V$ HP SR	$M_{p_T}^V$ LP SR	$H_{p_T}^V$ LP SR	$M_{p_T}^V$ CR	$H_{p_T}^V$ CR
Wbb	$79.3\% \pm 4.4\%$	$75.0\% \pm 8.6\%$	$77.4\% \pm 2.5\%$	$71.7\% \pm 4.5\%$	$68.0\% \pm 7.6\%$	$63.5\% \pm 14.0\%$
Wbc	$6.6\% \pm 0.9\%$	$3.4\% \pm 1.7\%$	$6.2\% \pm 0.5\%$	$5.3\% \pm 0.9\%$	$14.5\% \pm 3.2\%$	$3.4\% \pm 3.2\%$
Wbl	$3.9\% \pm 0.9\%$	$11.4\% \pm 3.5\%$	$4.5\% \pm 0.5\%$	$8.7\% \pm 1.4\%$	$9.8\% \pm 2.2\%$	$9.1\% \pm 3.8\%$
Wcc	$5.1\% \pm 1.7\%$	$6.8\% \pm 2.4\%$	$7.1\% \pm 1.0\%$	$6.3\% \pm 1.4\%$	$4.2\% \pm 2.4\%$	$12.3\% \pm 7.0\%$
Wcl	$2.3\% \pm 1.4\%$	$2.4\% \pm 2.1\%$	$3.4\% \pm 0.7\%$	$5.2\% \pm 1.5\%$	$2.6\% \pm 1.5\%$	$3.4\% \pm 2.1\%$
Wl	$2.9\% \pm 1.0\%$	$0.9\% \pm 1.6\%$	$1.3\% \pm 0.7\%$	$2.8\% \pm 0.7\%$	$0.9\% \pm 0.6\%$	$8.4\% \pm 5.1\%$
Events	187.5 ± 7.7	38.2 ± 3.1	429.5 ± 10.0	97.8 ± 4.2	33.8 ± 2.5	8.3 ± 1.2

Table 7.5: 0-lepton $W+jets$ nominal sample flavour composition and total event yield [172].

Sample	$M_{p_T}^V$ HP SR	$H_{p_T}^V$ HP SR	$M_{p_T}^V$ LP SR	$H_{p_T}^V$ LP SR	$M_{p_T}^V$ CR	$H_{p_T}^V$ CR
Wbb	$77.2\% \pm 2.6\%$	$72.4\% \pm 4.3\%$	$77.8\% \pm 1.8\%$	$69.3\% \pm 2.5\%$	$64.6\% \pm 4.9\%$	$53.5\% \pm 6.3\%$
Wbc	$7.4\% \pm 0.7\%$	$7.3\% \pm 1.1\%$	$6.6\% \pm 0.4\%$	$6.3\% \pm 0.6\%$	$13.7\% \pm 1.9\%$	$16.4\% \pm 3.7\%$
Wbl	$4.0\% \pm 0.5\%$	$6.7\% \pm 1.1\%$	$5.1\% \pm 0.3\%$	$8.7\% \pm 0.8\%$	$10.3\% \pm 1.7\%$	$14.6\% \pm 3.0\%$
Wcc	$6.2\% \pm 1.1\%$	$5.5\% \pm 1.7\%$	$6.6\% \pm 0.6\%$	$6.4\% \pm 0.7\%$	$4.5\% \pm 1.7\%$	$9.5\% \pm 3.0\%$
Wcl	$3.6\% \pm 0.8\%$	$4.2\% \pm 1.8\%$	$2.8\% \pm 0.5\%$	$6.2\% \pm 0.8\%$	$4.6\% \pm 1.2\%$	$4.4\% \pm 1.5\%$
Wl	$1.5\% \pm 0.5\%$	$3.9\% \pm 1.3\%$	$1.1\% \pm 0.2\%$	$3.1\% \pm 0.5\%$	$2.3\% \pm 1.2\%$	$1.6\% \pm 0.6\%$
Events	477.1 ± 11.7	147.5 ± 6.4	784.7 ± 12.3	301.8 ± 7.2	68.7 ± 3.5	26.9 ± 2.0

Table 7.6: 1-lepton $W+jets$ nominal sample flavour composition and total event yield [172].

Channel	$M_{p_T}^V$ HP SR	$H_{p_T}^V$ HP SR	$M_{p_T}^V$ LP SR	$H_{p_T}^V$ LP SR	$M_{p_T}^V$ CR	$H_{p_T}^V$ CR
Zbb	84.56%	81.84%	82.37%	76.06%	66.12%	63.18%
Zbc	6.03%	6.98%	5.80%	7.46%	15.04%	14.30%
Zbl	4.06%	6.55%	3.83%	6.59%	12.66%	12.81%
Zcc	3.68%	3.40%	5.82%	3.75%	3.36%	3.38%
Zcl	1.23%	0.44%	1.47%	3.97%	1.82%	4.95%
Zl	0.44%	0.78%	0.70%	2.16%	1.00%	1.38%
Events	259.91 ± 4.86	66.12 ± 2.04	420.45 ± 5.73	141.97 ± 2.50	43.49 ± 1.73	16.07 ± 0.83

Table 7.7: 0-lepton $Z+jets$ nominal sample flavour composition and total event yield [172].

Channel	$M_{p_T}^V$	$H_{p_T}^V$	p_T^V inclusive
Zbb	80.80%	76.95%	79.76%
Zbc	8.10%	6.26%	7.60%
Zbl	4.95%	7.06%	5.52%
Zcc	3.97%	4.46%	4.10%
Zcl	1.61%	3.60%	2.14%
Zll	0.57%	1.68%	0.87%
Events	115.49 ± 2.42	42.42 ± 1.27	157.92 ± 2.73

Table 7.8: 2-lepton $Z+jets$ nominal sample flavour composition and total event yield [172].

2254 **Acceptance Uncertainties**

2255 Several different types of acceptance uncertainties have been calculated and imple-
 2256 mented as nuisance parameters in the fit. These account for uncertainty in the overall
 2257 number of events in each channel, and for the migration of events between different
 2258 analysis regions. The acceptance uncertainties relevant to the $V+jets$ processes are
 2259 summarised below.

2260 • **Overall normalisation:** only relevant where normalisation cannot be left
 2261 floating (determined as part of the fit). The $V+hf$ component is left floating in
 2262 the fit. For other components, independent normalisations used for $W+hf$ and
 2263 $Z+hf$. The contributions are mainly determined by the 1-lepton (for $W+hf$)
 2264 and 2-lepton (for $Z+hf$) SRs respectively and then extrapolated to 0-lepton
 2265 channel.

2266 • **SR-to-CR relative acceptance:** the uncertainty on the normalisation of the
 2267 signal region due to events migrating between the signal and control regions.

2268 • **HP-to-LP relative acceptance:** the uncertainty on the normalisation of the
 2269 high-purity (HP) signal region due to events migrating between the high- and
 2270 low-purity signal regions.

2271 • **Medium-to-high p_T^V relative acceptance:** describes any shape effect in p_T^V
 2272 distribution, given that the analysis only uses two p_T^V bins (medium and high).

2273 • **Flavour relative acceptance:** for each flavour $V+xx$, where $xx \in \{bc, bl, cc\}$
 2274 the ratio of $V+xx/V+bb$ events is calculated. This corresponds to the uncer-
 2275 tainty of Vbb events due to the miss-tagging of other flavours Vxx .

2276 • **Channel relative acceptance:** corresponding to the uncertainty in the nor-
 2277 malisation of $V+jets$ events events due to the migration of events between
 2278 channels.

2279 The uncertainties arising from the different sources described in Section 7.2.1 are
 2280 summed in quadrature to give a total uncertainty on each region. A summary of the
 2281 different acceptance uncertainties that were derived in this way and subsequently
 2282 applied in the fit are given in Table 7.9. An effort has been made, wherever possible,
 2283 to harmonise similar uncertainties across different analysis regions and channels.

V+jets Acceptance Uncertainties				
Boson	W		Z	
Channel	0L	1L	0L	2L
Vbb Norm.	30%	-	-	-
SR/CR	90% [†]	40% [†]	40%	-
HP/LP	18%		18%	-
High/Medium p_T^V	30%	10%*	10%	
Channel Extrap.	20%	-	16%	-
Vbc/Vbb	30%			
Vbl/Vbb	30%			
Vcc/Vbb	20%			
Vcl Norm.	30%			
Vl Norm.	30%			

Table 7.9: V+jets acceptance uncertainties [172]. W+jets SR and CR uncertainties marked with a superscript † are correlated. The 1L W+jets H/M uncertainty marked by * is applied as independent and uncorrelated NPs in both HP and LP signal regions. The 0L W+jets Wbb Norm uncertainty is only applied when a floating normalisation for Wbb cannot be obtained from the 1L channel. A 30% uncertainty for $Z \rightarrow b\bar{b}$ norm is applied in the 1L channel when a floating normalisation for $Z \rightarrow b\bar{b}$ cannot be obtained from the 0L or 2L channels.

2284 Shape Uncertainties

2285 In order to derive shape uncertainties (which as the name suggests affect shapes but
2286 not overall normalisations of distributions), the following procedure is carried out.
2287 Normalised distributions of the reconstructed large- R Higgs candidate jet mass m_J
2288 are compared for the nominal sample and variations. For each variation, the ratio of
2289 the variation to nominal is calculated, the up and down variations are symmetrised,
2290 and an analytic function is fit to the symmetrised ratio. If different analysis regions
2291 or channels show the same pattern of variation, a common uncertainty is assigned.
2292 An example of a significant source of uncertainty, arising from choice of factorisation
2293 scale μ_R is shown in Fig. 7.2. HP SRs split into medium and high p_T^V bins are shown
2294 for the 0-lepton channel for $W+\text{hf}$ and $Z+\text{hf}$ jets. The 0- and 1-lepton channels for
2295 the $W+\text{hf}$ contribution and the 0- and 2-lepton channels for the $Z+\text{jets}$ contribution
2296 are merged, since the shapes in m_J are consistent across channels. An exponential
2297 function $e^{p_0 + p_1 x} + p_2$ has been fitted to the ratio of the normalised distributions.
2298 The magnitude of the variation does show p_T^V dependence, and so two separate
2299 uncertainties are added in the fit, and applied individually in each p_T^V region.

2300 The shape uncertainties for μ_R were derived on the SRs but are also applied to the
2301 CRs, as the low statistics in the CRs make it difficult to derive dedicated shape
2302 uncertainties. All the shape uncertainties are fully correlated accross regions.

2303 A comparison of the m_J shapes between SHERPA and MADGRAPH is shown in
2304 Fig. 7.3. The plots are split by process and channel, but merged in SR purity and p_T^V
2305 bins reflecting similarities between the m_J shapes across these regions. Due to the low
2306 statistics available for the alternate MADGRAPH sample, and the lack of statistically
2307 significant variation between the samples, no associated shape uncertainty is added
2308 to the fit in this case.

2309 The impacts of variations in the factorisation scale μ_F and the choice of PDF set on
2310 m_J shape were also found to be negligible in comparison with μ_R and are hence not
2311 associated uncertainty was added to the fit.

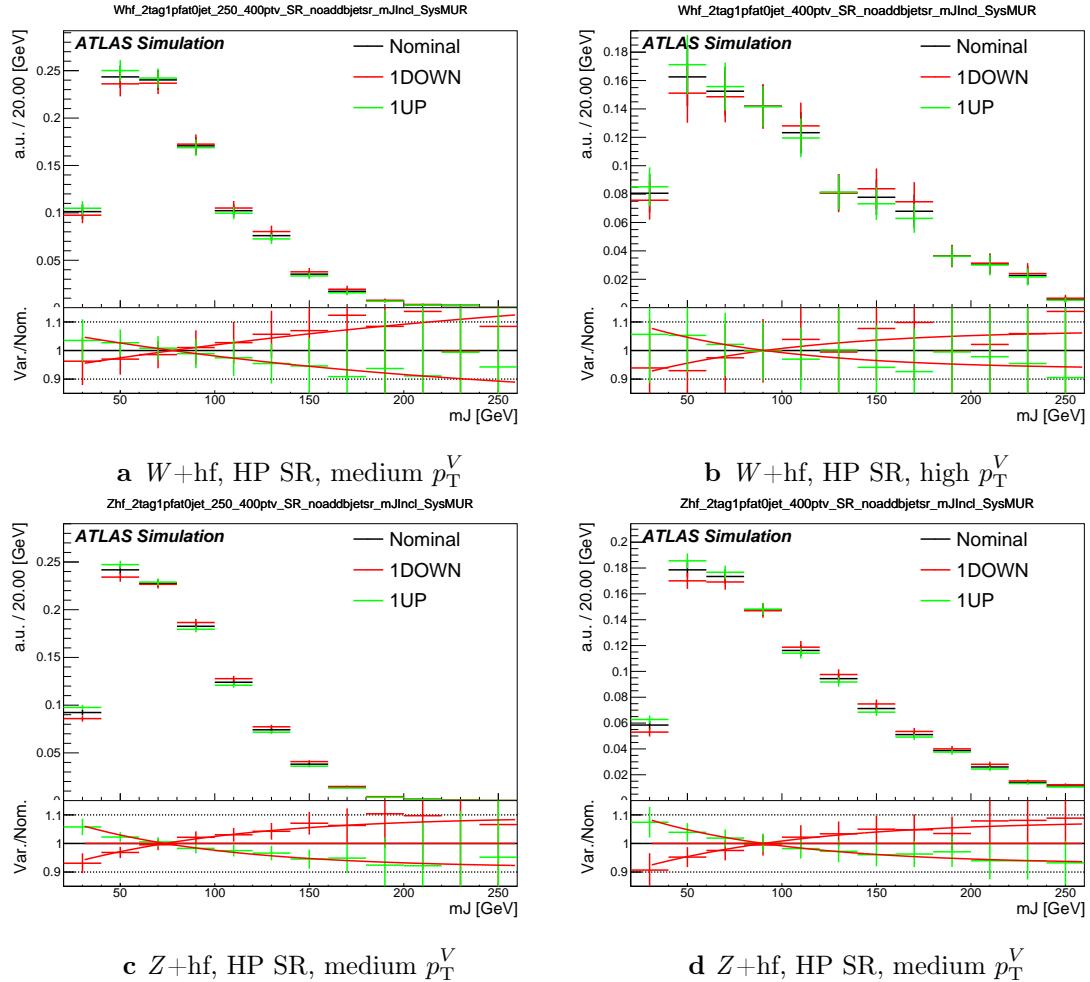


Figure 7.2: Normalised leading large- R jet mass distribution from Z and $W + hf$ processes in the HP SR of the 0-lepton channel [172]. The renormalisation scale μ_r has been varied by a factor of 2 (1up) and 0.5 (1down). An exponential function is fitted to the ratio between the nominal and variation samples.

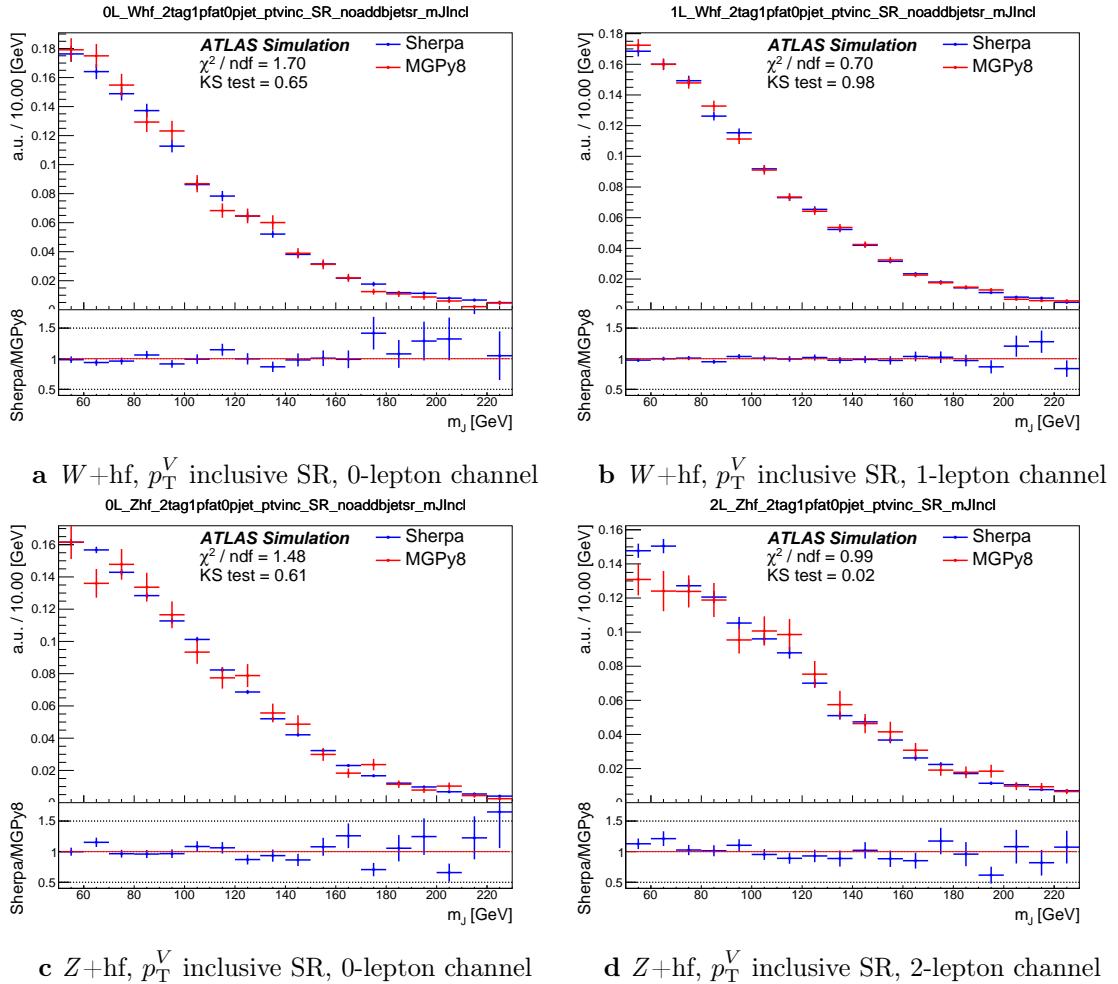


Figure 7.3: The comparison on m_J shapes between SHERPA and MADGRAPH samples from $V+hf$ process in p_T^V inclusive signal regions [172]. The Kolmogorov-Smirnov test and χ^2/ndf are shown on the plots.

2312 7.2.4 Diboson Modelling

2313 The uncertainties for the diboson background generally follows that of $V+jets$. How-
2314 ever an alternative sample was generated using POWHEG interfaced with PYTHIA8,
2315 using the AZNLO shower tune with the CTEQ6L1 PDFs [173]. Unlike SHERPA,
2316 POWHEG models the off-shell Z contribution at NLO.

2317 Acceptance and shape uncertainties are derived in an analogous fashion to $V+jets$
2318 as described below.

2319 Acceptance Uncertainties

2320 Diboson acceptance uncertainties are summarised in Table 7.10. Variations from μ_R ,
2321 μ_F , PDF choice and alternative generator are considered and are combined combined
2322 through a sum in quadrature as described in Section 7.2.3. The largest modification
2323 to the nominal acceptance results from the POWHEG+PYTHIA8 alternate sample,
2324 which modifies several parts of the generative model at the same time. Since the
2325 diboson contribution to the $t\bar{t}$ control region is small, no SR-to-CR relative acceptance
2326 uncertainty is required.

2327 For the WZ contribution, uncertainties are derived using the 1-lepton channel and
2328 applied to all three channels. An additional 8% channel migration uncertainty
2329 is applied on the 0-lepton channel. For the ZZ contribution, the normalisation
2330 uncertainty is calculated using the 2-lepton channel and applied to all three channels.
2331 The 0- and 1-lepton channels have a similar HP-to-LP relative acceptance uncertainty
2332 of 18%. The 1-lepton medium-to-high p_T^V relative acceptance is based off the value
2333 obtained from the 2-lepton channel. 30% and 18% channel migration uncertainties
2334 are applied in the 0- and 1-lepton channels respectively.

2335 Since the contribution from WW is small, dedicated studies are not performed, but
2336 a 25% normalisation uncertainty is applied in all the three channels which is based
2337 on the modelling studies performed for the previous analysis [110].

Diboson Acceptance Uncertainties						
Bosons	WZ			ZZ		
Channel	0L	1L	2L	0L	1L	2L
Normalisation	16%			10%		
HP/LP	18%			18%		
High/Medium	10%			6%	18%	
Channel Extrap.	8%	-	-	30%	18%	-

Table 7.10: Diboson acceptance uncertainties [172]. All uncertainties except channel extrapolation uncertainties are fully correlated between ZZ and WZ processes and channels.

2338 Shape Uncertainties

2339 Diboson shape uncertainties are derived in a similar fashion to $V+jets$. Only the
 2340 uncertainties associated with systematic variation of μ_R and the event generator
 2341 have a non-negligible impact on the m_J shape. Variation of μ_R produces consistent
 2342 m_J shape impacts across all regions and channels, and hence only a single associated
 2343 uncertainty is derived, shown in Fig. 7.4. A hyperbolic tangent is fitted to the
 2344 symmetrised ratio.

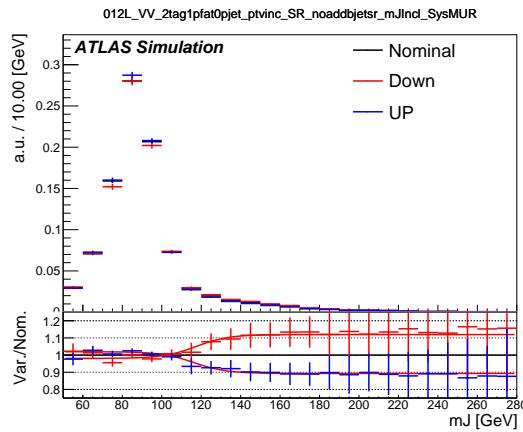


Figure 7.4: Normalised leading large- R jet mass distribution from WZ and ZZ process, merged among all the signal regions and lepton channels [172]. The renormalisation scale μ_R has been varied by a factor of 2 (1up) and 0.5 (1down). The red line shape shows the fitting results of the hyperbolic tangent function.

2345 The comparison between the nominal SHERPA and alternative POWHEG+PYTHIA
 2346 8 samples is shown in Fig. 7.5 for the 0- and 1-lepton channels for both WZ and

2347 ZZ processes. For these channels, the shape of m_J varies in opposite directions
2348 in the LP and HP signal regions. Shapes are similar between p_T^V bins, the 0- and
2349 1-lepton channels and for WZ and ZZ . A third order polynomial is fitted to the
2350 ratio, and this function transitions to a constant piecewise function in the high
2351 mass region to accurately represent the shape taking into account large statistical
2352 uncertainties. Dependence on event generator was found to be negligible within
2353 statistical uncertainty in the 2-lepton channel. All diboson shape uncertainties are
2354 fully correlated in the fit.

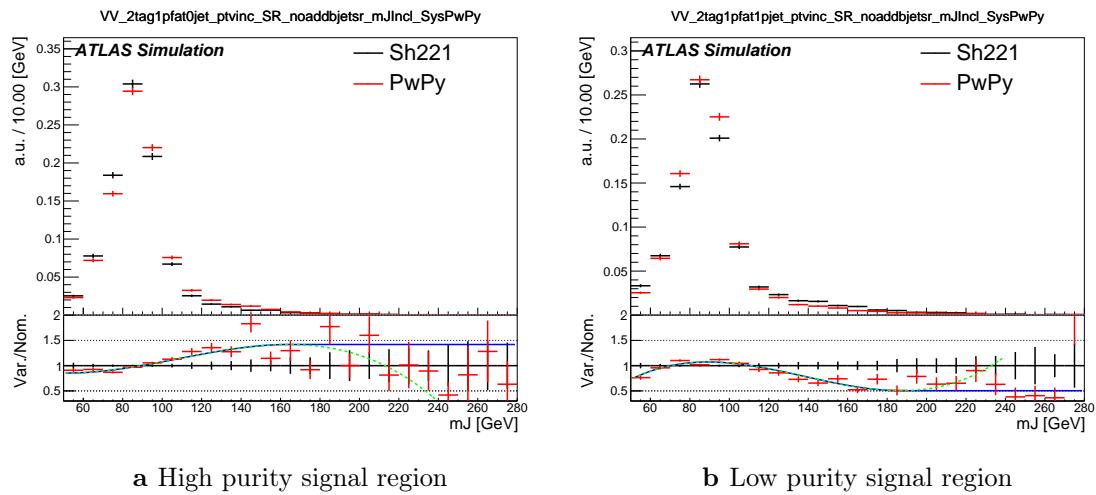


Figure 7.5: The comparison on m_J shapes between SHERPA and POWHEG+PYTHIA 8 samples from WZ and ZZ process in high and low purity signal regions [172]. p_T^V regions and 0- and 1-lepton channels are merged. The dashed green line shows the fitted third order polynomial function and the blue lines show the function after a protection is added in the high mass region.

2355 7.3 Statistical Treatment

2356 Selected events are used to perform a statistical test of the background-only hy-
2357 pothesis, i.e. a model which does not include the VH , $H \rightarrow b\bar{b}$ process. The test
2358 involves a binned global maximum-profile-likelihood fit from the model to the data
2359 using the m_J distribution, and combines all the analysis regions defined in Table 7.1.
2360 The test is based on the profile likelihood ratio test statistic. The signal strength
2361 $\mu = \sigma/\sigma_{\text{SM}}$ is defined as the ratio between the observed and predicted cross-sections,
2362 where $\mu = 0$ corresponds to the background-only hypothesis and $\mu = 1$ corresponds

2363 to the SM prediction. It is a parameter of interest (POI) which acts to scale the
2364 total number of signal events.

2365 The present analysis makes use of two POIs. The first, μ_{VH}^{bb} , is the signal strength
2366 for the VH , $H \rightarrow b\bar{b}$ process, the primary process under investigation. The diboson
2367 production strength μ_{VZ}^{bb} for the VZ , $Z \rightarrow b\bar{b}$ process is measured simultaneously
2368 and provides a validation of the analysis apparatus used for the primary $H \rightarrow b\bar{b}$
2369 measurement. Alongside the two POIs, the predictive model depends on several
2370 uninteresting parameters which are not the primary target of measurement. These
2371 parameters are called nuisance parameters (NPs), collectively referred to as θ . Freely
2372 floating background normalisations are implemented as NPs and are also extracted
2373 during the fitting processes.

2374 7.3.1 Likelihood Function

2375 The statistical setup treats each bin as a Poisson counting experiment and is based on
2376 the ROOSTATS framework [174]. The combined likelihood over N bins is constructed
2377 as the product of Poisson probabilities in each bin. Considering the simplified case
2378 of a single signal strength parameter μ , and neglecting sources of systematic or
2379 statistical uncertainty, this is given by

$$\mathcal{L}(\mu) = \prod_{i=1}^N \frac{(\mu s_i + b_i)^{n_i}}{n_i!} \exp[-(\mu s_i + b_i)], \quad (7.1)$$

2380 where s_i (b_i) is the expected number of signal (background) events in bin i , and n_i is
2381 the number of observed data events in bin i .

2382 Treatment of Uncertainties

2383 Systematic uncertainties can modify the predicted signal and background yields s_i
2384 and b_i . Each source of systematic uncertainty is taken into account by adding an
2385 additional NP θ_j to the likelihood in the form of a Gaussian cost function. The

2386 combined effect of the NPs is then

$$\mathcal{L}(\theta) = \prod_{j=1}^{N_\theta} \frac{1}{\sqrt{2\pi}\sigma_j} \exp \left[\frac{-(\bar{\theta}_j - \theta_j)^2}{2\sigma_j^2} \right], \quad (7.2)$$

2387 where N_θ is the number of NPs, $\bar{\theta}_j$ is the nominal value of the j th NP, θ_j is the fitted
2388 value, and σ_j is the corresponding associated prior uncertainty on θ_j . As the fitted
2389 value of the θ_j deviates from its nominal value, a cost is introduced. The presence
2390 of NPs modifies the likelihood as

$$\mathcal{L}(\mu) \rightarrow \mathcal{L}(\mu, \theta) = \mathcal{L}(\mu)\mathcal{L}(\theta). \quad (7.3)$$

2391 The predicted signal and background yields are also modified by the presence of the
2392 NPs with

$$s_i \rightarrow s_i(\theta), \quad b_i \rightarrow b_i(\theta). \quad (7.4)$$

2393 For NPs which are left freely floating in the fit, no corresponding Gaussian constraint
2394 is added to the likelihood.

2395 Statistical uncertainty is also present, and implemented using a dedicated NP for
2396 each bin which can scale the background yield in that bin. Statistical NPs are also
2397 implemented using a Gaussian constraint.

2398 Smoothing and Pruning

2399 Systematic uncertainties are smoothed and pruned in the fit. Smoothing accounts
2400 for the large statistical uncertainty present in some bins that are subject to large
2401 fluctuations. The smoothing procedure relies on the assumption that the impact of
2402 systematics should be approximately monotonic and correlated between neighbouring
2403 bins.

2404 In addition to smoothing, pruning is the process of removing from the fit those
2405 systematics which only have a very small effect. This improves the stability of the
2406 fit by reducing the number of degrees of freedom. Acceptance uncertainties are
2407 pruned in a given region if they have a variation of less than 0.5%, or if the up and
2408 down variations have the same sign in that region. Shape uncertainties are pruned

²⁴⁰⁹ in a given region if the deviation in each bin is less than 0.5% in that region. In
²⁴¹⁰ addition, acceptance and shape uncertainties are neglected in a given region for any
²⁴¹¹ background which makes up less than 2% of the total background in a given region.

²⁴¹² Fit Procedure and Statistical Tests

²⁴¹³ The best-fit value of μ , denoted $\hat{\mu}$, is obtained via an unconditional maximisation
²⁴¹⁴ of the likelihood. The likelihood is also used to construct a statistical test which can
²⁴¹⁵ confirm or reject the background-only hypothesis. The test statistic q_μ is constructed
²⁴¹⁶ from the profile likelihood ratio, as in

$$q_\mu = -2 \ln \frac{\mathcal{L}(\mu, \hat{\theta}_\mu)}{\mathcal{L}(\hat{\mu}, \hat{\theta})} \quad (7.5)$$

²⁴¹⁷ where $\hat{\mu}$ and $\hat{\theta}$ are chosen to maximise the likelihood \mathcal{L} , and the profile value $\hat{\theta}_\mu$ is
²⁴¹⁸ obtained from a conditional maximisation fo the likelihood for a specific choice of
²⁴¹⁹ $\mu = 0$ corresponding to the background-only hypothesis.

²⁴²⁰ The test statistic is used to construct a p -value which is used to confirm or accept
²⁴²¹ the background-only hypothesis. The p -value is typically reported in terms of the
²⁴²² significance Z , defined as the number of standard deviations for a Gaussian Normal
²⁴²³ distribution which will produce a one-sided tail integral equal to the p -value, as in

$$p = \int_Z^\infty \frac{1}{\sqrt{2\pi}} e^{-x^2/2} dx = 1 - \Phi(Z). \quad (7.6)$$

²⁴²⁴ Typically a value of $Z = 3$ constitutes *evidence* of a processes, while $Z = 5$ is required
²⁴²⁵ for a *discovery*. Alongside the p -value, the best-fit value of the signal strength $\hat{\mu}$ and
²⁴²⁶ its corresponding uncertainty are typically quoted, and compared to their expected
²⁴²⁷ values (see Section 7.3.3).

²⁴²⁸ 7.3.2 Background Normalisations

²⁴²⁹ The normalisation of the largest backgrounds are left floating and are determined in
²⁴³⁰ the fit. The corresponding postfit background normalisations are listed in Table 7.11.
²⁴³¹ A single normalisation factor is used for $W+\text{hf}$ and $Z+\text{hf}$, which constitue more

2432 than 90% of the total $V + \text{jets}$ background, since the use of independent factors in
2433 different channels were found to be compatible.

Process	Normalisation factor
$t\bar{t}$ 0-lepton	0.88 ± 0.10
$t\bar{t}$ 1-lepton	0.83 ± 0.09
$W + \text{hf}$	1.12 ± 0.14
$Z + \text{hf}$	1.32 ± 0.16

Table 7.11: Factors applied to the nominal normalisations of the $t\bar{t}$, $W + \text{hf}$, and $Z + \text{hf}$ backgrounds, as obtained from the likelihood fit [126]. The errors represent the combined statistical and systematic uncertainties.

2434 The normalisations and shapes of all other backgrounds, with the exception of the
2435 multijet background which is estimated using a data driven technique, are initialised
2436 using the simulated samples.

2437 7.3.3 Asimov Dataset & Expected Results

2438 The Asimov dataset is constructed by replacing the data with the sum of the signal
2439 and background predictions $n_i = s_i + b_i$. A fit to this dataset using the nominal
2440 values of the NPs from the simulation will recover the input values and is useful for
2441 studying constraints on and correlations between the NPs.

2442 Alternatively, a conditional fit to the Asimov dataset can be performed using values
2443 of the background NPs which are determined from an unconditional fit to data. The
2444 signal NPs and POIs are fixed at their nominal values from the SM simulation. The
2445 result of this fit can be used to calculate expected (median) significances, which can
2446 be compared to their observed values, as is done in Section 7.4.2.

2447 7.4 Results

2448 In the present analysis, the two signal strength parameters μ_{VH}^{bb} and μ_{VZ}^{bb} are extracted
2449 from a simultaneous maximisation of the likelihood described in Section 7.3. The
2450 results of the analysis are summarised in this section. Post-fit m_J distributions are

2451 shown in Section 7.4.1. The observed signal strengths are given in Section 7.4.2,
2452 along with observed and expected significances. Finally in Section 7.4.3 the impact
2453 of systematic uncertainties on the results is examined.

2454 7.4.1 Post-fit Distributions

2455 In addition to the observed significance and signal strength, it is also useful to study
2456 the post-fit m_J distributions to compare the simulation and data using the best-fit
2457 values $\hat{\mu}$ and $\hat{\theta}$. Post-fit m_J distributions are given for the signal regions in the 0-,
2458 1- and 2-lepton channels in Fig. 7.6. The LP and HP regions are merged for the
2459 0- and 1-lepton channels. The plots show large falling backgrounds, predominantly
2460 made up of W -jets and Z -jets events, and a signal distribution corresponding to
2461 the Standard Model Higgs boson peaking around $m_H = 125$ GeV. In general there is
2462 a good level of agreement between the simulation and data, indicating the fit model
2463 is performing as expected. Fig. 7.7 shows the post-fit plots for the $t\bar{t}$ control regions.
2464 Again, a good level of agreement is observed given the statistical uncertainties on
2465 the distributions.

2466 7.4.2 Observed Signal Strength & Significance

2467 The measured signal strength is computed as the ratio between the measured signal
2468 yield to the prediction from the SM. The combined result for all three lepton channels
2469 and all analysis regions is given for μ_{VH}^{bb} in Eq. (7.7), and for μ_{VZ}^{bb} is given in Eq. (7.8).
2470 Both results include a full breakdown of the systematic and statistical uncertainties.

$$\mu_{VH}^{bb} = 0.72^{+0.39}_{-0.36} = 0.72^{+0.29}_{-0.28}(\text{stat.})^{+0.26}_{-0.22}(\text{syst.}) \quad (7.7)$$

2471

$$\mu_{VZ}^{bb} = 0.91^{+0.29}_{-0.23} = 0.91 \pm 0.15(\text{stat.})^{+0.24}_{-0.17}(\text{syst.}) \quad (7.8)$$

2472 The results for μ_{VH}^{bb} and μ_{VZ}^{bb} agree with the expectation from the SM within their
2473 combined uncertainty. The μ_{VH}^{bb} measurement is dominated by statistical uncertainty,
2474 while the μ_{VZ}^{bb} measurement is dominated by systematic sources of uncertainty. These
2475 measured signal strength for μ_{VZ}^{bb} corresponds to an observed significance of 2.1
2476 standard deviations, with an expected (median) significance given the SM prediction

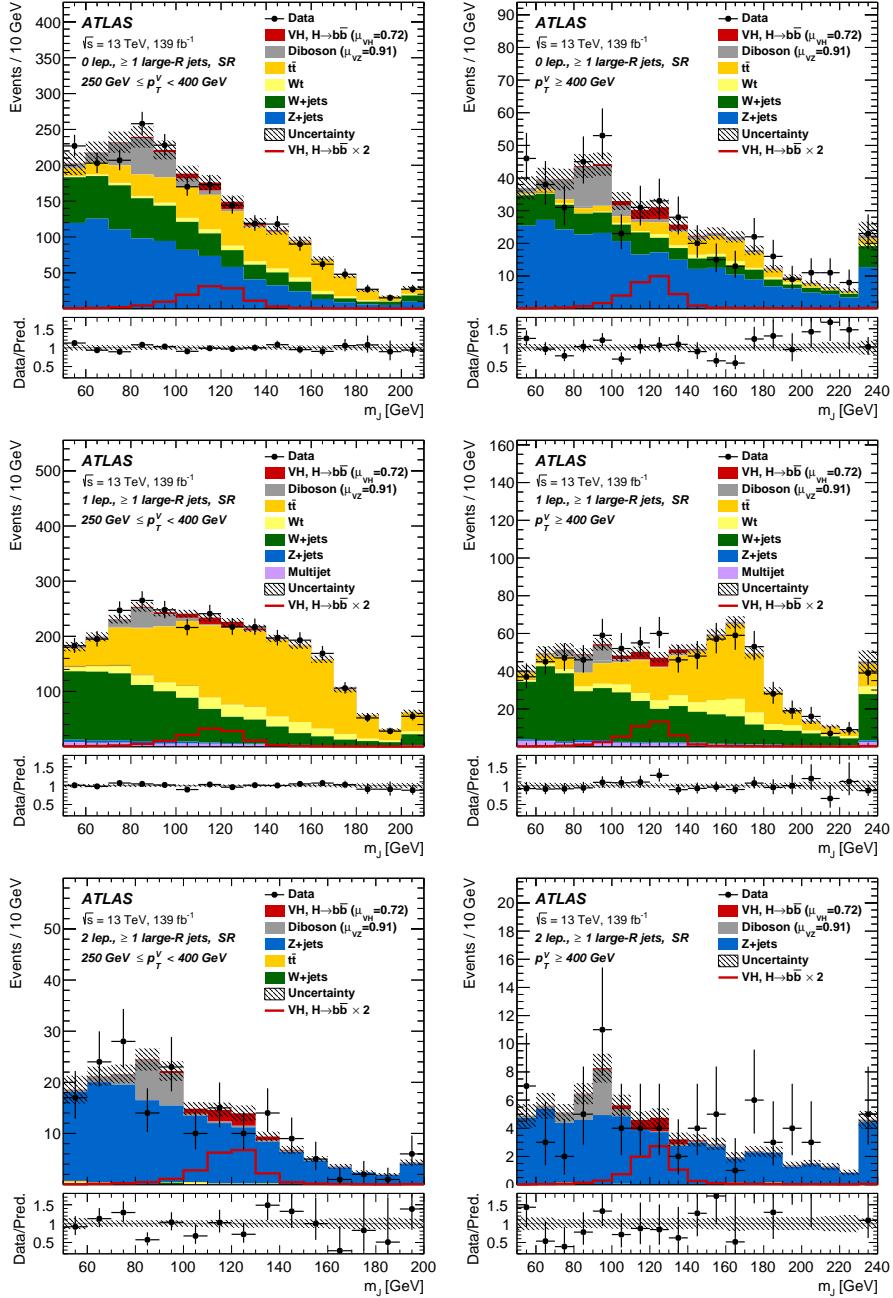


Figure 7.6: The m_J post-fit distributions in (top) the 0-, (middle) 1- and (bottom) 2-lepton SRs for (left) $250 \text{ GeV} < p_T^V < 400 \text{ GeV}$ and (right) $p_T^V \geq 400 \text{ GeV}$ [126]. The LP and HP regions are merged for the 0-lepton and 1-lepton channels. The fitted background contributions are shown as filled histograms. The Higgs boson signal ($m_H = 125 \text{ GeV}$) is shown as a filled histogram and is normalised to the signal yield extracted from data ($\mu_{VH}^{bb} = 0.72$), and as an unstacked unfilled histogram, scaled by the SM prediction times a factor of two. The size of the combined on the sum of the fitted signal and background is shown in the hatched band. The highest bin contains the overflow.

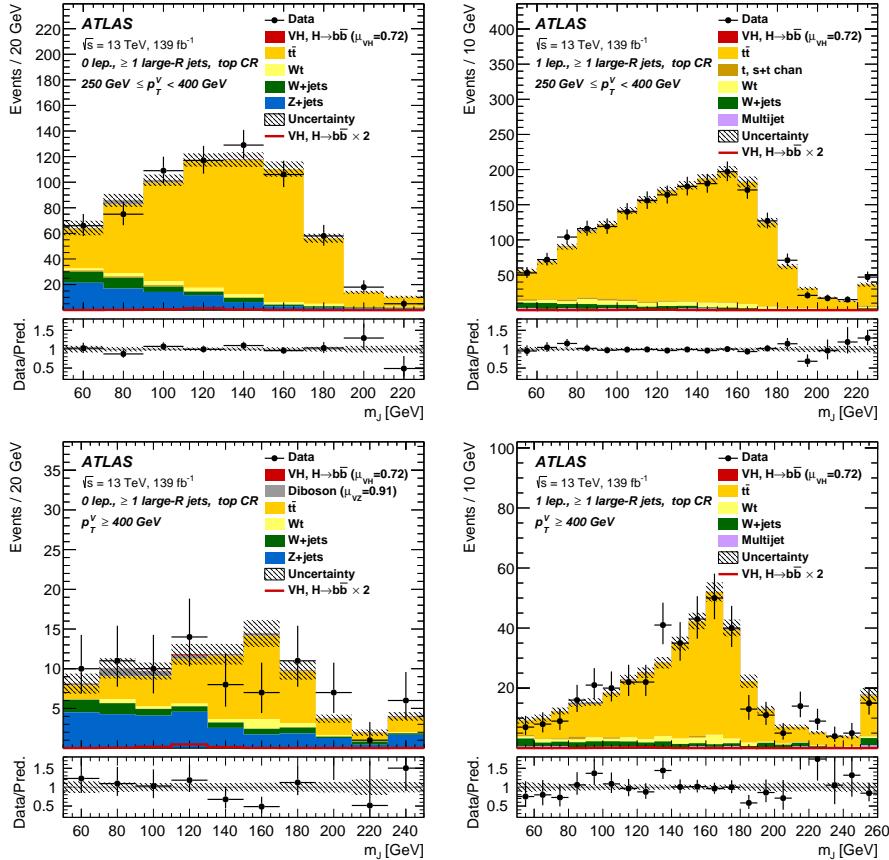


Figure 7.7: The m_J post-fit distributions in the $t\bar{t}$ control region for (top) the 0-lepton channel and the 1-lepton channel for $250 \text{ GeV} < p_T^V < 400 \text{ GeV}$ and (bottom) the 0-lepton channel and the 1-lepton channel for $p_T^V > 400 \text{ GeV}$ [126]. The background contributions after the likelihood fit are shown as filled histograms. The Higgs boson signal ($m_h = 125 \text{ GeV}$) is shown as a filled histogram on top of the fitted backgrounds normalised to the signal yield extracted from data ($\mu_{VH}^{bb} = 0.72$), and unstacked as an unfilled histogram, scaled by the SM prediction times a factor of 2. The size of the combined statistical and systematic uncertainty for the sum of the fitted signal and background is indicated by the hatched band. The highest bin in the distributions contains the overflow.

of 2.7 standard deviations obtained using the method described in Section 7.3.3. The diboson observed (expected) signal strength significance is 5.4 (5.7). These results are summarised in Fig. 7.8, which shows the background-subtracted m_J distribution. A clear signal excess is visible around the Higgs mass of $m_H = 125$ GeV.

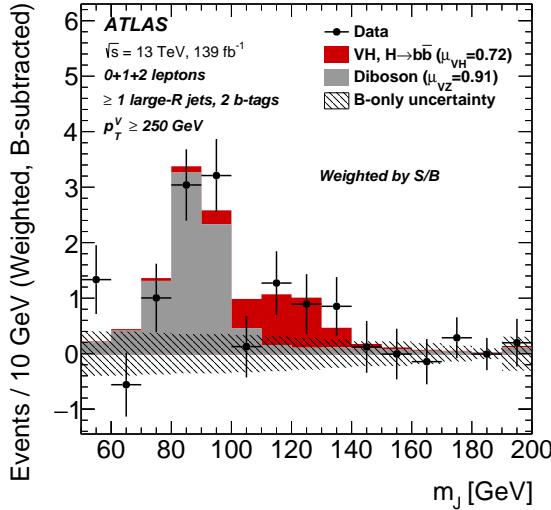


Figure 7.8: m_J distribution in data after subtraction of all backgrounds except for the WZ and ZZ diboson processes [126]. The contributions from all lepton channels and signal regions are summed and weighted by their respective values of the ratio of fitted Higgs boson signal and background yields. The expected contribution of the associated WH and ZH production of a SM Higgs boson with $m_H = 125$ GeV is shown scaled by the measured combined signal strength ($\mu_{VH}^{bb} = 0.72$). The diboson contribution is normalised to its best-fit value of $\mu_{VZ}^{bb} = 0.91$. The size of the combined statistical and systematic uncertainty is indicated by the hatched band. This error band is computed from a full signal-plus-background fit including all the systematic uncertainties defined in Section 7.2, except for the VH/VZ experimental and theory uncertainties.

2481 Compatability Studies

Alongside the standard 2-POI fit, a (3+1)-POI fit can be performed by splitting μ_{VH}^{bb} into three separate POIs, one for each channel. A simultaneous fit to the channel specific signal strengths can then be performed, which allows a comparison of the contributions from each channel. Fig. 7.9 compares the best-fit signal strengths. The 0- and 1-lepton channels show a signal strength which is consistent with the SM prediction, while the 2-lepton channel shows a small deviation within the 1σ

2488 uncertainty. Overall, good compatibility is observed via a χ^2 test with a corresponding
2489 p -value of 49%.

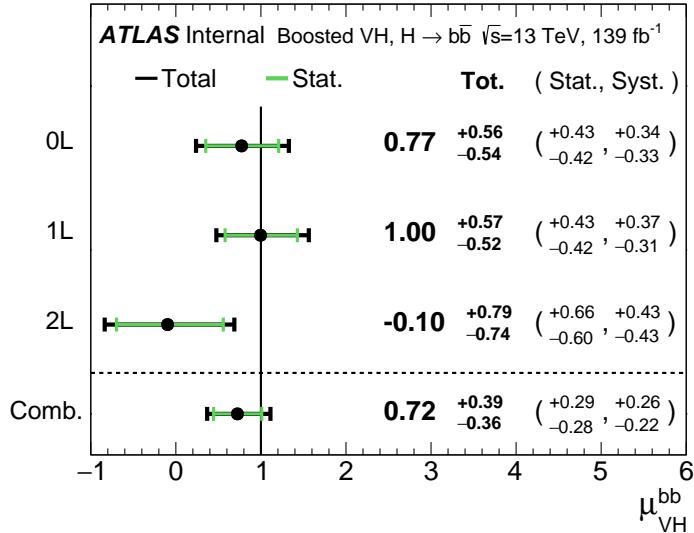


Figure 7.9: Signal strength compatibility test between the (3+1)-POI fit (with the three lepton channels splitted) and the default (1+1)-POI fit [126]. The compatibility of the three channels is evaluated via a χ^2 difference test and results in a p-value of 49%.

2490 7.4.3 Impact of Systematics

2491 The impact of systematic uncertainties on the final fitted value $\hat{\mu}_{VH}^{bb}$ is studied looking
2492 at the NP rankings, and the uncertainty breakdown.

2493 Fig. 7.10 shows the NP ranking, which is used to visualise which out of the many
2494 NPs involved in the fit have the largest impact on the sensitivity to the fitted POI.
2495 To obtain the ranking, a likelihood scan is performed for each NP θ_j . First, an
2496 unconditional fit is used to determine $\hat{\theta}_j$. From this best-fit point, the NP is varied
2497 in steps and the likelihood is recomputed until the $\pm 1\sigma_{\hat{\theta}_j}$ values are reached. For
2498 each corresponding value of θ_j , the change in the best-fit value of the POI, $\Delta\hat{\mu}_{VH}^{bb}$
2499 is calculated and used to rank the NPs. Also shown in Fig. 7.10 are the pulls and
2500 constraints for the highest ranked NPs.

2501 The experimental uncertainty on the signal large- R jet mass resolution (JMR) has
2502 the largest impact of any NP. It is a significant contributor to the overall uncertainty

2503 on μ_{VH}^{bb} in Eq. (7.7). JMR and jet energy scale (JES) uncertainties also have impacts
 2504 for the $V+jets$ background and for the diboson background. The freely-floating
 2505 $Z+hf$ normalisation is the second highest ranked NP, and is heavily constrained by
 2506 the fit. The VZ POI μ_{VZ}^{bb} is also a significant NP when considering the primary μ_{VH}^{bb}
 2507 measurement.

2508 The NP ranking highlights individual NPs which have a large impact on the POI
 2509 measurement sensitivity. Complementary information is provided at a higher level
 2510 by considering the overall impact of different groups of systematics. The groups
 2511 are constructed from NPs which have similar physical origin. The impact on each
 2512 group is calculated by running a fit with all the NPs in the given group fixed to their
 2513 nominal values. The uncertainty on the POI extracted from this fit is subtracted
 2514 in quadrature from the the uncertainty on the POI from the nominal fit, and the
 2515 resulting values are provided as the impact for each group. The full breakdown
 2516 for the observed impact of uncertainties on the μ_{VH}^{bb} signal strength is provided in
 2517 Table 7.12. The total systematic impact is the difference in quadrature between the
 2518 nominal uncertainty on μ_{VH}^{bb} and the combined statistical impact. The “data stat
 2519 only” group fixes all NPs at their nominal value, while the total statistical impact
 2520 fixes all NPs except floating normalisations. The floating normalisations group fixes
 2521 only the NPs associated with normalisation which are left floating in the fit. The
 2522 uncertainty on μ_{VH}^{bb} is dominated by combined statistcal effects (0.28), although the
 2523 combined impact of systematics (0.24) is of a comparable size. The signal largest
 2524 group is the data stat uncertainty (0.25), demonstrating that the analysis would
 2525 benefit from an increased integrated luminosity or improved efficiency to select signal
 2526 relevant events (recall from Section 7.1.3 the signal efficiency is in the range of
 2527 10%). Of the experimental systematic sources of uncertainty, the dominant impact
 2528 is the experimental uncertainties associated with the reconstruction of large- R jets
 2529 (0.13). Other experimental sources of uncertainty are small in comparison. Modelling
 2530 uncertainties also have a large contribution to the overall systematic uncertainty. The
 2531 biggest contribution to the overall uncertainty is the combined statistical uncertainty
 2532 on the simulated samples (0.09), which contain only a finite number of events. Out of
 2533 the backgrounds, the $W+jets$ and $Z+jets$ have the highest (0.06) and second-highest
 2534 (0.05) impact respectively.

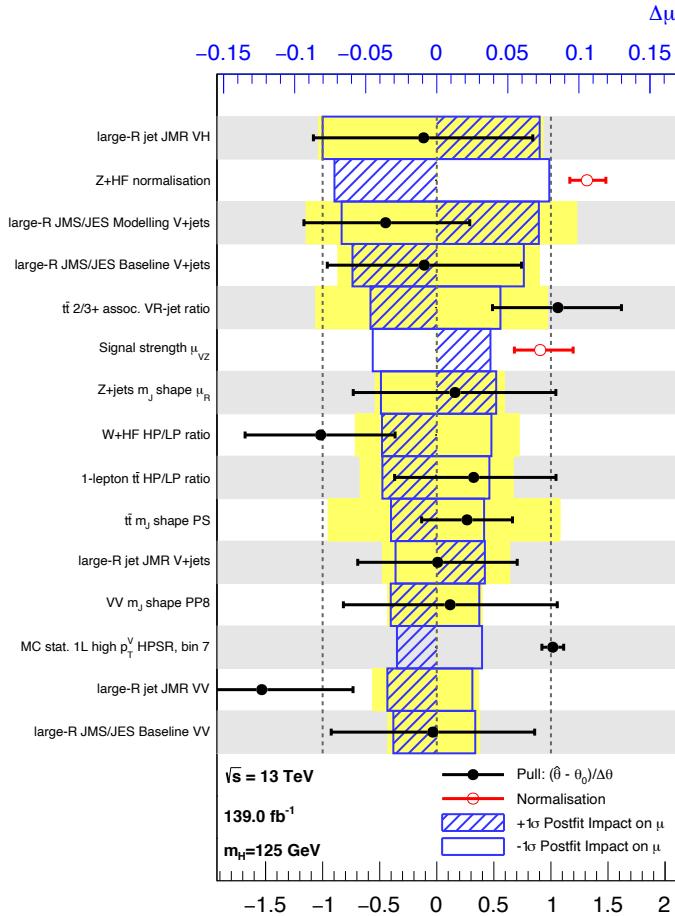


Figure 7.10: Impact of systematic uncertainties on the fitted VH signal-strength parameter μ_{VH}^{bb} sorted in decreasing order [172]. The boxes show the variations of $\hat{\mu}$, referring to the top x -axis, when fixing the corresponding individual nuisance parameter to its post-fit value modified upwards or downwards by its post-fit uncertainty, i.e. $\hat{\theta} \pm \sigma_{\hat{\theta}}$, and repeating the fit. The impact of up- and down-variations can be distinguished via the dashed and plane box fillings. The yellow boxes show the pre-fit impact (top x -axis) by varying each nuisance parameter by ± 1 . The filled circles show the deviation of the fitted value for each nuisance parameter, $\hat{\theta}$, from their nominal input value θ_0 expressed in standard deviations with respect to their nominal uncertainties $\Delta\theta$ (bottom x -axis). The error bars show the post-fit uncertainties on $\hat{\theta}$ with respect to their nominal uncertainties. The open circles show the fitted values and uncertainties of the normalization parameters that are freely floating in the fit. Pre-fit, these parameters have a value of one.

Source of uncertainty	Signed impact	Avg. impact
Total	+0.388 / -0.356	0.372
Statistical	+0.286 / -0.280	0.283
↔ Data stat only	+0.251 / -0.245	0.248
↔ Floating normalisations	+0.096 / -0.092	0.094
Systematic	+0.261 / -0.219	0.240
<hr/>		
Experimental uncertainties		
small-R jets	+0.041 / -0.034	0.038
large-R jets	+0.161 / -0.105	0.133
E_T^{miss}	+0.008 / -0.007	0.007
Leptons	+0.013 / -0.007	0.010
<i>b</i> -tagging	<i>b</i> -jets	+0.028 / -0.004
	<i>c</i> -jets	+0.012 / -0.011
	light-flavour jets	+0.009 / -0.007
	extrapolation	+0.004 / -0.005
Pile-up	+0.001 / -0.002	0.001
Luminosity	+0.019 / -0.007	0.013
<hr/>		
Theoretical and modelling uncertainties		
Signal	+0.073 / -0.026	0.050
Backgrounds	+0.106 / -0.095	0.100
↔ $Z + \text{jets}$	+0.049 / -0.047	0.048
↔ $W + \text{jets}$	+0.059 / -0.056	0.058
↔ $t\bar{t}$	+0.037 / -0.032	0.035
↔ Single top quark	+0.031 / -0.023	0.027
↔ Diboson	+0.034 / -0.029	0.032
↔ Multijet	+0.009 / -0.009	0.009
↔ MC statistical	+0.091 / -0.092	0.092

Table 7.12: Breakdown of the observed absolute contributions to the uncertainty on the signal strength μ_{VH}^{bb} obtained from the (1+1)-POI fit [172]. The average impact represents the average between the positive and negative uncertainties on μ_{VH}^{bb} . The sum in quadrature of the systematic uncertainties attached to the categories differs from the total systematic uncertainty due to correlations.

2535 7.5 Conclusion

2536 The analysis of the associated production of vector bosons with boosted Higgs bosons
2537 decaying to a pair of b -quarks using large- R jets is presented. The Higgs candidate is
2538 reconstructed as a large- R jet in order to improve sensitivity in the boosted regime
2539 in which the Higgs decay products are significantly collimated. The analysis is
2540 performed using 139 fb^{-1} of proton–proton collision data at $\sqrt{s} = 13\text{ TeV}$ collected
2541 throughout the duration of Run 2 of the LHC.

2542 In comparison with the null hypothesis, the Standard Model (SM) VH , $H \rightarrow b\bar{b}$
2543 process is found to have an observed significance of 2.1 standard deviations, whereas
2544 the corresponding expected significance is 2.7 standard deviations. The VH , $H \rightarrow b\bar{b}$
2545 process is measured simultaneously with the diboson VZ , $Z \rightarrow b\bar{b}$ process, which
2546 provide a cross-check for the main analysis. The observed (expected) significance for
2547 the diboson process is 5.4 (5.7).

2548 The statistical and systematic sources of uncertainty contribute a similar amount
2549 to the overall uncertainty on the result. This analysis would therefore likely benefit
2550 greatly from the improved b -tagging efficiency at high- p_{T} enabled by GN1 as discussed
2551 in Chapter 6, due to the associated reduction in statistical uncertainty provided by
2552 the increased number of events used in the analysis.

2553 Chapter 8

2554 Conclusion

2555 Recap why flavour tagging at high pT is important.

2556 Recap challenges

- 2557 • tracking suffers from several problems which might be improved by...

- 2558 • tracking might be improved by...

2559 algorithmic gains in flavour tagging can improve things. future work on that front:

- 2560 • use more info for flavour tagging (hits, calo info, leptons)

- 2561 • more aux tasks, energy, mass, lxy regression

2562 ultimately analyses will benefit greatly, in particualr boosted xbb tagging and dihiggs

2563 analysis

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