

HIGH ENERGY PHYSICS AT LOW(ER) ENERGIES: PRECISION MEASUREMENTS IN
TOP QUARK PHYSICS AT $\sqrt{s} = 5.02$ TeV

by

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Department of Physics
University of Toronto

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 $\sqrt{s} = 5.02 \text{ TeV}$

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Abstract

The top quark is the heaviest of all known subatomic particles with a mass similar to that of a tungsten atom. Furthermore, it has the shortest lifetime of all quarks and is the only one that can be studied as a “free” quark. With the discovery of the Higgs boson at the Large Hadron Collider (LHC) in 2012 and no sign of any physics beyond the Standard Model (SM), measurements of the top quark provide an alternate approach to understanding and testing the SM. This thesis will present two measurements of the top quark at a centre-of-mass energy of 5.02 TeV with 257 pb^{-1} of proton-proton collision data collected by the ATLAS detector. The first is a $t\bar{t}$ cross-section measurement that is used to constrain the gluon Parton Distribution Function (PDF) at high Bjorken x and the second is a search for t -channel single-top-quark production. The pair-production cross-section was measured individually in both the dilepton and single-lepton channels of the $t\bar{t}$ decay before being combined. The measurement in the single-lepton channel is currently the most precise measurement of the top-quark pair-production cross-section by the ATLAS Collaboration to date. The t -channel cross-section is measured in the semi-leptonic decay of the top quark and is the first observation of this process at $\sqrt{s} = 5.02 \text{ TeV}$.

To Mama and Papa, thank you.

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Chapter 1

Introduction

In the quest to understand our universe, the field of particle physics made significant and recent contributions to human knowledge. Within a century and a half, the Standard Model of particle physics (SM) was developed on the shoulders of atomic theory through the simultaneous progression of both theoretical and experimental particle physics.

A keystone of the SM was laid in 1897 by Thomson’s discovery of the electron [1], while studying cathode rays. This discovery was quickly followed by Planck’s law [2] of blackbody radiation which would mark the beginnings of quantum theory. Quantum mechanics would end up forming the bedrock of modern particle physics in conjunction with the ideas of relativity that were introduced by Einstein in the early 20th century [3, 4]. Einstein would also introduce the idea of “light quanta”, now known as a photon, in order to explain the photoelectric effect [5]. In parallel to Einstein, theoretical physicists such as Bohr, Heisenberg, Schrödinger, Dirac, and many more were developing quantum mechanics as a theory to explain experimental results at small distance scales (or equivalently, high energy scales). A prime example of this is the atomic structure of the hydrogen atom, after the nucleus [6] was discovered by Rutherford with his gold foil scattering experiments.

One of the consequences of the advancement on quantum mechanics was Dirac’s postulate of positrons, an “antiparticle” which shares the same quantum numbers as the electron but has opposite charge. Solutions to the Dirac equation [7] would lead Dirac to propose the hole theory with an infinite number of electrons in the vacuum and that positrons must arise whenever the vacuum is not perfectly filled. Although Dirac’s hole theory would turn out to be incorrect (although consistent with quantum field theory that it was replaced by), it would lead to the prediction and eventual discovery of the positron by Anderson in 1932 [8] while studying cosmic rays with cloud chambers. Antiparticles have now been discovered for all subatomic particles that have been confirmed to satisfy the Dirac equation. Anderson would eventually discover the muon with Neddermeyer in 1936 [9], a fundamental particle analogous to the electron, also while studying cosmic rays but without any prior theoretical postulate.

The electron neutrino was the next fundamental particle proposed, by Pauli in 1930 and it was introduced in order to explain the continuous spectrum of β -decay seen by Chadwick in 1914 [10]. The electron neutrino would eventually be discovered in 1956 by Cowan and Reines [11], while studying the inverse β -decay using neutrinos expected to be produced in nuclear reactors. A muon neutrino would also be discovered by Lederman, Schwartz, and Steinberger using a synchrotron [12] without any existing theoretical predictions. Similarly, the tau lepton was discovered by Perl [13] in electron-positron collisions and the tau neutrino was discovered by the DONUT Collaboration at Fermilab in 2000 [14].

By 1935, Yukawa would predict the existence and mass of a “meson”, which would act as force carriers for the strong force [15]. Various mesons have been discovered over the decades since Yukawa’s initial proposal and found to behave according to Bose-Einstein statistics. However, at the time, the pion [16] was the one to match Yukawa’s theory. Similar to mesons, various additional “baryons”, composite particles which obey Fermi-Dirac statistics (such as protons and neutrons), were discovered in the 20th century. It was with these discoveries in mind that Gell-Mann and Zweig would propose the existence of the up, down, and strange quarks, along with the gluon [17, 18]. Quarks, as constituents of the proton, were eventually discovered in 1968 during scattering experiments probing the structure of protons at SLAC [19]. The charm quark was eventually discovered through the observation of the J/ψ meson by Richter and Ting and the gluon would finally be discovered in three “jet” (collections of particles in a geometric region that typically arise from quarks and gluons) events seen in electron-positron collisions at DESY in 1978 [20]. The final pair of quarks, the bottom and top quarks, were postulated by Kobayashi and Maskawa in 1973 in order to explain CP violation observed in kaon decays. The bottom quark would be discovered by Lederman at Fermilab in 1977 [21] and the top quark by the D0 and CDF collaborations in 1995 [22, 23], also at Fermilab.

In 1968, Glashow, Weinberg, and Salam proposed a mechanism to unify the electromagnetic and weak nuclear forces [24–26]. The mechanism relied on the introduction of a scalar (spin 0) field, first predicted in the 1960s, known as the Higgs boson [27–32]. In addition to the Higgs boson, this mechanism predicted the existence of two additional force mediators (the W and Z bosons) similar to the photons. Both bosons were discovered by the UA1 and UA2 collaborations in proton-antiproton collisions at CERN [33–36] and the Higgs boson was eventually discovered by the ATLAS and CMS collaborations [37, 38] using the large hadron collider at CERN.

With the discovery of the Higgs boson, the SM as we know it today was complete albeit with some shortcomings such as its inability to explain dark matter, the fine-tuning of the Higgs boson mass, the absence of gravity, and its eventual breakdown at energies near the Planck scale¹. As of now, searches for physics beyond the SM (BSM) are done through direct searches of new particles or through precision measurements and subsequent comparison with SM predictions. Searches for BSM physics typically occur through astronomical, collider, measurements of low-energy systems, and neutrino-based experiments. Although no BSM physics has been found, anomalies which may hint at BSM physics, have been observed in certain measurements. Recent such anomalies include possible violation of lepton flavour universality in b-quark decays [39], a five standard deviation

¹The SM could break at lower energy scales as well.

discrepancy between select predictions of the muon magnetic moment and the observed value [40], and the W boson mass measurement made by the CDF Collaboration in 2022 [41]. The W boson mass measurement is particularly intriguing as it is larger than the SM prediction by seven standard deviations, much larger than the other anomalies, and is a contentious measurement within the field. The confirmation of such anomalies could indicate either a hidden flaw in our understanding of the SM or perhaps even BSM physics that might be visible at the LHC

Continued effort on searches for BSM physics and measurements at hadron colliders, like the LHC and HL-LHC, are based on our understanding of proton substructure. The uncertainty in the proton substructure is typically one of the dominant systematic uncertainties in both the theoretical predictions of SM cross-sections (i.e. Higgs boson production cross-sections [42]) and experimental measurements (i.e. the W boson mass measurement by CDF [41]). The proton substructure is typically probed through specialized scattering experiments but it is also possible to probe it through precision measurements of the SM. Two such measurements are the inclusive cross-sections of top quarks produced as top and antitop-quark pairs, or in processes where only a single-top-quark is produced. Measurements of these cross-sections at different centre-of-mass energies provide a unique way of increasing our understanding of PDFs.

This thesis summarizes both of these measurements which were performed using data collected by the ATLAS detector at CERN at a centre-of-mass energy of $\sqrt{s} = 5.02$ TeV in pp collisions. A summary of all the work performed over the course of this thesis is summarized in Appendix A. Chapter 2 provides an overview of the theory behind both measurements and is followed by Chapter 3 which describes the LHC and the ATLAS detector. Reconstruction and calibration algorithms are discussed in Chapter 4 and are followed by algorithms for flavour tagging in Chapter 5. The pair-production cross-section measurement is presented in Chapter 6 and is followed by the t -channel cross-section measurement in Chapter 7. Finally, Chapter 8 concludes the thesis.

Chapter 2

Theoretical Overview

The SM of particle physics is a quantum field theory describing the various particles in nature and their interactions with each other. With 17 different fundamental constituents, the SM describes the electromagnetic interactions, weak interactions, and the interactions via the strong nuclear force. Although the SM is incomplete, it shows remarkable agreement with data in various tests and no evidence of new physics has yet been found. Section 2.1 provides an overview of the SM and is followed by a discussion on the phenomenology of the top quark in Section 2.2. Sections 2.3 and 2.4 present the physics at hadron colliders and the physics during and after the collision of hadrons. Finally, Section 2.5 gives a small overview of relevant simulation programs used in particle physics.

2.1 The Standard Model

The SM predicts the existence of two sets of fundamental particles: one set with half-integer spin obeying Fermi-Dirac statistics (fermions) and the other set with integer spin obeying Bose-Einstein statistics (bosons). Fermions are split into two types depending on their possible interactions. Fermions capable of interacting with the strong and electroweak forces have both an electric charge and a colour charge, and are denoted as quarks. Conversely, fermions that only interact with the electroweak force and have only an electric charge are called leptons.

There are a total of six quarks (of different “flavours”), three “up-type” quarks and three “down-type” quarks. Additionally, there are three flavours of neutral leptons (lepton neutrinos) and three flavours of charged leptons. A chiral structure of the fermions of the SM is needed to describe the weak interaction. The left-handed up-type quarks and neutral leptons have a weak isospin number of $1/2$, the down-type quarks and charged leptons have a weak isospin of $-1/2$, and all right-handed fermions in the SM have a weak isospin of 0. Fermions can be further categorized into three generations with two quarks and two leptons, each of different type, in a single generation. The three flavours of

up-type quarks are: up, charm, and top (u , c , and t) whereas the three flavours of down-type quarks are: down, strange, and bottom (d , s , and b). Similarly, the electron, muon, and tau leptons (e , μ , and τ) are the three flavours of charged leptons and the electron neutrino, muon neutrino, and tau neutrino (ν_e , ν_μ , and ν_τ) are the three flavours of lepton neutrinos in the SM.

The four gauge bosons that mediate the forces are the gluon (g) for the strong nuclear force, the photon (γ) for the electromagnetic force, and the W and Z bosons for the weak nuclear force. These bosons are denoted as gauge bosons since they are adjoint representations of the $SU(3)$ symmetry of the SM for the gluon and the mixing of the $U(1)$ and $SU(2)_L$ gauge bosons for the others. An additional scalar boson (with a spin of 0) - the Higgs boson, arises from the Brout-Englert-Higgs mechanism [27–32] of electroweak symmetry breaking.

All quarks, all leptons, and the W boson in the SM have a respective anti-particle with the same quantum numbers and mass but opposite charge. Figure 2.1 shows a cartoon of all particles in the SM and their respective quantum numbers. Sections 2.1.1 and 2.1.2 present Quantum Chromodynamics (QCD), the theory describing interactions of quarks and gluons, and the electroweak sector of the SM, respectively.

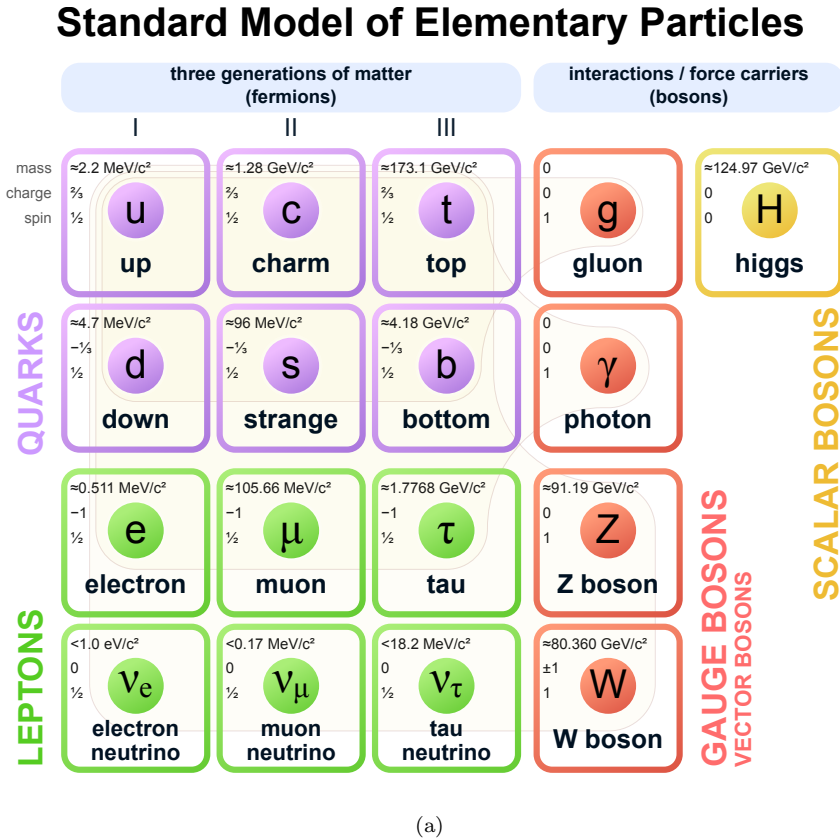


Figure 2.1: A cartoon showing the various fermions and bosons that make up the SM.

2.1.1 Quantum Chromodynamics

The Lagrangian¹ describing the interactions between quarks and gluons is defined a free quark field that satisfies the Dirac equation and also satisfies a local $SU(3)$ gauge transformation. The theory for a free field (ψ) that satisfies the Dirac equation (i.e. it is a spin 1/2 particle) is given by

$$\mathcal{L}_{\text{Dirac}} = \bar{\psi} (i\cancel{D} - m) \psi \quad (2.1)$$

If the Lagrangian is to be invariant under local $SU(3)$ transformations², the partial derivative must be replaced with the covariant derivative (D_μ)

$$\partial_\mu \rightarrow D_\mu = \partial_\mu - \frac{1}{2} i g_s \lambda_a G_\mu^a \quad (2.2)$$

Here, G_μ^a are the gluon fields and under the $SU(3)$ transformation, they are required to transform as

$$G_\mu^a \rightarrow G_\mu^{a'} = G_\mu^a + \frac{1}{g_s} \partial_\mu \theta_a - f_{abc} \theta_b G_\mu^c \quad (2.3)$$

Here, f_{abc} is the structure constant for the $SU(3)$ group that is defined according to: $[\lambda_a, \lambda_b] = i f_{abc} \lambda_c$. By defining such fields, the resulting Lagrangian is invariant under all local $SU(3)$ and can be written as

$$\begin{aligned} \mathcal{L}_{\text{QCD}} &= -\frac{1}{4} G_{\mu\nu}^a G_a^{\mu\nu} + \bar{\psi}_j (i\cancel{D} - m_j) \psi_j \\ G_{\mu\nu}^a &= \partial_\mu G_\nu^a - \partial_\nu G_\mu^a + g_s f_{abc} G_\mu^b G_\nu^c \end{aligned} \quad (2.4)$$

Here, the index j runs over the various fermions that experience colour charge (in the SM it is the quarks). Note that at tree level, the Lagrangian permits interactions of two quarks and one gluon, three gluons, and four gluons. Furthermore, due to the Gell-Mann matrices being 3×3 matrices, the quark fields must be expressed as vectors in the colour space (colour triplets): $\psi_j = (\psi_j^R, \psi_j^G, \psi_j^B)^T$. Here, the superscripts represent the red, green, and blue colour charges, respectively.

Since QCD is a renormalizable theory, one can incorporate UV divergences into the coupling that changes based on the energy scale of an interaction. This scale is denoted as the renormalization scale μ_r . The strong coupling constant α_s in QCD is expressed as

$$\alpha_s(\mu_r) = \frac{g_s(\mu_r)}{4\pi} = \frac{12\pi}{(33 - 2n_f) \ln \left(\frac{\mu_r}{\Lambda_{\text{QCD}}} \right)} \quad (2.5)$$

Here, n_f refers to the flavours of quarks and Λ_{QCD} is the energy scale where perturbation theory in QCD breaks down ($\sim 200 \text{ MeV}$). With such a structure, the coupling strength approaches 0 as

¹Technically this is a Lagrangian density

²This can be expressed as $\psi \rightarrow \psi' = e^{i g_s \lambda_a \theta_a / 2} \psi$. Here, g_s is the strong coupling constant, λ_a are the eight Gell-Mann matrices, and θ_a is an infinitesimally small angle. Note that the index runs over the eight Gell-Mann matrices which are also generators of the $SU(3)$ group.

$\mu_t \rightarrow \infty$ and approaches ∞ when $\mu_t \rightarrow 0$. These two properties of QCD are called asymptotic freedom and colour confinement, respectively. Asymptotic freedom allows one to consider quarks as free particles at high energies and short distances since interactions at such scales can be neglected. Colour confinement on the other hand, ensures that it is impossible to find free quarks at low energies. In the perturbative regime, QCD along with the other Quantum Field Theories (QFTs) that make up the SM, can be expanded as a power series of the coupling constant (denoted as “perturbation theory”). The expansion can then be used to determine theoretical cross-section of various processes at a given order [43, 44].

2.1.2 Electroweak Sector and Electroweak Symmetry Breaking

The electroweak sector of the SM is analogous to QCD. However, it requires special treatment in order to match the parity violation seen in weak decay. Since the weak decay was experimentally observed for left-handed fermions, the Lagrangian must be invariant under local $SU(2)$ transformations but only for the left-handed fermions (denoted as $SU(2)_L$). Unlike the charged current interaction, the electromagnetic interaction can be formulated by requiring the Lagrangian be invariant under local $U(1)$ transformations and since parity is not violated under electromagnetism, the $U(1)$ transformation must be applied to both the left- and right-handed components of the fermions.

The free Lagrangian from Section 2.1.1 can be written according to the chiralities of the fermion, but the mass term must be dropped for the Lagrangian to satisfy the $SU(2)_L$ symmetry. In this form, the free Lagrangian is

$$\mathcal{L} = i\bar{\psi}_L \not{\partial} \psi_L + i\bar{\psi}_R \not{\partial} \psi_R \quad (2.6)$$

The Lagrangian is then required to be invariant under the following local transformations

$$\begin{aligned} \psi_L &\rightarrow \psi'_L = e^{i\frac{\tau_j}{2}\alpha_j} e^{iY\beta} \psi_L \\ \psi_R &\rightarrow \psi'_R = e^{iY\beta} \psi_R \end{aligned} \quad (2.7)$$

Here, ψ_R and ψ_L are projections of the fermionic field into its right- and left-handed components, respectively³, τ_j are the three Pauli matrices that are generators of the $SU(2)$ group, Y is the weak hypercharge, and α and β are the rotation angles. The Lagrangian is locally invariant under $SU(2)_L \times U(1)$ if the following is satisfied

$$\begin{aligned} D_\mu \psi_L &= \left(\partial_\mu - \frac{1}{2}ig\tau^j W_\mu^j - \frac{1}{2}ig'YB_\mu \right) \psi_L \\ D_\mu \psi_R &= \left(\partial_\mu - \frac{1}{2}ig'YB_\mu \right) \psi_R \end{aligned} \quad (2.8)$$

Here, three gauge fields (W_μ^j) arise from the $SU(2)_L$ symmetry and one (B_μ) from the $U(1)$ symmetry. The constants g and g' represent the coupling strengths of these gauge fields. A transformation on

³ $\psi_R = \frac{1}{2}(1 + \gamma^5)$ and $\psi_L = \frac{1}{2}(1 - \gamma^5)$

the gauge fields similar to the one shown in Section 2.1.1 is necessary to ensure gauge invariance and in doing so, the Lagrangian can be written as

$$\mathcal{L} = -\frac{1}{4}W_{\mu\nu}^i W_i^{\mu\nu} - \frac{1}{4}B_{\mu\nu}B^{\mu\nu} + i\bar{\psi}_L \not{D}\psi_L + i\bar{\psi}_R \not{D}\psi_R \quad (2.9)$$

Note that the left-handed fermions are represented as doublets in the weak isospin (τ_3) space whereas the right-handed fermions are represented as singlets. The weak hypercharge and weak isospin of a given particle determine the electric charge it experiences and is defined by the Gell-Mann-Nishijima formula [45, 46]

$$Q = \tau_3 + Y \quad (2.10)$$

Note that the fermions do not have any mass terms and if one were to manually include them as seen in the Dirac equation, it would violate the $SU(2)_L$ gauge invariance. Thus, the ‘‘Higgs mechanism’’ of spontaneous symmetry breaking is used to incorporate the mass terms without violating gauge invariance. This is done by including a complex scalar doublet field (the Higgs field ϕ) that is invariant under $SU(2)_L \times U(1)$, as follows

$$\mathcal{L}_{\text{Higgs}} = D_\mu \phi D^\mu \phi^\dagger - V(\phi) \quad (2.11)$$

$$V(\phi) = \mu^2 \phi^2 + \lambda \phi^4 \quad (2.12)$$

Such a potential has a non-trivial minima at $\phi^2 = v = \sqrt{\frac{-\mu^2}{\lambda}}$ provided that $\mu^2 < 0$. Such a potential looks like a ‘‘Mexican hat’’ in two dimensions, as seen in Figure 2.2. The $SU(2)_L \times U(1)$ symmetry that the Lagrangian with the Higgs field is invariant under, will be broken if the value of the field drops to the minima. Defining h as an excitation around the minima vacuum expectation value v , and using the unitary gauge⁴, part of the Higgs Lagrangian can be written as

$$\mathcal{L}_{\text{Higgs}} = g^2 \frac{v^2}{8} \left[(W_\mu^1)^2 + (W_\mu^2)^2 + \left(\frac{g'}{g} B_\mu - W_\mu^3 \right)^2 \right] \quad (2.13)$$

$$\mathcal{L}_{\text{Higgs}} = \frac{1}{2} W^T \cdot \vec{M}^2 \cdot W \quad (2.14)$$

$$M^2 = \frac{v^2}{4} \begin{pmatrix} g^2 & 0 & 0 & 0 \\ 0 & g^2 & 0 & 0 \\ 0 & 0 & g^2 & -gg' \\ 0 & 0 & -gg' & g'^2 \end{pmatrix} \quad (2.15)$$

Here, the vector $W^T = (W_\mu^1, W_\mu^2, W_\mu^3, B_\mu)$ and M is the mass matrix. The mass matrix can be diagonalized by performing a unitary transformation on W and defining the fields $W^\pm = (W^1 \mp iW^2)/\sqrt{2}$, $Z = \frac{gW^3 - g'B}{\sqrt{g^2 + g'^2}}$, and $A = \frac{g'W^3 + gB}{\sqrt{g^2 + g'^2}}$. Here, the $W^\pm$ fields correspond to two charged bosons (the W bosons) which mediate the charged current and have a mass of $gv/2$, the Z boson which mediates the neutral current and has a mass of $v\sqrt{g^2 + g'^2}/2$, and the photon field A which has no mass.

⁴This is a gauge transformation that removes mixing terms between the Goldstone bosons and the Higgs field [47, 48]

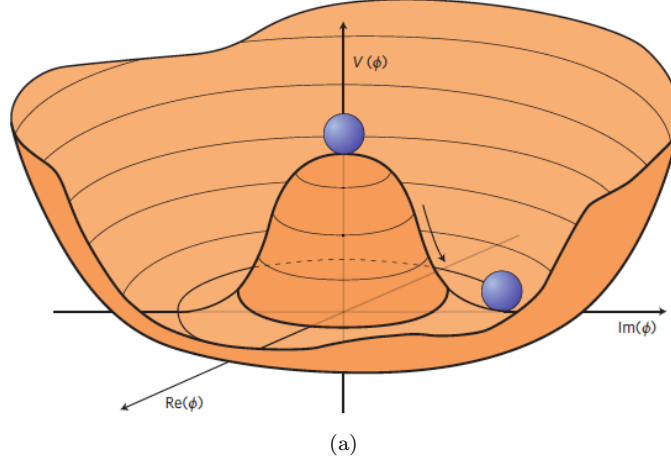


Figure 2.2: A figure showing the potential energy of the Higgs field in two dimensions [49].

Mass terms in the Lagrangian can arise through spontaneous symmetry breaking if one were to add Yukawa interactions between the Higgs field and the fermions. Such an interaction can be written as

$$\mathcal{L}_{\text{Yukawa}} = y (\bar{\psi}_L \phi \psi_R + \bar{\psi}_R \bar{\phi} \psi_L) \quad (2.16)$$

After spontaneous symmetry breaking, such Yukawa interactions yield mass terms similar to $\frac{1}{\sqrt{2}} y v (\bar{\psi}_L \psi_R + \bar{\psi}_R \psi_L)$. With this formalism, the kinetic terms of fermions result in the mixing of mass eigenstates of left-handed quarks with other left-handed quarks and the mixing of lepton neutrinos with other lepton neutrinos. In the quark sector, mixing is governed by the Cabibbo–Kobayashi–Maskawa (CKM) matrix. For neutrinos, the Pontecorvo–Maki–Nakagawa–Sakata (PMNS) matrix is used to parametrize the mixing. Equation 2.17 shows the various terms of the CKM matrix, their best known values, and their associated uncertainty [50].

$$V_{\text{CKM}} = \begin{pmatrix} |V_{ud}| & |V_{us}| & |V_{ub}| \\ |V_{cd}| & |V_{cs}| & |V_{cb}| \\ |V_{td}| & |V_{ts}| & |V_{tb}| \end{pmatrix} = \begin{pmatrix} 0.97373 \pm 0.00031 & 0.2243 \pm 0.0008 & 0.00382 \pm 0.00020 \\ 0.221 \pm 0.004 & 0.975 \pm 0.006 & 0.0408 \pm 0.0014 \\ 0.0086 \pm 0.0002 & 0.0415 \pm 0.0009 & 1.014 \pm 0.029 \end{pmatrix} \quad (2.17)$$

2.2 Top-quark Phenomenology

The top quark is an up-type quark with a charge of $+2/3$ and is the heaviest of all known fermions, with a mass of $172.69 \pm 0.30 \text{ GeV}$ [50]. Such a large mass means that the top quark has the largest coupling to the Higgs field. Furthermore, the top quark has a width of $1.42^{+0.19}_{-0.15} \text{ GeV}$ [50] which means that it decays before it has a chance to form a meson or baryon bound state. Thus, the top quark is effectively the only quark one can study in its free state. The top quark will decay almost always into a W boson and a b -quark due to the large value of the V_{tb} term in the CKM matrix. Due to this property, one can identify top quark decays by searching for evidence of a W boson and

a b -quark through their decay products. Due to these properties, top quark measurements provide unique probes of the SM and the theory of QCD.

The dominant form of top-quark production in hadron colliders is pair production through quark-antiquark annihilation ($q\bar{q} \rightarrow t\bar{t}$) and gluon-gluon fusion ($gg \rightarrow t\bar{t}$), as seen in Figure 2.4. Small contributions also arise from quark-gluon interactions. At lower centre-of-mass energies, quark-antiquark annihilation dominates the production whereas gluon-gluon fusion dominates at higher energies. Figure 2.3 shows the “next-to-leading-order” (NLO) $t\bar{t}$ pair-production cross-sections, in pp collisions, as a function of $\sqrt{s}$. At $\sqrt{s} = 5.02$ TeV, $q\bar{q} \rightarrow t\bar{t}$ ($gg \rightarrow t\bar{t}$) is $\sim 22\%$ ($\sim 78\%$) of the total cross-section but drops (rises) to $\sim 10\%$ ($\sim 90\%$) at $\sqrt{s} = 13$ TeV.

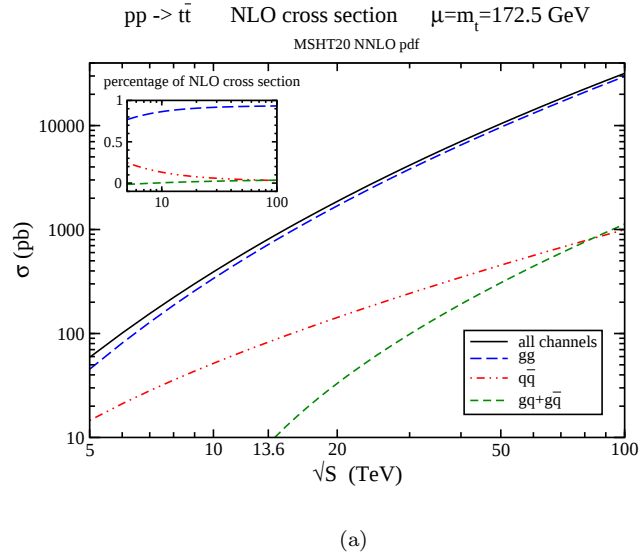


Figure 2.3: The NLO $t\bar{t}$ pair-production cross-sections, in pp collisions, as a function of $\sqrt{s}$. The total (solid black line), $q\bar{q} \rightarrow t\bar{t}$ (dashed blue line), $gg \rightarrow t\bar{t}$ (dashed red line), and $gg \rightarrow t\bar{t}$ (dashed green line) cross-sections are shown. The percentage of the NLO cross-section for each channel is plotted on the sub-figure at the top left. A special thanks to Nikolaos Kidonakis for this plot [51].

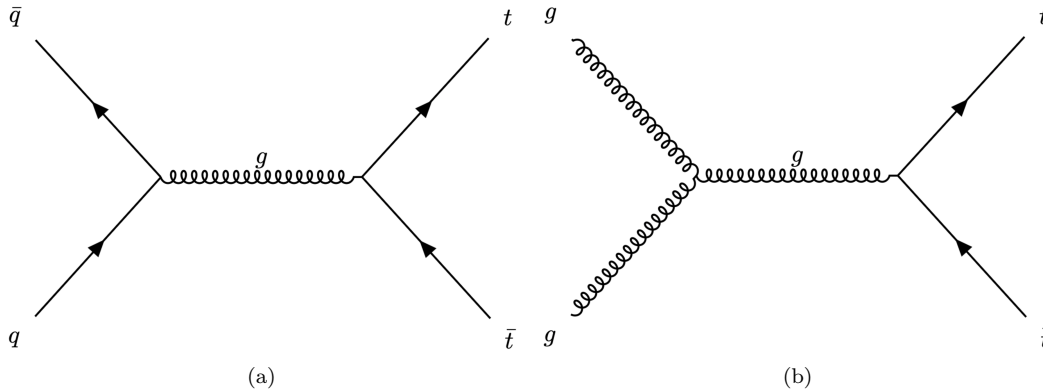


Figure 2.4: Feynman diagrams at leading-order in the strong coupling constant α_s for the dominant sources of top-quark pair production via (a) quark-antiquark annihilation and (b) gluon-gluon fusion.

Final states from top quark pairs can be categorized into three distinct categories depending on the decay topology of the two daughter W bosons - the dilepton, lepton+jets, and all-hadronic final states. The dilepton final state occurs when both W bosons decay into leptons⁵, the lepton+jets final state occurs when one W boson decays into two leptons and the other into two quarks (which eventually form hadrons), and the all-hadronic final state occurs when both W bosons decay into quarks. The dilepton final state occurs $\sim 10\%$, lepton+jets at 45% ($\sim 15\%$ for each type of lepton), and the all-hadronic $\sim 45\%$. The next largest source of top-quark production is through electroweak processes (single-top-quark production), and is then followed by more rare associated production modes such as $t\bar{t}Z$, $t\bar{t}W$, $t\bar{t}H$, and $t\bar{t}t\bar{t}$.

The $|V_{tb}|$ term of the CKM matrix can be measured by measuring the t -channel single-top-quark production cross-section ($\sigma(tq + \bar{t}q)$), thus many t -channel measurements have been performed at various centre-of-mass energies over the years. The dominant process for electroweak single-top-quark production is the t -channel exchange where a light quark from one of the colliding protons interacts with a b -quark from another proton through the exchange of a virtual W boson. Single-top-quarks or anti-top-quarks are produced depending on the weak isospin of the light quark. In pp collisions, the two-to-one ratio of up-type quarks to down-type valence quarks in a proton leads to a higher production cross-section of single-top-quarks ($\sigma(tq)$) as compared to anti-top production ($\sigma(\bar{t}q)$). The ratio of the two individual cross-sections, R_t can be measured in conjunction with the total t -channel cross-section. Two additional processes for single-top-quark production are the s -channel and tW associated production. Feynman diagrams for all three sources of single-top-quark production at leading-order in the strong (α_s) and electroweak (α_{EW}) coupling constants are shown in Figure 2.5.

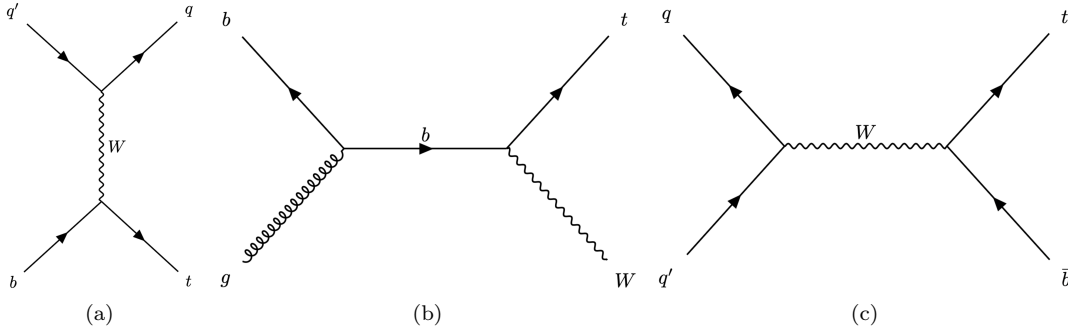


Figure 2.5: Feynman diagrams at leading-order in the strong coupling constant α_s and electroweak coupling constant for the sources of single-top-quark production via (a) t -channel, (b) tW associated, and (c) s -channel production.

2.3 Physics at Hadron Colliders

Experiments in high energy particle physics probe the behaviour of fundamental particles by colliding known initial states and then observing the final states. Given two beams with an initial state

⁵Technically this includes the τ lepton. However, since the τ leptons are more difficult to detect when compared with electrons and muons, they are not typically considered as part of the lepton+jets channel.

denoted as i , the rate of events scattered from their interaction that result a specific final state j can be expressed as

$$\frac{dN_j}{dt} = \sigma(i \rightarrow j) \cdot \mathcal{L} \quad (2.18)$$

Here, σ is the cross-section and represents the probability of state i transitioning to state j and $\mathcal{L}$ is the luminosity, a factor that encodes the flux of particles in the state i colliding with one another. The formula can be integrated to get the total number of events observed and since the cross-section is time-independent, it factors out. The integral over time of $\mathcal{L}$ is denoted as the integrated luminosity ($\mathcal{L}_{\text{int}}$). The cross-section of a process is often either measured or calculated from first-principles. The energy scale of the physics interaction is thus identified with the centre-of-mass energy ($\sqrt{s}$) in particle colliders.

At the LHC, the particle beams being collided are not continuous streams of particles. Instead, “bunches” of protons are collided with each other. Assuming beams with Gaussian transverse profiles, the instantaneous luminosity at the LHC can be expressed as

$$\mathcal{L} = \frac{N_1 N_2 f_r N_b}{4\pi\sigma_x\sigma_y} F \quad (2.19)$$

Here, N_1 and N_2 represent the number of protons in the two bunches being collided, N_b is the number of bunches in the machine, f_r is the revolution frequency, σ_x is the horizontal Gaussian width, σ_y is the vertical Gaussian width, and F is a form factor that accounts for beam crossing angle and other second-order interactions. The number of events observed by a detector which recorded a given integrated luminosity can thus be expressed as: $N_j = \sigma(i \rightarrow j) \cdot \mathcal{L}_{\text{int}} \cdot \epsilon$. Here, ϵ represents the selection efficiency of the detector to detect the final state j . Note that one can increase the number of observed events by either increasing the efficiency, or increasing the luminosity by collecting more data.

The coordinate system employed in this thesis is a right-handed one with the z -axis is parallel to the beamline, the x -axis points towards the centre of the LHC, and the y -axis points upwards. Final state particles are typically parametrized in spherical coordinates, with ϕ being the azimuthal angle around the z -axis, and θ is the longitudinal angle measured from the z -axis (i.e. $\theta = 0$ is along the z -axis). An alternative variable to represent the angle relative to the beam is the pseudorapidity (η) which is defined as $\eta = -\ln\left(\tan\left(\frac{\theta}{2}\right)\right)$ ⁶.

Multiple pp collisions are to be expected during a bunch crossing since there is more than one proton per bunch. Thus, a selection must be made to choose that “hard scatter”. The hard scatter is the pp collision in a bunch crossing that collided with the largest p_T at an energy scale larger than $\mathcal{O}(\text{GeV})$. Collisions of protons other than the hard scatter are referred to as “pileup” and can be categorized as “in-time pileup” and “out-of-time pileup”. In-time pileup is additional pp collisions from the same bunch crossing whereas out-of-time pileup arises from pp collisions of a different bunch crossing.

⁶With this transformation, a particle with $\theta = 90^\circ$ has $\eta = 0$ and a particle travelling along the positive z -axis has $\eta = \infty$.

2.4 The Hard Scatter with Hadrons

Since hadrons like protons are composite objects and not fundamental particles in the SM, a new formalism must be considered if one is to compute cross-sections from hadron collisions. The key to the formalism for a hard scatter is to realize that one can factorize the effects from perturbative QCD that arise from interactions of quarks and gluons, and the non-perturbative QCD effects that govern the internal structure of the proton. Figure 2.6 shows a cartoon of two protons colliding and leading to an interaction with a final state j . In this formalism, the cross-section for pp (or any hadron collision) can be factorized [52] as

$$\sigma(pp \rightarrow j) = \sum_{a,b} \int dx_a dx_b f_a(x_a, Q^2) f_b(x_b, Q^2) \hat{\sigma}(ab \rightarrow j, \mu_r) \quad (2.20)$$

The indices a and b represent the partons of the two proton beams (i.e. quarks and gluons), the variable x_i represents the fractional momentum carried by a parton i . f_i is the Parton Distribution Function (PDF) which specifies the probability to find a parton i with a momentum fraction (also called the Bjorken- x) x_i at the four-momentum transfer scale Q^2 (also denoted as the factorization scale, μ_f). Finally, $\hat{\sigma}(ab \rightarrow j)$ is the partonic cross-section calculated to a certain level in perturbative QCD with a renormalization scale μ_r , of partons a and b interacting to form the final state j . Effectively, this equation sums all contributions that partons can make to the cross-section with a final state j .

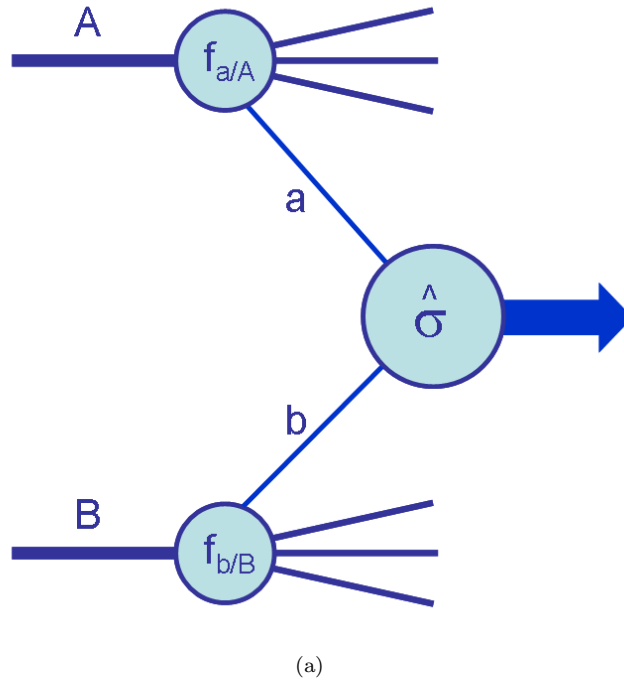


Figure 2.6: A cartoon showing how two protons collide in the parton model [52].

In the factorization formalism, the partonic cross-section and sum over partons are typically

calculated using Feynman rules and Monte Carlo (MC) numerical integration techniques. However, the PDFs cannot be determined from first-principles and are instead derived from fits to data. The data typically comes from Deep Inelastic Scattering (DIS) experiments which probe the proton structure at lower energies by colliding them with leptons although LHC data can be used to constrain PDFs as well. The fits to data are undertaken by various collaborations within the high energy physics community, such as the NNPDF Collaboration [53–56], CTEQ Collaboration [57–59], and even the ATLAS Collaboration [60]. For a given physics process at an energy scale E and rapidity y , the Bjorken- x can be parametrized [52] as

$$x \sim \frac{E}{\sqrt{s}} e^y \quad (2.21)$$

Thus, a good understanding of the high Bjorken- x region is necessary if one wants to probe BSM physics at higher energy scales. It should be noted that the high Bjorken- x region can be probed by SM measurements at lower centre-of-mass energies. Figure 2.7 shows the $Q^2 - x$ plane as probed by DIS experiments. Note that a clear gap is visible at the energy scale relevant to LHC physics. Luckily, the energy scale dependence of PDFs can be determined by solving the Dokshitzer-Gribov-Lipatov-Altarelli-Parisi (DGLAP) equations [61–63] even though the Bjorken- x dependence of PDFs is measured in-situ. Figure 2.8 shows a set of proton PDFs for $Q^2 = 10 \text{ GeV}^2$ and $Q^2 = 10\,000 \text{ GeV}^2$ [56]. At both energy scales, the sea of quarks and gluons dominate at low Bjorken- x whereas at high Bjorken- x , it is the valence quarks.

2.4.1 Parton Shower and Hadronization

Whenever free quarks and gluons are produced, the colour confinement property of QCD will lead to the radiation of quarks and/or gluons before the hard scatter or after (this is called the “parton shower” or PS). Emissions before are termed initial state radiation (ISR) and emissions after are termed final state radiation (FSR). The cross-section of a final state j emitting an additional parton can be expressed as: $\sigma_{j+1} \sim \sigma_j \cdot \frac{dE}{E} \frac{d\theta^2}{\theta^2}$. Note the singularities at low energy and angle of the emitted particle. This divergence implies that only variables which are “infrared and collinear safe” (i.e. insensitive to the presence of soft and collinear partons) can be determined using perturbative QCD.

Below the energy scale of $\sim 1 \text{ GeV}$, partons start clustering into bound states of hadrons (“hadronization”) since colour confinement is at a scale where the strong coupling constant is large and perturbative calculations are unreliable. Thus, one must use models tuned to observed data for hadronization instead of first-principle theoretical calculations that could be used for the parton shower. Dedicated programs are used to simulate the parton shower and hadronization and since a priori there is an uncertainty in the tuned parameters, one must consider modelling uncertainties in a measurement that uses parton showers. A similar method is used to model the “underlying event” interactions between the remnant protons of a hard scatter.

An additional problem arises in the “matching” of the partonic cross-section to the parton shower itself. Since higher-order corrections to the partonic cross-section include parton shower emissions, a

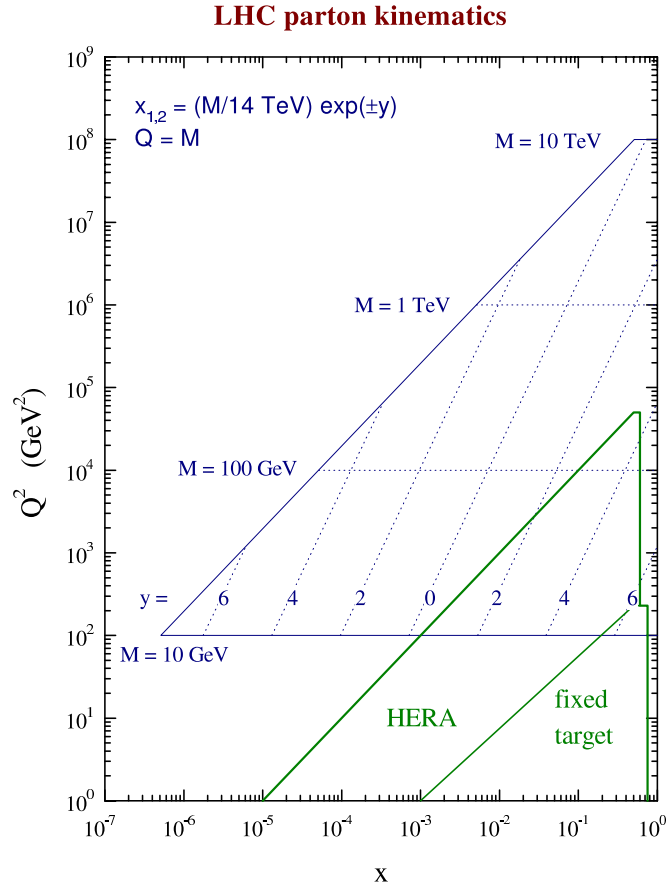


Figure 2.7: Graphical representation of the relationship between the parton variables (Bjorken- x and scale Q^2) and the kinematic variables (mass M and rapidity y) of a final state produced at the LHC assuming a $\sqrt{s} = 14$ TeV [52].

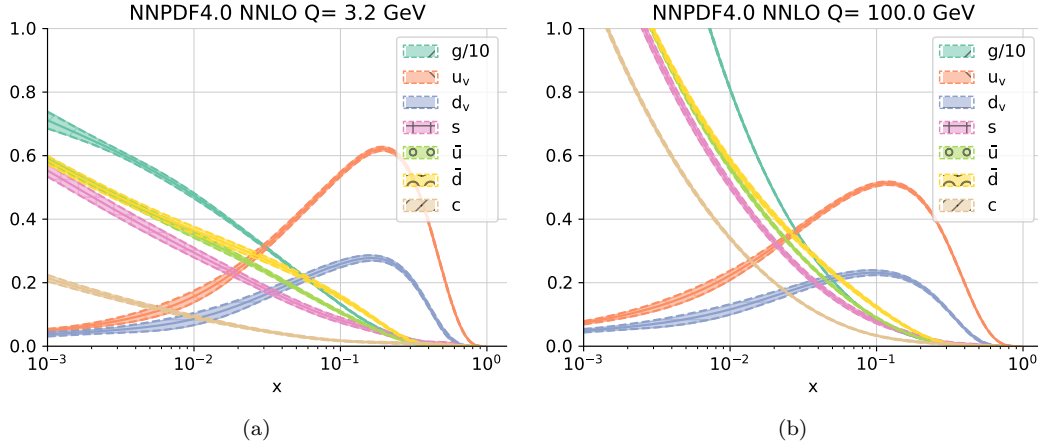


Figure 2.8: The NNPDF4.0 next-to-next-to-leading-order (NNLO) proton PDFs as determined by the NNPDF Collaboration plotted on the y-axis as a function of the Bjorken x , for (a) $Q^2 = 10 \text{ GeV}^2$ and (b) $Q^2 = 10\,000 \text{ GeV}^2$. The teal band represents the gluon PDF scaled by $\frac{1}{10}$, the orange and purple bands show the PDFs of the up and down valence quarks in a proton whereas the pink and green bands are the PDFs of the strange and anti-up quarks found in the sea of quarks. Finally, the yellow and brown bands are the PDFs of the anti-down and charm quarks found in the sea of quarks, respectively. A detailed description of the calculation of the PDFs and their uncertainties is discussed in Ref. [56].

matching algorithm must be used to prevent potential double counting. This is best illustrated in Figure 2.9 which shows a diagram of $t\bar{t}$ production at NLO. This diagram is one that would appear for a parton emission with $t\bar{t}$ production at “leading-order” (LO). An uncertainty in the matching algorithm is assessed by using different combinations of matrix element (ME) and parton shower algorithms or by changing certain parameters in the simulation of the parton shower.

2.5 Simulation of Physics Processes

The software used to simulate particle interactions relevant to this thesis are discussed below. The POWHEG BOX v2 [64–67], MADGRAPH5_AMC@NLO [68, 69] (referred hereafter as AMC@NLO) [68], and SHERPA 2.2.5 [70] NLO matrix element generators are used. The POWHEG BOX v2 generates the hardest emission at NLO before passing the event to the parton shower simulation. Conversely, AMC@NLO and SHERPA subtract contributions of terms associated with a parton shower from the NLO calculation before applying the parton shower simulation.

In conjunction with the matrix element generators, the PYTHIA 8 [71], SHERPA 2.2.5 [72], and HERWIG 7 [73, 74] programs are used to simulate the parton shower and hadronization. The PYTHIA and SHERPA programs treat hadronization by connecting the final state quarks with a string (denoted as the Lund string model) that models a linear potential and represents the colour fields. Hadronization is then assumed to occur through $q\bar{q}$ production at whenever the string “breaks” ($\mathcal{O}(1 \text{ GeV})$). HERWIG on the other hand is based on the cluster hadronization model which attempts

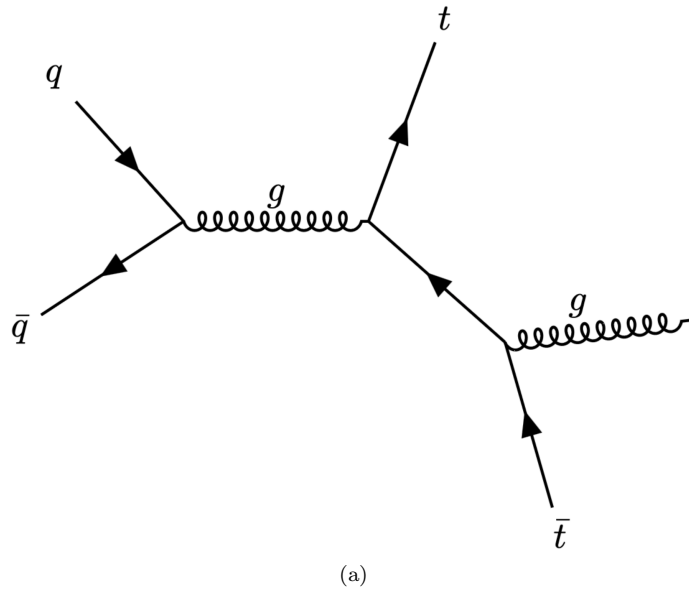


Figure 2.9: Feynman diagram that is NLO in the strong coupling constant α_s for $t\bar{t}$ pair production.

to cluster quarks into colourless mesons and baryons during hadronization. After the parton shower and hadronization, the EVTGEN program [75] is used to handle the decays of b - and c -flavoured hadrons.

All stable particles ($\tau \sim 30$ ps) then undergo a detailed detector simulation based on the GEANT4 framework [76]. This program can simulate the passage of particles through matter and the expected detector response.

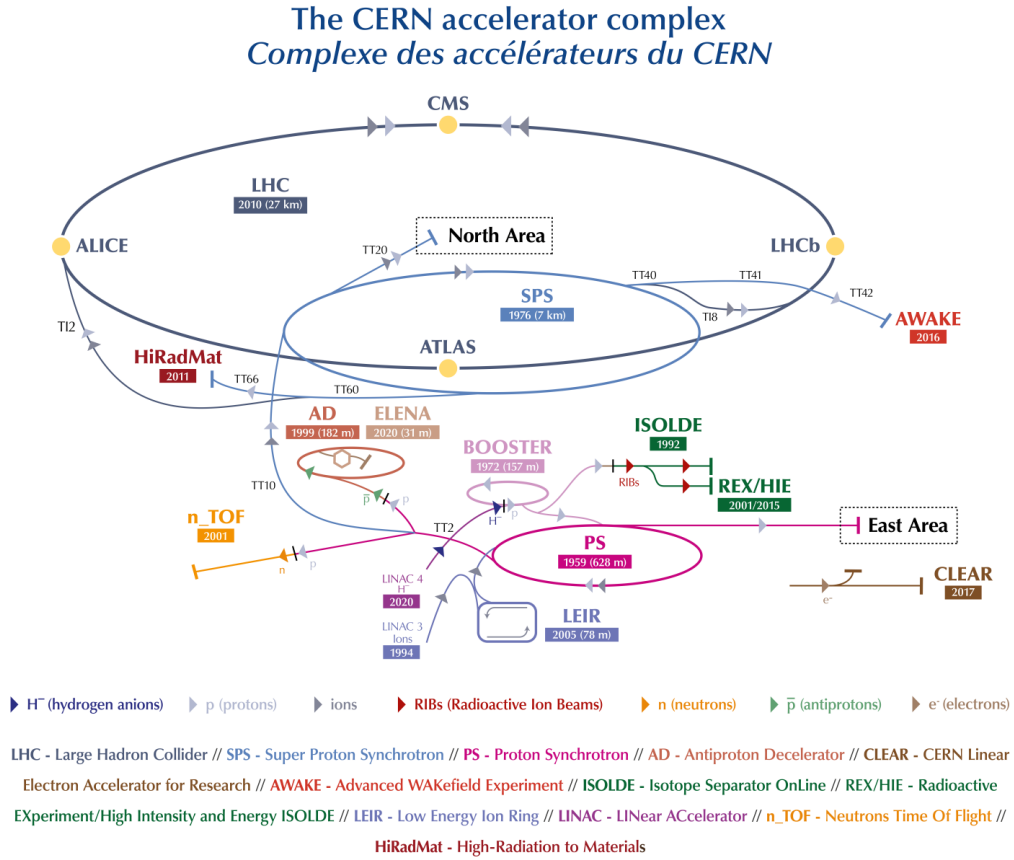
Chapter 3

The LHC and the ATLAS Detector

The LHC [77] is the largest and most energetic particle accelerator ever built. It was constructed by the Conseil Européen pour la Recherche Nucléaire (CERN), in a ~ 27 km long tunnel underneath the Franco-Swiss border near Meyrin, Switzerland. The LHC provides proton-proton and heavy ion collisions to nine different experiments: A Toroidal LHC ApparatuS (ATLAS) [78], Compact Muon Solenoid (CMS) [79], Large Hadron Collider beauty (LHCb) [80], A Large Ion Collider Experiment (ALICE) [81], TOTal Elastic and diffractive cross-section Measurement (TOTEM) [82], LHC forward (LHCf) [83], Monopole and Exotics Detector At the LHC (MoEDAL) [84], ForwArd Search ExpeRiment (FASER) [85], and the Scattering and Neutrino Detector (SND) [86]. Since this thesis presents two analyses based on data collected by the ATLAS detector during pp collisions at the LHC, Section 3.1 will present the LHC machine while Section 3.2 presents the ATLAS detector.

3.1 The Large Hadron Collider

The LHC is a synchrotron designed to achieve centre-of-mass energies of $\sqrt{s} = 14$ TeV in pp collisions. Proton beams used for the collisions are created by ionizing hydrogen gas in the duoplasmatron, extracting the electrons, and then passing on the plasma of protons to the LINAC2 linear accelerator. Protons in LINAC2 are accelerated to 50 MeV and fed to a set of three synchrotrons, the proton synchrotron booster (PS Booster), the proton synchrotron (PS), and the super proton synchrotron (SPS). The three synchrotrons accelerate the protons to 1.4 GeV, 25 GeV, and 450 GeV, respectively. The protons are then fed to the LHC in bunches spaced a minimum of 25 ns apart in two beams which are accelerated to their final centre-of-mass energies using radio-frequency cavities, while dipole superconducting magnets bend the beam. The beams are then focussed using quadrupole magnets and collided at interaction points that are surrounded by the detectors. Figure 3.1 shows a schematic of the LHC injection complex.



(a)

Figure 3.1: A schematic showing the CERN accelerator complex and how certain components feed into the LHC.

Although the LHC was designed to accelerate protons to $\sqrt{s} = 14$ TeV, the LHC has only operated at lower centre-of-mass energies due to limitations in the maximum operating current of the dipole magnets. In the first round of LHC collisions (denoted as Run 1), ATLAS recorded $\sim 5 \text{ fb}^{-1}$ at $\sqrt{s} = 7$ TeV and $\sim 21 \text{ fb}^{-1}$ at $\sqrt{s} = 8$ TeV. Run 1 ran from 2010 to 2012 and provided the data that led to the discovery of the Higgs Boson [37, 38]. Run 1 was followed by a shutdown period (LS1) for detector upgrades, accelerator repairs, and improvements. Run 2 ran between 2015 and 2018, and ATLAS recorded a total of $\sim 140 \text{ fb}^{-1}$ at $\sqrt{s} = 13$ TeV. Beyond the main pp runs in Run 2, the LHC provided additional heavy ion collisions (Pb-Pb, p -Pb, and Xe-Xe) at lower centre-of-mass energies. In anticipation of these heavy ion runs, special pp runs were taken with low-pileup conditions at $\sqrt{s} = 5.02$ TeV and $\sqrt{s} = 13$ TeV, to be used as a reference dataset. The low-pileup $\sqrt{s} = 5.02$ TeV run was taken in 2017 and ATLAS recorded 255 pb^{-1} whereas in the low-pileup $\sqrt{s} = 13$ TeV runs, 338 pb^{-1} was recorded. The LHC provided 273 pb^{-1} worth of $\sqrt{s} = 5.02$ TeV data in 2017 and ATLAS recorded 270 pb^{-1} . Out of the recorded dataset, 95.2% is considered good for physics after applying data quality requirements [87]. The $\sqrt{s} = 5.02$ TeV physics runs were taken between the 12th and 20th of November, with various bunch settings that gave a peak instantaneous luminosity between $0.5 \text{ nb}^{-1} \text{ s}^{-1}$ and $1.3 \text{ nb}^{-1} \text{ s}^{-1}$. The pileup was constrained to a $\langle\mu\rangle$ between 0.5 and 4, which is an order of magnitude smaller than the average pileup used for most of the 13 TeV pp run [87, 88]. Run 2 was followed by a long shutdown period (LS2) where additional upgrades to the detectors were carried out. Collisions were restarted with Run 3 in 2022, at a $\sqrt{s} = 13.6$ TeV. Run 3 is expected to continue until 2025 and provide $\sim 150 \text{ fb}^{-1}$ worth of data to the ATLAS detector.

3.2 The ATLAS Detector

The ATLAS detector is one of two general-purpose detectors (the other being CMS) at the LHC designed to study the SM and search for BSM effects. It was designed and is operated by the ATLAS Collaboration, which is one of the largest international scientific collaborations, with over 3000 scientists from a total of 5700 individual members, from 182 institutions in 42 countries. The ATLAS detector is cylindrically symmetric around the LHC beam pipe and almost hermetically covers the 4π solid angle. Due to the beam pipe, it is impossible to fully cover the entire interaction point, hence the slight lack of coverage. The detector is approximately 44 m long, has a diameter of 25 m, and weighs 7000 tons.

Figure 3.2 shows the various concentric subdetectors and components that comprise the ATLAS detector [78]. Starting from the beamline and moving radially outward, a particle will first encounter a set of three detectors that reconstruct particle tracks and are collectively called the Inner Detector (ID). To measure particle momenta and achieve charge identification, the ID is immersed in a 2 T axial magnetic field from a solenoid. After passing through the solenoid field, the particle encounters the Liquid Argon (LAr) and Tile calorimeters which are used to measure the particle energy. Beyond the calorimeters, a particle will encounter the Muon Spectrometer (MS) which is surrounded by a magnetic field, up to 3.5 T, from an air-core toroid that helps measure the momenta of muons. Sections 3.2.1, 3.2.2, and 3.2.3 provide additional details on the ID, calorimeters, and the MS,

respectively. Section 3.2.4 summarizes the set of forward detectors that allow for beam conditions and luminosity measurements whereas Section 3.2.5 discusses the trigger and data acquisition system that selects and saves interesting physics events.

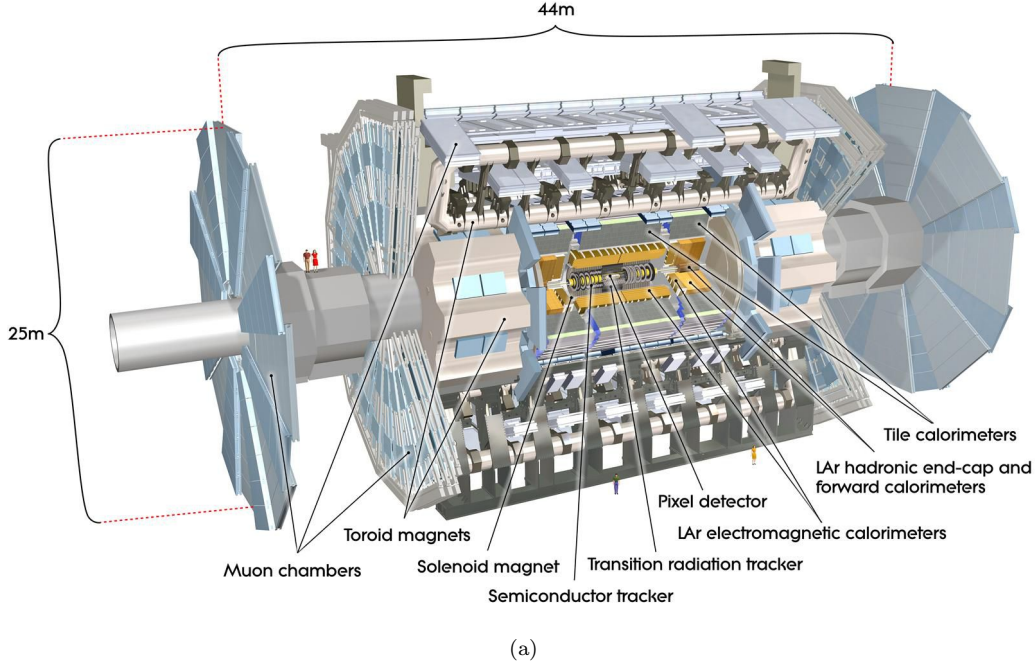


Figure 3.2: A schematic diagram showing the various components of the ATLAS detector.

3.2.1 Inner Detector

The three ID subdetectors are contained within a cylinder of length 3.512 m and radius 1.150 m, and can provide full coverage in ϕ , up to a $|\eta| < 2.5$. Tracks with $p_T > 0.4$ GeV are measured (although tracks with $p_T > 0.1$ GeV can also be measured), in the ID through the complementary reconstruction of “hits” in the pixel detector, the silicon microstrip detector (SCT), and Transition Radiation Tracker (TRT). Figure 3.3 shows two views of the ID and its various subdetectors. Overall, the ID is design to have a momentum resolution of $\frac{\sigma(p_T)}{p_T} = 0.05\% \cdot p_T \oplus 1\%$.

Pixel Detector

The pixel detector consists of individual silicon pixels, 90% of them with a size of $50 \times 400 \mu\text{m}^2$ in the $R - \phi \times z$ plane¹ and a thickness of $250 \mu\text{m}$. Each pixel is a reverse-biased p-n junction bonded to a readout channel, that in the presence of a charged particle will create multiple electron-hole pairs

¹Slightly larger pixels of $50 \times 600 \mu\text{m}^2$, $\sim 10\%$ of all pixels, can be found in the regions at the front-end chips on a module.

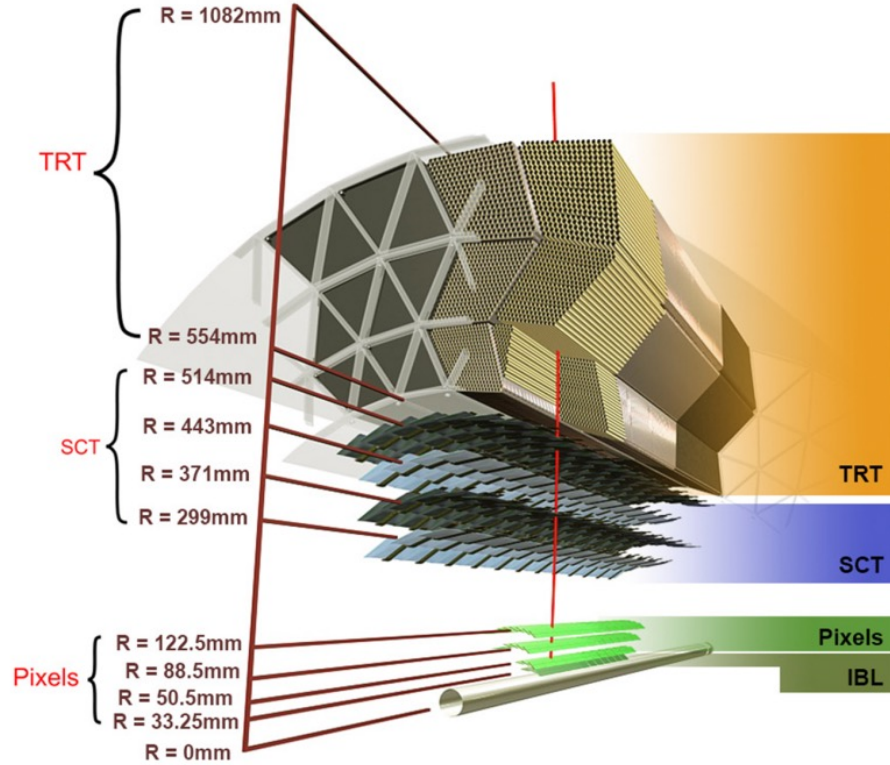
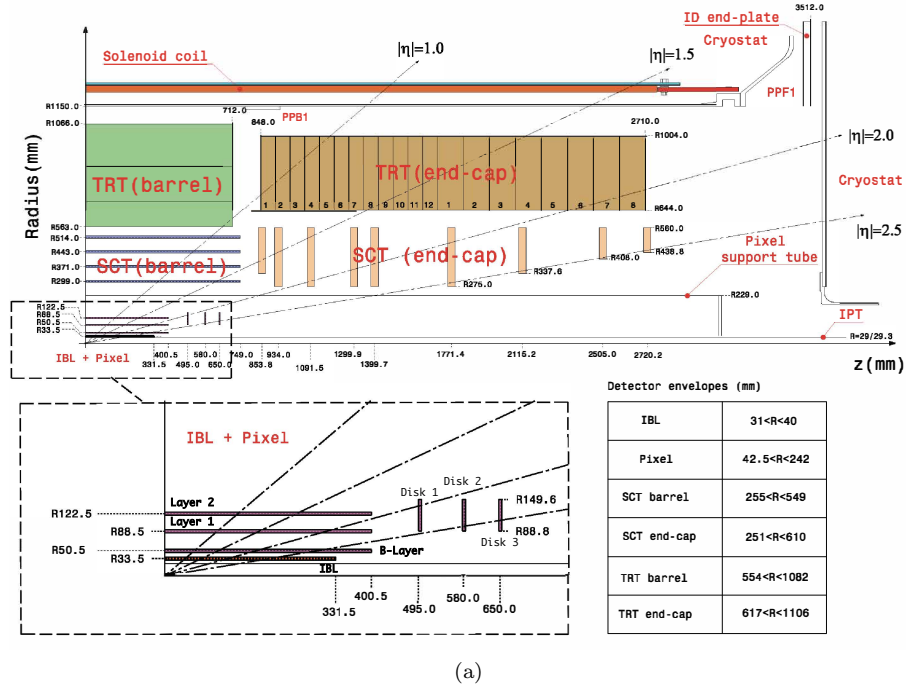


Figure 3.3: (a) schematics of the ID along the $R - z$ plane and (b) a 3D computer generated image of the ID, as seen at an angle. In (a), the dashed lines represent lines of constant pseudorapidity. In (b), $R = 0\text{mm}$ is the beam line and the red line represents the trajectory of a particle arising from a collision in the beamline.

which produce an electrical signal by travelling to their respective electrodes. The electric signal can be read through more than 80 million channels and constitutes a hit in the pixel detector if it is above a certain threshold. The pixel detector consists of three layers arranged in concentric cylindrical rings in the barrel and radial disks in the endcap. The layers have an intrinsic resolution of $10\mu\text{m}$ in the $R - \phi$ plane and $115\mu\text{m}$ along the z -axis for the barrel and $115\mu\text{m}$ in R for the endcap. An additional “Insertable B Layer” (IBL) was added to the pixel detector in LS1 in order to improve and in some cases, maintain the tracking resolution at higher instantaneous luminosity seen in Run 2 [89]. The IBL provides coverage up to $|\eta| < 3.0$ and is based on pixels of size $50 \times 250\mu\text{m}^2$ in the $R - \phi \times z$ plane. The IBL has ~ 12 million readout channels and achieves an intrinsic resolution of $10\mu\text{m}$ in the $R - \phi$ plane and $66.5\mu\text{m}$ along the z -axis [90]. Its inclusion in ATLAS provides increased tracking efficiencies, primary vertex reconstruction efficiencies, and a $\mathcal{O}(10\%)$ increase in the efficiency to identify b -hadron associated jets, for a given rejection factor for light and c -hadron associated jets (b -jet identification and its concepts are further discussed in Chapter 5). The IBL (pixel) detector averages approximately one (four) hits per track in both data and MC [91].

SCT Detector

The SCT detector follows the same principle and a similar geometry to the pixel and IBL detectors but consists of eight (nine) layers of silicon strips in the barrel (endcap) region. This detector uses small angle (40mrad) stereo strips that have an average pitch of $\sim 80\mu\text{m}$. This allows for a measurement of both the $R - \phi$ and z -coordinates. The geometry of the SCT detector provides an intrinsic resolution of $17\mu\text{m}$ in the $R - \phi$ plane and $580\mu\text{m}$ along the z -axis in the barrel, and on R for the endcaps. Typically, the SCT records between four and twelve hits for a track through its ~ 6.3 million readout channels.

TRT Detector

The TRT detector is a gaseous detector that consists of 144 cm (37 cm) long “straw tubes” made of Kapton in the barrel (endcap) regions. The tubes have a diameter of 4 mm , and contain a $31\mu\text{m}$ tungsten wire plated in gold, and a gas mixture². The wire, an anode, is held at a potential difference of 1.5 kV with respect to the straw shell, a cathode. Both the wire and shell can be used to collect ions from the gas mixture, after a particle has ionized it by travelling through it. The electrical signal measured can then be used to define a hit in the TRT. 73 (160) layers of straw tubes are placed parallel to the beamline for a total of 52544 (122880) straws in the barrel (endcap), that are readout using ~ 350000 readout channels.

The TRT has an intrinsic resolution of $130\mu\text{m}$ per straw. However, due to its geometry it can only provide measurements in the $R - \phi$ plane and only to a $|\eta| < 2.0$. Although the resolution is

²The original gas mixture was a 70% Xe, 27% CO_2 , and 3% O_2 mixture. However, due to leaks, the mixture was changed in Run 2 to a less expensive 70% Ar and 30% CO_2 mixture.

worse for the TRT than the pixel or SCT detectors, the TRT typically provides 36 hits per track and can also be used for particle identification.

The space between the straw tubes is filled with “radiator material” comprised of polypropylene which has a different dielectric constant than its surroundings. When a highly boosted particle with $\gamma \gtrsim 1000$ passes through such inhomogeneous materials, it releases transition radiation [92]. Since the electron and pion mass differs by two orders of magnitude, there is a region of p_T ($p_T \lesssim m_\pi \cdot 1000$) where the presence of transition radiation would indicate the presence of an electron. Transition radiation photons produced in the TRT can be detected through the ionization of the gas in the straw tubes. The gas is chosen to have a high efficiency of absorbing transition radiation. Low p_T particles can also be isolated by studying the time of the signals seen in the straw in conjunction with the transition radiation [93].

3.2.2 Calorimetry in ATLAS

Two distinct types of calorimeters are used in ATLAS. The first is a LAr calorimeter system for both electromagnetic (EM) and hadronic calorimetry. LAr performs EM calorimetry the barrel ($|\eta| < 1.5$), endcap ($1.375 < |\eta| < 3.2$), and forward ($3.2 < |\eta| < 4.9$) regions and hadronic calorimetry in the $1.5 < |\eta| < 3.2$ and forward region. The second calorimeter used in ATLAS is a Tile hadronic calorimeter in the central region ($|\eta| < 1.7$). Both calorimeters are sampling calorimeters with different passive and active materials. Particles from the collision interact with the passive material and create a cascade of energetic particles that result in what is known as a shower. This cascade of particles is then detected by their interaction with the active material. Table 3.1 summarizes the various layers and geometric regions of the LAr and Tile calorimeters. The relative calorimeter energy resolutions can be expressed as $\frac{\sigma(E)}{E} = \frac{a}{\sqrt{E}} \oplus \frac{b}{E} \oplus c$, where a is a stochastic term, b is a term representing electronics and pileup noise, and c is a constant term. The relative energy resolution can be measured in both test beams and collision data.

LAr Calorimeter

The LAr calorimeter is an EM calorimeter in the barrel (EMB) whereas in the endcap (EMEC and HEC) and forward (FCAL) regions not covered by the Tile hadronic calorimeter, it is both a EM and hadronic calorimeter. The LAr EM calorimeter is designed with an accordion geometry to ensure full coverage in ϕ and a fast extraction of the signal in the EMB and EMEC, as seen by the schematic shown in Figure 3.4. Different passive materials are used in the various geometric regions but liquid Argon is the active material across the entire LAr detector. Lead is used as the passive material in the EMB and EMEC segments whereas the HEC uses copper, and the FCAL uses a combination of copper and tungsten. The shower generated by particle interaction with the passive material ionizes the liquid Argon, and the signal is readout using electrodes that are kept under a potential difference.

Table 3.1: Table showing the various geometric sections of the LAr and Tile calorimeters. The EM calorimeter components in the barrel (endcap) are denoted as EMB (EMEC) and the LAr hadronic calorimeter in the endcap is denoted as the HEC. The LAr forward calorimeter is denoted as the FCAL.

		Barrel	End-cap	
EM calorimeter				
Number of layers and $ \eta $ coverage				
Presampler	1	$ \eta < 1.52$	1	$1.5 < \eta < 1.8$
Calorimeter	3	$ \eta < 1.35$	2	$1.375 < \eta < 1.5$
	2	$1.35 < \eta < 1.475$	3	$1.5 < \eta < 2.5$
			2	$2.5 < \eta < 3.2$
Granularity $\Delta\eta \times \Delta\phi$ versus $ \eta $				
Presampler	0.025×0.1	$ \eta < 1.52$	0.025×0.1	$1.5 < \eta < 1.8$
Calorimeter 1st layer	$0.025/8 \times 0.1$	$ \eta < 1.40$	0.050×0.1	$1.375 < \eta < 1.425$
	0.025×0.025	$1.40 < \eta < 1.475$	0.025×0.1	$1.425 < \eta < 1.5$
			$0.025/8 \times 0.1$	$1.5 < \eta < 1.8$
			$0.025/6 \times 0.1$	$1.8 < \eta < 2.0$
			$0.025/4 \times 0.1$	$2.0 < \eta < 2.4$
			0.025×0.1	$2.4 < \eta < 2.5$
			0.1×0.1	$2.5 < \eta < 3.2$
Calorimeter 2nd layer	0.025×0.025	$ \eta < 1.40$	0.050×0.025	$1.375 < \eta < 1.425$
	0.075×0.025	$1.40 < \eta < 1.475$	0.025×0.025	$1.425 < \eta < 2.5$
			0.1×0.1	$2.5 < \eta < 3.2$
Calorimeter 3rd layer	0.050×0.025	$ \eta < 1.35$	0.050×0.025	$1.5 < \eta < 2.5$
Number of readout channels				
Presampler	7808		1536 (both sides)	
Calorimeter	101760		62208 (both sides)	
LAr hadronic end-cap				
$ \eta $ coverage			$1.5 < \eta < 3.2$	
Number of layers			4	
Granularity $\Delta\eta \times \Delta\phi$			0.1×0.1	$1.5 < \eta < 2.5$
			0.2×0.2	$2.5 < \eta < 3.2$
Readout channels			5632 (both sides)	
LAr forward calorimeter				
$ \eta $ coverage			$3.1 < \eta < 4.9$	
Number of layers			3	
Granularity $\Delta x \times \Delta y$ (cm)			FCal1: 3.0×2.6	$3.15 < \eta < 4.30$
			FCal1: $\sim$ four times finer	$3.10 < \eta < 3.15,$ $4.30 < \eta < 4.83$
			FCal2: 3.3×4.2	$3.24 < \eta < 4.50$
			FCal2: $\sim$ four times finer	$3.20 < \eta < 3.24,$ $4.50 < \eta < 4.81$
			FCal3: 5.4×4.7	$3.32 < \eta < 4.60$
			FCal3: $\sim$ four times finer	$3.29 < \eta < 3.32,$ $4.60 < \eta < 4.75$
Readout channels			3524 (both sides)	
Scintillator tile calorimeter				
	Barrel		Extended barrel	
$ \eta $ coverage	$ \eta < 1.0$		$0.8 < \eta < 1.7$	
Number of layers	3		3	
Granularity $\Delta\eta \times \Delta\phi$	0.1×0.1		0.1×0.1	
	Last layer 0.2×0.1		0.2×0.1	
Readout channels	5760		4092 (both sides)	

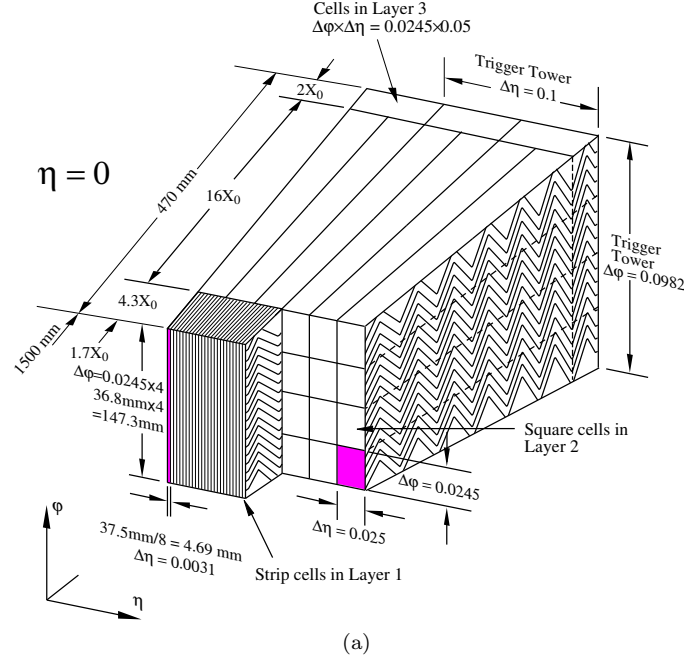


Figure 3.4: A barrel module of the LAr calorimeter where the cells in different layers and their granularity is shown. A trigger tower is the object used to make trigger decisions in Run 2 from the calorimeter and is a set of calorimeter cells that are summed together.

At the LHC energies, interactions in the EM calorimeter are dominated by bremsstrahlung and electron-positron pair production, both of which cause interactions characterized by the radiation length X_0 . After traversing one radiation length, an electron is expected to retain only $\frac{1}{e}$ of its original energy. Thus, EM calorimeters must be designed to have a large radiation length so that they may fully contain an EM shower. The analogue for hadronic showers is the nuclear interaction length (λ), which is the mean distance travelled by a hadronic particle before undergoing a nuclear interaction. Figure 3.5 shows the radiation length of the EM calorimeter layers and the interaction length for the entire detector before the MS, as a function of $|\eta|$. Note the EM “crack region” with low X_0 between $1.37 < |\eta| < 1.52$ due to the transition between the barrel and endcap cryostats that enclose the calorimeter. With respect to the rest of the detector, this region typically has a worse performance for identifying electrons.

The relative energy resolution was measured for the various components of the LAr calorimeter using electron test beams and determined to be: $\frac{\sigma(E)}{E} = \frac{10.1\%}{\sqrt{E[\text{GeV}]}} \oplus 0.17\%$ for the EMB and EMEC, $\frac{\sigma(E)}{E} = \frac{21\%}{\sqrt{E[\text{GeV}]}} \oplus 0\%$ for the HEC, and $\frac{\sigma(E)}{E} = \frac{29\%}{\sqrt{E[\text{GeV}]}} \oplus 3.1\%$ for the FCAL. A separate energy resolution was also determined using pion beams for the HEC, $\frac{\sigma(E)}{E} = \frac{71\%}{\sqrt{E[\text{GeV}]}} \oplus 5.8\%$, and the FCAL, $\frac{\sigma(E)}{E} = \frac{94\%}{\sqrt{E[\text{GeV}]}} \oplus 7.5\%$. The noise term was measured to be 1.6%, in a separate test beam with both the LAr and Tile calorimeters [78].

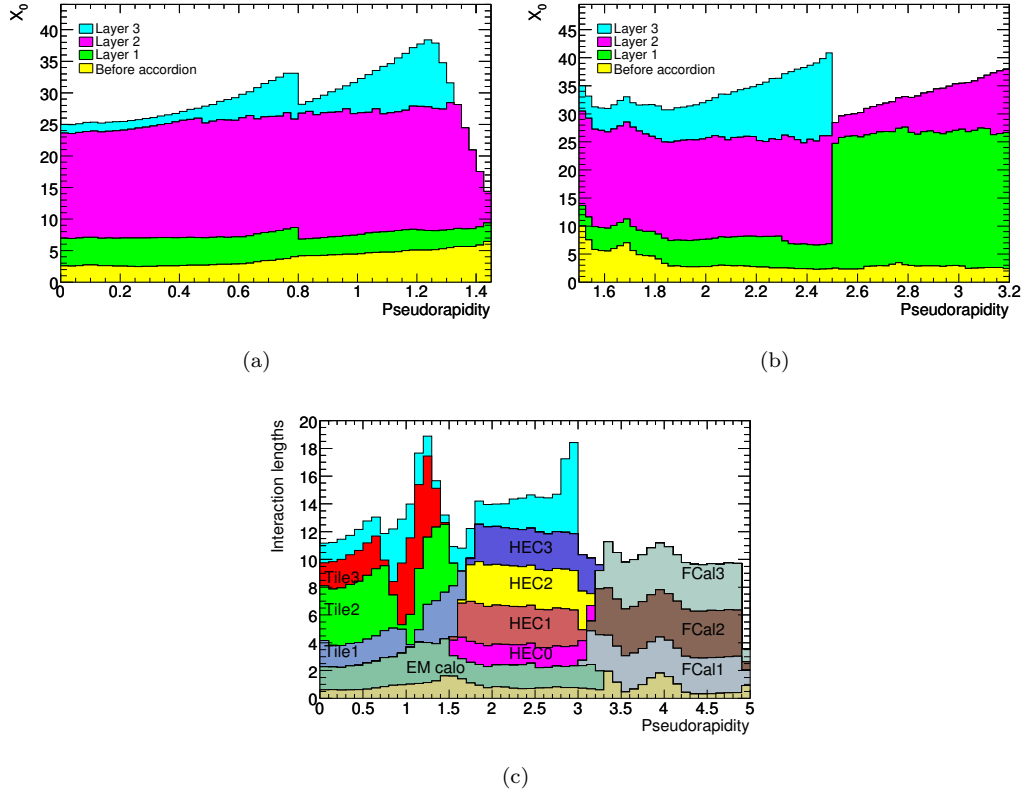


Figure 3.5: The radiation length in the EM (a) barrel and (b) endcap calorimeters, as well as the (c) interaction length for the entire detector. All plots are shown as functions of $|\eta|$. The different labelled colours in the three figures represent different layers of the LAr and Tile (only for (c)) calorimeters. In (c), the unlabelled tan represents the material before the calorimeters whereas the unlabelled cyan band represents material after the calorimeter layers but before the MS.

Tile Calorimeter

The Tile calorimeter uses steel as the passive material and polystyrene scintillator tiles as the active material. Charged particles cause the tiles to scintillate, releasing ultraviolet photons which are converted to visible light by wavelength-shifting fluors, and then readout by photomultiplier tubes (PMTs). Figure 3.6 shows a schematic of a Tile calorimeter module. The relative energy resolution of the Tile calorimeter was measured using pions from test beams, and determined to be $\frac{\sigma(E)}{E} = 56\%/\sqrt{E[\text{GeV}]} \oplus 5.5\%$ [78].

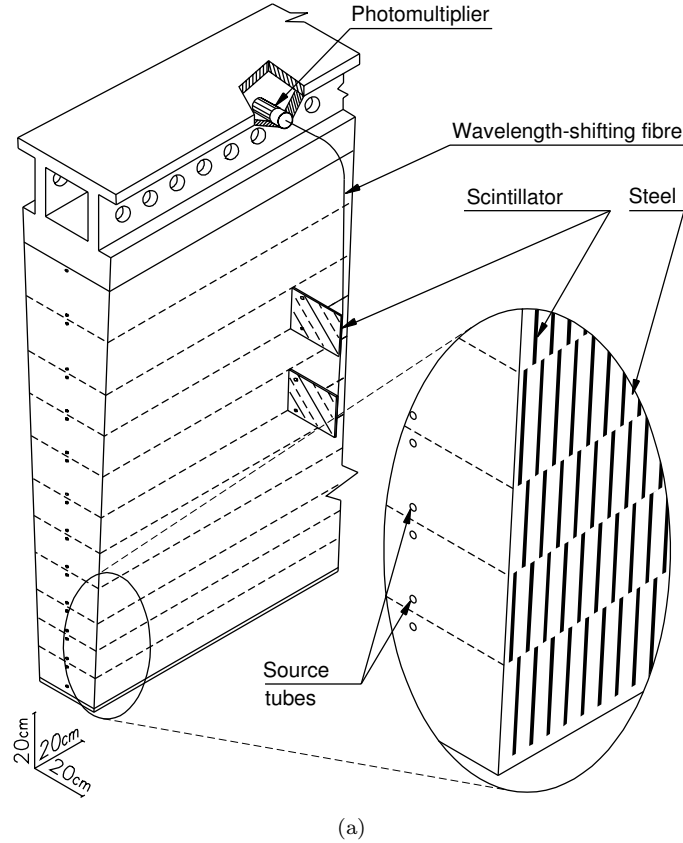


Figure 3.6: Schematic showing a Tile calorimeter module.

3.2.3 Muon Spectrometer

The MS consists of four subsystems immersed in the toroid's magnetic field: the Monitored Drift Tubes (MDT), Cathode Strip Chambers (CSC), Resistive Plate Chambers (RPC), and the Thin Gap Chambers (TGC). Muon tracks with $|\eta| < 2.7$ are observed as hits in each of the subdetectors and can thus be reconstructed whereas tracks with $|\eta| < 2.4$ can be used as inputs to the trigger system. A small gap (MS crack region) near $|\eta| = 0$ exists to allow for services to the solenoid magnet, the calorimeters, and the ID. Figure 3.7 shows schematics of the muon detectors in the $r - \phi$ and $r - z$ planes. The relative muon momentum resolution is designed to be $\sim 8\%$ ($\sim 2\%$) for a muon with a

p_T of 1 TeV (100 GeV) [94].

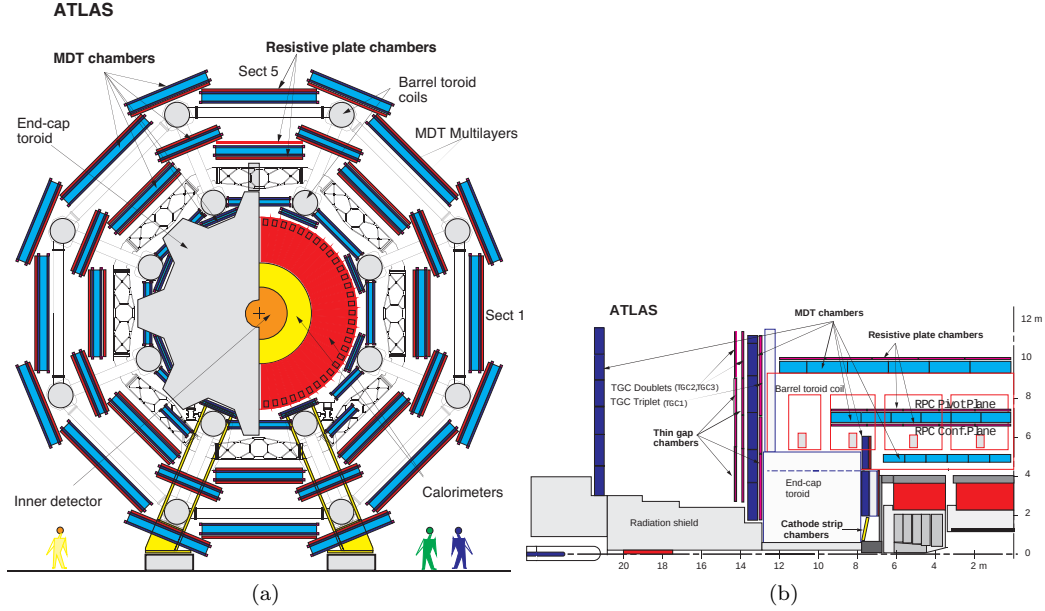


Figure 3.7: Schematics of the MS, as seen in the (a) $R - \phi$ and (b) $R - z$ planes. (b) only shows one half of the detector along the negative z -axis, with the origin defined in the bottom right corner. The inner, middle and outer chamber layers are denoted as BI, BM, BO in the barrel and EI, EM, EO in the endcap, respectively [95].

Monitored Drift Tubes

The MDT detector follows the same principles as the TRT detector but is constructed using 30 mm long tubes made of aluminum, and with an inner cable made of a gold-plated tungsten-rhenium alloy that is kept at a potential difference of 3080 V. The gas mixture used is 93% Ar and 7% CO₂. Three to eight layers of drift tubes are stacked together, pointing along ϕ , to create MDT chambers. The chambers are further stacked on top of each other, to form three layers around the ATLAS detector. The MDT is made of 1150 chambers and covers $|\eta| < 2.7$. This corresponds to 354000 individual drift tubes, each with their own measurement channel. Each tube is designed to have a spatial resolution along the z -axis, of 80 μm , which corresponds to a resolution of 35 μm for an MDT chamber. Muons are expected to leave approximately 20 hits in the MDT detector. Although the MDT has a high number of hits per track, it cannot be used for triggering due to a large drift time which gives a timing resolution of 700 ns.

Cathode Strip Chambers

The CSCs are approximately 7 m from the interaction point and are multi-wire drift chambers that fall between $2.0 \leq |\eta| \leq 2.7$, and replace first layer for the MDTs in this region. This is due to

their ability to endure a larger particle flux and better time resolution. Copper strips, acting as a cathode, are oriented radially and a gold-plated Tungsten wire, the anode, is placed in an intersecting chequerboard fashion with respect to the cathode strip. The anode wires are spaced 2.5 mm apart from each other and the cathode strip. The anode and cathode are held at a potential difference of 1.9 kV and immersed in a gas mixture of Ar (80%) and CO₂ (20%). The CSC detector is constructed with 32 chambers that correspond to 30700 channels, with each chamber providing a resolution of 40 μ m along the z -axis and 5 mm in the $R - \phi$ plane. Muons are expected to leave four measurements per track in the CSC. Although the CSC have a drift time resolution of 7 ns, they are not used as inputs for triggering.

Resistive Plate Chambers

The RPCs are parallel resistive plates constructed from a phenolic-melaminic plastic laminate, that are kept 2 mm away from each other. A gas mixture³ is placed in between the plates and an electric field of 4.9 kV m⁻¹ is applied. When a particle traverses through the plates, particles created from the ionization of the gas will move towards the anode, and will be recorded as a signal. RPCs are used to measure muon momenta and trigger for muons in the barrel region of $|\eta| < 1.05$. They consist of three concentric cylindrical layers around the beam axis. The RPC detector is constructed with 606 chambers which correspond to 373000 channels. Each RPC chamber has a drift time resolution of 1.5 ns which allows it to be used for triggering but has a resolution of 10 mm along both the z -axis and $R - \phi$ plane. Muons are expected to leave six hits per track in the RPC.

Thin Gap Chambers

The TGC are multi-wire proportional chambers which use a gas mixture of 55% CO₂ and 45% n-pentane. To allow for spatial separation of signal, the anode wires in the TGC are held 1.4 mm from the graphite cathode and 1.8 mm from other wires. A potential difference of 2.9 kV between the anode and cathode leads to a timing resolution of 4 ns. The TGC is organized into two concentric rings covering $1.05 < |\eta| < 1.92$ and $1.92 < |\eta| < 2.4$. A total of 3588 chambers corresponding to 318000 channels are used to achieve a resolution of 2-6 mm along R and 3-7 mm in ϕ . Muons are expected to leave nine hits per track in the TGC.

3.2.4 Forward Detectors

Four additional detectors are located in the forward region (high values of $|z|$) in order to measure the luminosity and provide a physics program for diffractive collisions. The luminosity in Run 2 was measured using the LUMinosity measurement using Cerenkov Integrating Detector (LUCID) [78, 96] with some information from the Beam Conditions Monitor (BCM) [97]. Other forward detectors

³The mixture comprises 92.7% C₂H₂F₄, 5% isobutane, and 0.3% SF₄.

include the Absolute Luminosity For ATLAS (ALFA) detector [98] which allows one to provide a luminosity calibration by measuring the total elastic pp cross-section through the optical theorem [99], the Zero Degree Calorimeter (ZDC) [78] which measured forward neutrons in heavy ion collisions, and the ATLAS Forward Proton (AFP) detector [100] which was used to study elastic pp collisions⁴. For the analyses presented in this thesis, only the LUCID and BCM detectors were involved in the luminosity calibrations so only these two detectors will be described below.

LUCID Detector

The LUCID detector is located ± 17 m from the ATLAS interaction point and can detect inelastic pp scattering in the forward region. With this, LUCID can measure the integrated luminosity and provide measures of the beam conditions and the instantaneous luminosity. The detector is made up of twenty 1.5 m long aluminum tubes with a diameter of 1.5 mm, that have PMTs at one end. The aluminum tubes are placed in a container filled with C_4F_{10} , and the container is placed 10 cm above the beamline ($|\eta| \approx 5.8$). When a particle transits through the gas, it will release Cerenkov radiation that is detected by the PMTs. The number of hits measured in LUCID in combination with a track counting algorithm and calorimeter inputs can be used to determine the luminosity [88, 101].

BCM Detector

The BCM detector is placed approximately ± 180 cm away from the interaction point, along the z -axis, and ~ 20 mm above the beam pipe ($|\eta| \approx 4.2$). The BCM is designed to detect abnormal beam conditions in order to prevent any damage to the detector. Since it counts the rate of particle interactions, data from the BCM can also be used to supplement luminosity measurements [88, 101]. The BCM detector does this by following the same principles as the silicon based Pixel detector but uses four 500 μ m thick 8×8 mm² diamond sensors, with a potential difference of 1 kV.

3.2.5 Trigger and Data Acquisition

The ATLAS trigger and data acquisition system is used to select only the interesting collisions out of all the pp collisions seen by ATLAS. This is a necessity since there is neither enough bandwidth, storage space, nor processing power to transfer, save, and analyze all information seen with the 40 MHz rate of LHC collisions. Thus, a two stage trigger is used to reduce the collision rate to a manageable 1 kHz. The first tier is a hardware based “Level-1” trigger that uses partial information from the calorimeters and muon detectors to select for electrons, photons, τ leptons, muons, and missing transverse energy (E_T^{miss})⁵. The level-1 trigger algorithms cut the rate to ~ 100 kHz. Events passing the level-1 trigger are then passed on to a High Level Trigger (HLT) which reconstructs the

⁴Collisions where one or both protons have not fragmented

⁵Transverse energy that is not detected by the detector but must exist due to conservation of energy.

event using the full ATLAS reconstruction chain based on the Athena software framework [102]. A decision is then made by the HLT based on various algorithms whether to save an event. The rate of events passing this trigger system is less than 1 kHz [103, 104].

Chapter 4

Object Reconstruction and Calibration in ATLAS

In the ATLAS detector, it is possible to reconstruct “objects” such as particle tracks, vertices, electrons, and muons, and jets of particles. This section summarizes the various algorithms and calibrations that are used by the ATLAS Collaboration to define and select these objects. Section 4.1 present the track reconstruction and vertex finding algorithms. Section 4.2 and Section 4.3 summarize the reconstruction, identification, isolation, and calibration algorithms for electrons and muons, respectively. Finally, Sections 4.4 and 4.5 summarize the reconstruction and calibration algorithms used for collimated sprays of particles and the missing transverse energy (E_T^{miss}), respectively.

4.1 Track and Vertex Reconstruction

In an event, all hits from the ID can be used to reconstruct particle tracks. Furthermore, the track information can be used to determine “vertices” which are defined by multiple charged tracks and could be associated with the hard scatter (denoted as the primary vertex) or the result of particle decays. The helical trajectory of a particle moving in a uniform magnetic field can be parametrized [105, 106] using the five variables shown in Equation 4.1. Thus, the ATLAS track reconstruction algorithms attempt to efficiently reconstruct tracks and accurately determine the five variables.

$$\hat{r} = \left(d_0, z_0, \theta, \phi, \frac{q}{p} \right) \quad (4.1)$$

Here, d_0 is the transverse impact parameter, z_0 is the longitudinal impact parameter¹, θ is the polar angle, ϕ is the azimuthal angle, and $\frac{q}{p}$ is the charge to momentum ratio of the track.

Initially, hits in the inner detectors are clustered together from hits that are geometrically nearby and a single “space point”, the point where the particle passed through, is determined. Sets of three space points are then used to form seeds for the track reconstruction algorithm. Additional cuts on the momentum, impact parameter, and the requirement of additional space point in a separate layer, are then used to increase the chances to build the final track candidates from the seeds, while also considering additional space points in the remaining layers. After tracks have been constructed, an ambiguity resolution step is performed by identifying sets of tracks that are likely to be duplicates with a score based on track properties and χ^2 fits. Furthermore, a track extension algorithm is used to add hits from the TRT detector to the tracks. Further details on the ambiguity resolution algorithms can be found in Ref. [105].

Primary vertices that define a pp collision with multiple tracks, are determined in ATLAS using an iterative algorithm [107]. A seed vertex is placed at the estimated mode of all tracks in an event, along the z -axis. This seed is used as a starting point and the various tracks are used to determine the best vertex position using an iterative χ^2 fit. In each iteration, tracks are weighted based on the quality of match to the vertex. Once a vertex position is determined, tracks that were inconsistent with the primary vertex based on their contribution to the χ^2 are then used in the determination of other vertices, and this process is repeated with all tracks of an event. The primary vertex arising from the hard scatter is defined as the vertex with the largest sum of squared track p_T .

4.2 Electron Reconstruction and Calibration

The measurements discussed in this thesis rely on the reconstruction and identification of isolated electrons and positrons². This is achieved by dedicated reconstruction, identification, and isolation algorithms discussed in Section 4.2.1. Corrections to the electron spectra, determined using $\sqrt{s} = 13$ TeV data are discussed in Section 4.2.2 and Section 4.2.3, while Section 4.2.4 discusses corrections relevant for measurements using $\sqrt{s} = 5.02$ TeV data. Further details on the electron reconstruction, identification, isolation, and corrections can be found in Appendix B.1 and B.2.

4.2.1 Reconstruction, Identification, and Isolation

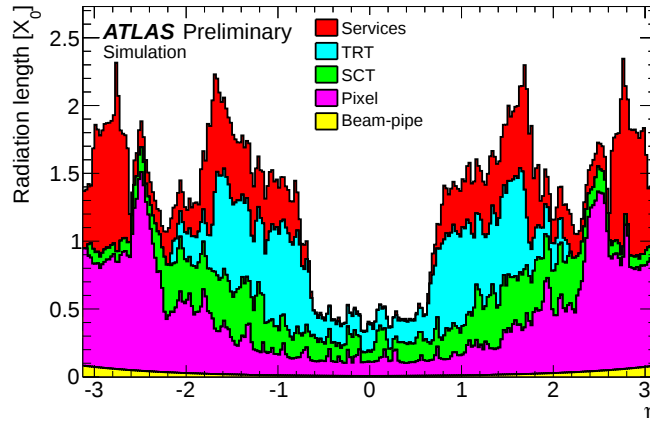
Electron candidate reconstruction in ATLAS is performed by identifying clusters of energy deposits in the EM calorimeter and matching them with tracks in the inner detector. Calorimeter cells with

¹The transverse (longitudinal) impact parameter is defined as the shortest distance in the $R - \phi$ plane (along the z -axis) between an extrapolated track and a reference point that is typically the interaction point or the primary vertex.

²Positron reconstruction, identification, and isolation is the exact same as electrons and so a positron is referred to as an “electron” in this thesis, unless explicitly stated.

an energy above a noise threshold are used as seeds whose neighbours are summed, if they measure energy above a looser noise threshold. A dedicated algorithm, discussed in Ref. [108], is used to prevent overlaps of cells. Clusters passing such requirements are termed “EM topo-clusters”.

Due to the size of the ID in the radial direction, bremsstrahlung radiation emitted from electrons passing through the ID materials can lead to inefficiencies in electron reconstruction and the degradation of tracking parameter resolution. This is visible in Figure 4.1, which shows the radiation length X_0 traversed by a straight track through the ID, as a function of η [109]. After traversing the ID, high energy electrons decaying only through bremsstrahlung radiation, are expected to lose $\sim 40\%$ of their energy in the least dense region around $|\eta| \sim 0$, and $\sim 90\%$ of their energy in the transition region³. To correct for bremsstrahlung effects, a Gaussian-sum filter (GSF) fitting procedure [109–111] is applied to tracks that loosely match a calorimeter cluster barycenter⁴ and have at least four silicon hits.



(a)

Figure 4.1: Distribution of the ID material thickness in radiation length X_0 , given separately for each sub-detector and as a function of η . This is the description used to simulate the ATLAS detector.

The GSF track is then matched to the calorimeter topo-cluster and ambiguities arising from the fact that the electron candidate could be a valid photon candidate are treated according to the algorithms defined in Ref. [78, 108, 112]. Calorimeter topo-clusters are then expanded by a variable window size that depends on whether a track can be matched to only the seed-cluster or to multiple energy clusters [108]. This new cluster is called the “supercluster”. Further details of this algorithm are discussed in Ref. [108]. The track matching is performed again, and electron candidate tracks with the GSF fit are required to match the superclusters. The electron candidate four-vector can now be defined using the calibrated energy of the supercluster and track information from the track best matched to the new supercluster object. Figure 4.2 shows a cartoon of an electron passing through the ATLAS detector and the various inputs required for electron candidate reconstruction [113].

³Electrons with an energy greater than the critical energy decay predominantly through bremsstrahlung effects. Since the fractional energy loss increases linearly (logarithmically) for bremsstrahlung (ionization), energies much higher than the critical energy follow this rule

⁴An energy weighted position point in the $\eta - \phi$ plane.

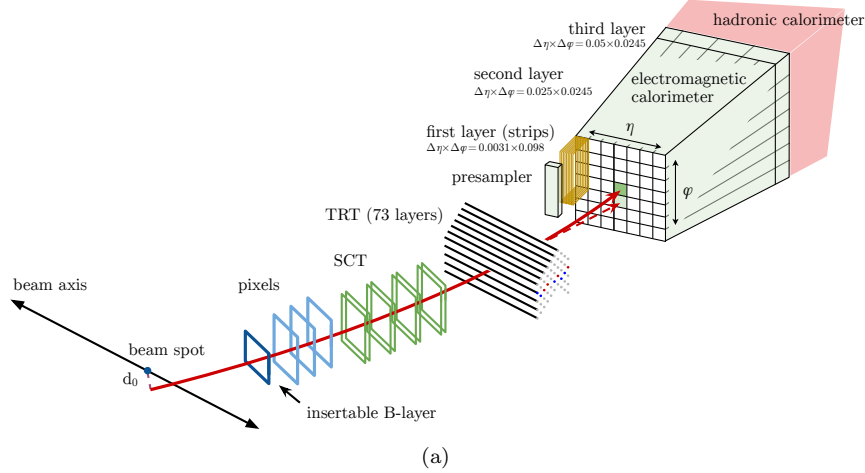


Figure 4.2: An illustration of the path taken by an electron (solid red line) through the various layers comprising the ATLAS detector. The dashed red line shows the path of a possible photon produced via bremsstrahlung effects while traversing detector material

According to the Neyman Pearson lemma [114], under certain conditions the optimal discriminant for a classifier is the likelihood ratio between the signal and background. Thus, electron identification is performed by using a likelihood-based discriminant d_L . The signal (L_S) and background (L_B) likelihood functions are first defined as the product of probability distributions for a given set of variables, and the functions can be written as

$$L_j(x_i) = \prod_i P_{ij}(x_i)$$

Here, L_j is the signal or background likelihood, the index i runs over the various input parameters, P_{ij} are the probability distributions for the input parameter i and likelihood type j , and x_i represents the value of the input parameter i . The list of input variables can be found in Ref. [108]. The functions are determined in bins of the electron candidate's E_T and $|\eta|$, using $Z \rightarrow ee$ and $J/\psi \rightarrow e^+e^-$ events in data. The selection employs the “tag-and-probe” method that is further discussed in Section 4.2.2 and Ref. [108]. The probability distributions are all smoothed to avoid non-physical effects from low statistics [108]. Working points with a fixed electron identification efficiency are defined by applying cuts on d_L as a function of E_T and $|\eta|$ such that a slightly falling efficiency curve is observed as a function of the number of primary vertices. A linearly falling efficiency is chosen over a constant efficiency in order to reduce large background efficiencies seen in the latter approach. The **LooseAndBLayer** and **Medium** working points are typically used in analyses and are defined by cuts on d_L and additional track parameter requirements [108, 113].

Electrons arising from semi-leptonic decays of heavy quarks (i.e. b-quarks), hadronic jets misidentified as leptons, and electrons from photon conversions can lead to a significant misidentified lepton background. This background is controlled by selecting for isolated electrons using calorimeter and tracking information.

Contributions from misidentified leptons can be reduced by examining the summed E_T of the electron candidate and topological clusters [115] whose barycenters fall within $\Delta R = \sqrt{\Delta\phi^2 + \Delta\eta^2} = 0.2$. The calorimeter isolation energy ($E_{T, \text{cone}}^{\text{isol}}$) can then be calculated by subtracting the electron candidate energy $E_{T, \text{core}}$, energy associated with leakage effects $E_{T, \text{leakage}}$, and energy from pileup events $E_{T, \text{pileup}}$.

Since decays tend to be more collimated at higher p_T ⁵, a cone size that decreases at higher p_T would be less sensitive to contamination from tracks arising from collimated decays than a fixed radius cone. Thus, the track based isolation variable $p_{T, \text{cone}}^{\text{var20}}$ is determined by first summing the p_T from all tracks found in a variable sized cone of $\Delta R = \min\left(\frac{10 \text{ GeV}}{p_T [\text{GeV}]}, 0.2\right)$ around the electron candidate track. The p_T corresponding to the electron candidate track is then subtracted from the summed p_T [113]. The **FixedCutLoose** isolation requirement is used to calculate the trigger efficiency and is defined using the following cuts: $E_{T, \text{cone}}^{\text{isol}} < 0.20p_T$ and $p_{T, \text{cone}}^{\text{var20}} < 0.15p_T$. The **FixedCutTight** requirement that is used by the analyses discussed in this thesis requires both cuts to be less than $0.06p_T$.

4.2.2 Efficiency Measurement

The electron spectra predicted by MC generators is an imperfect simulation the true electron p_T spectrum and detector response. Thus, it must be corrected before the electron objects can be used in measurements. The corrections can be determined by measuring the efficiencies related to electron reconstruction, identification, isolation, and trigger in both data and MC.

The efficiency to trigger on an electron can be factorized according to

$$\epsilon_{\text{Total}}^X = \epsilon_{\text{Cluster}}^{\text{MC}} \cdot \epsilon_{\text{Reco}}^X \cdot \epsilon_{\text{ID}}^X \cdot \epsilon_{\text{Isol}}^X \cdot \epsilon_{\text{Trigger}}^X = \frac{N_{\text{Cluster}}^{\text{MC}}}{N_{\text{All}}^{\text{MC}}} \cdot \frac{N_{\text{Reco}}^X}{N_{\text{Cluster}}^X} \cdot \frac{N_{\text{ID}}^X}{N_{\text{Reco}}^X} \cdot \frac{N_{\text{Isol}}^X}{N_{\text{ID}}^X} \cdot \frac{N_{\text{Trigger}}^X}{N_{\text{Isol}}^X} \quad (4.2)$$

Here, the superscript X represents whether the efficiency is measured in data or MC. $\epsilon_{\text{Cluster}}$ is the efficiency to produce EM clusters associated with electrons and is the number of EM clusters seen in MC events divided by the total MC events. Note that this efficiency is measured in MC only [113]. ϵ_{Reco} is the reconstruction efficiency and is determined by dividing the number of successfully reconstructed electron candidates with the number of EM clusters seen in an event. The identification efficiency ϵ_{ID} can then be determined by taking the number of electron candidates passing the identification cuts and dividing by the number of electron candidates reconstructed. Similarly, the isolation efficiency can be determined by taking the number of identified electron candidates passing the isolation requirements and dividing by the total candidates identified. Finally, trigger efficiencies are determined by the ratio of online trigger objects (discussed in Section 3.2.5) to the number of isolated electron candidates in an event.

The relevant corrections (also denoted as “scale factors”) for the various effects discussed in

⁵Such decays or objects are denoted as “boosted” decays or objects since they have a large Lorentz factor.

Equation 4.2 can be expressed as: $SF_i = \frac{\epsilon_i^{\text{Data}}}{\epsilon_i^{\text{MC}}}$. The scale factors are typically measured in bins of E_T and η , and are applied to MC in order to correct for any mis-modelling from physics and detector effects. Note that by applying the scale factors, the MC efficiencies will be equal to the efficiencies measured in data. Since the scale factors are always applied to MC simulation, the uncertainties associated with the efficiency measurements (and thus the scale factor measurements) are considered in an analysis as systematic uncertainties.

The efficiencies are typically measured using the tag-and-probe method in $Z \rightarrow ee$ and $J/\psi \rightarrow e^+e^-$ events and a selection sensitive to dilepton events decaying from either resonance is applied. A strict definition on one of the leptons (the “tag”) is then used to create a sample of unbiased leptons (the “probe”), with which one can measure the efficiencies.

4.2.3 Electron Energy Scale Calibrations

The reconstructed electron energy needs to be calibrated before it can be used for physics analyses. The calibration procedure starts by training a multivariate analysis (MVA) using MC, to estimate the generator level electron energy (E_{gen}) while using detector level variables as inputs [108, 116, 117]. Separate MVAs are trained in bins of E_T and η , and the output from the MVA is denoted as E_{calib} . The uncertainty in the calibrated energy, $\sigma(E_{\text{calib}})$ is determined by converting the interquartile range of the $E_{\text{calib}}/E_{\text{gen}}$ distributions to a standard deviation. Figure 4.3 shows the relative electron energy resolution ($\sigma(E_{\text{calib}})/E_{\text{gen}}$) using single electron MC samples, as a function of η for various E_T ranges [117]. Note that the electron energy resolution is larger in the transition region regardless of the E_T and improves at higher electron energies.

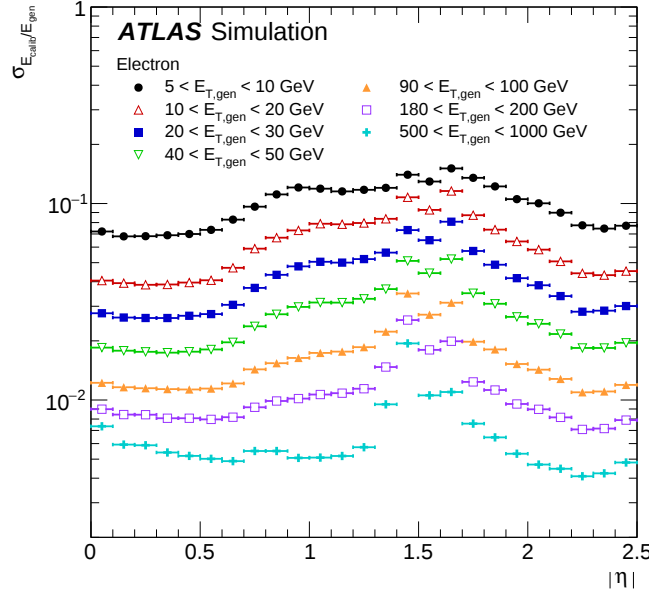
Before the MVA can be applied to data, corrections are applied to the different calorimeter layers to ensure a uniform energy response across the layers, and corrections that account for energy shifts induced by pileup. After these two corrections, the MVA is applied to data and followed by additional corrections from: energy loss between the barrel calorimeter module and the effect of high voltage inhomogeneities in the calorimeter. These corrections are further discussed in Ref. [117] and [108].

The residual differences between the corrected data and simulation in η bin i , can be expressed as an additional energy scale correction (α_i) and an additional constant uncertainty on the relative energy resolution (c_i). These corrections can be expressed as Equation 4.3.

$$E^{\text{data}} = E^{\text{MC}} \cdot (1 + \alpha_i) \quad (4.3)$$

$$\left(\frac{\sigma(E)}{E} \right)^{\text{data}} = \left(\frac{\sigma(E)}{E} \right)^{\text{MC}} \oplus c_i$$

Both corrections can be determined using a χ^2 fit to $Z \rightarrow ee$ decays that are well-defined, back-to-back in ϕ , and have electrons in the i and j η regions. This is done by assuming a massless electron, and writing the dilepton invariant mass observed in data, to first-order in α_i and α_j . With



(a)

Figure 4.3: The relative calibrated energy resolution $\sigma(E_{\text{calib}})/E_{\text{gen}}$, as a function of electron $|\eta|$, for various ranges of generator electron E_T . The uncertainty on E_{calib} is determined by converting the interquartile range of the $E_{\text{calib}}/E_{\text{gen}}$ distributions, to a standard deviation.

these assumptions and the relations in Equation 4.3, it is possible to write the dielectron invariant mass as: $m_{ij}^{\text{data}} = m_{ij}^{\text{MC}} \cdot \left(1 + \frac{\alpha_i + \alpha_j}{2}\right)$. Similarly, by using error propagation rules, the relative invariant mass resolution can be written as: $\left(\frac{\sigma(E)}{E}\right)^{\text{data}} = \left(\frac{\sigma(E)}{E}\right)^{\text{MC}} \cdot \left(1 + \frac{c_i \oplus c_j}{2}\right)$. Thus, it is possible to probe the electron energy scale and the electron energy resolution by using the tag and probe method in $Z \rightarrow ee$ decays. Ref. [117] provides further details on the electron energy scale calibrations, simulated samples, selection requirements, background estimation, and validation for $\sqrt{s} = 13$ TeV data taken in 2015 and 2016.

Note that the correction on the energy scale is applied on data such that the energy scale matches MC whereas the relative resolution in simulation is smeared to match data. Systematic uncertainties from the selection, background treatment, and choice of algorithm are propagated to the scale and resolution measurements, as discussed in Ref. [117].

The $Z \rightarrow ee$ calibration can be interpreted as fixing the relative energy scale as a function of η at a E_T equal to the average E_T seen in all $Z \rightarrow ee$ events ($\langle E_{Zee} \rangle$). Thus, the relative effect of a systematic uncertainty for an arbitrary electron E_T and η can be estimated by taking the relative change in uncorrected energy for a systematic variation and subtracting the relative change evaluated at $\langle E_{Zee} \rangle$. The effect on the relative resolution is determined similarly, but the subtraction is done in quadrature. Details of the systematic uncertainties considered are presented in Ref. [116, 117].

Figure 4.4 shows the electron energy scale uncertainty and the relative electron energy resolution as a function of E_T , for an electron with $|\eta| = 0.3$ and a slightly different⁶ reconstruction algorithm [117] than the one discussed in Section 4.2.1. For an electron with $E_T = 20$ GeV and $|\eta| = 0.3$, the energy scale is known to an accuracy of 1% and has a relative energy resolution of $\sim 4\%$ that is known to an accuracy of $\sim 10\%$ [117].

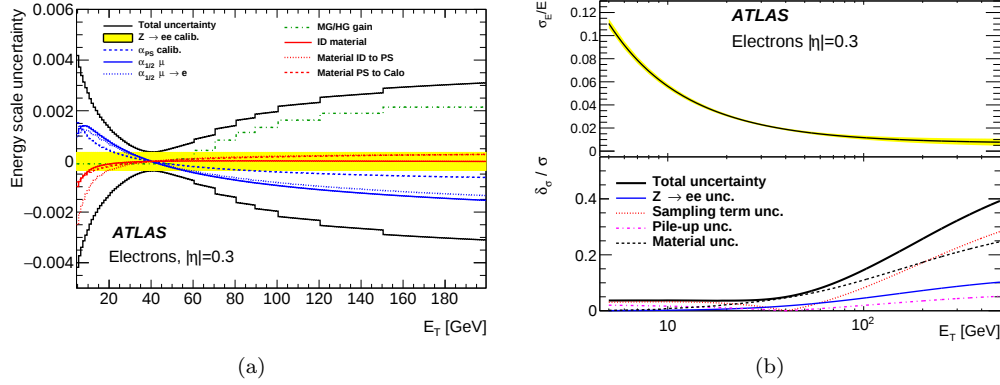


Figure 4.4: (a) shows the relative electron energy scale uncertainty as a function of E_T and an electron $|\eta| = 0.3$. The total uncertainty (solid black curve) is shown as well as the main contributions, which are represented by the signed impact of a one-sided variation of the corresponding uncertainty. The total uncertainty is shown as a two-sided variation. (b) shows the relative electron energy resolution $\sigma(E)/E$, as a function of E_T and an electron $|\eta| = 0.3$. The yellow band in the top panel shows the total uncertainty in the relative resolution. The lower panel shows a breakdown of the relative uncertainties in the energy resolution (δ_σ/σ). The black curve in the lower panel represents the total uncertainty.

4.2.4 $\sqrt{s} = 5.02$ TeV Corrections

Since the detector response and experimental conditions at $\sqrt{s} = 5.02$ TeV are different from the ones at $\sqrt{s} = 13$ TeV, the electron energy scale and various efficiencies needed to be studied and validated with $\sqrt{s} = 5.02$ TeV data. In some cases, the $\sqrt{s} = 13$ TeV data was found to model the $\sqrt{s} = 5.02$ TeV environment without any additional corrections (like the trigger efficiency discussed in Section 4.2.2) whereas in other cases, a new calibration needed to be derived and applied. Details on the derivation and validation of these corrections are discussed in Ref. [118]. Typically, scale factors measured at $\sqrt{s} = 5.02$ TeV have a significantly larger uncertainty than the ones measured using high-pileup $\sqrt{s} = 13$ TeV data, due to the lower statistics of the $\sqrt{s} = 5.02$ TeV sample. If the high-pileup scale factors and calibrations at $\sqrt{s} = 5.02$ TeV are found to agree with $\sqrt{s} = 5.02$ TeV data then they are preferred as the former can take advantage of higher statistics.

Figure 4.5 shows a comparison of the electron reconstruction efficiency as a function of E_T , for an electron reconstructed in the EM barrel and endcap calorimeters. The plots compare the

⁶Electron energy scale uncertainties and the electron energy resolution are expected to be smaller with the reconstructed algorithm [108] discussed in Section 4.2.1. Unfortunately, the energy scale uncertainty and the relative energy resolution plots were not produced in Ref [108], hence the old plots from Ref. [117] are shown in this thesis.

reconstruction efficiency observed in MC for the 5.02 TeV, low-pileup 13 TeV, and high-pileup 13 TeV datasets. The 5.02 TeV simulation generally agrees with the high-pileup 13 TeV simulation, within statistical uncertainty. The reconstruction scale factors between the high-pileup 13 TeV data and $\sqrt{s} = 5.02$ TeV data were further compared and found to differ by $\sim 0.15\%$. The excellent agreement motivated the use of high-pileup 13 TeV electron reconstruction scale factors and their uncertainties, with an additional uncertainty of 0.2% that accounts for any possible mis-modelling from this extrapolation.

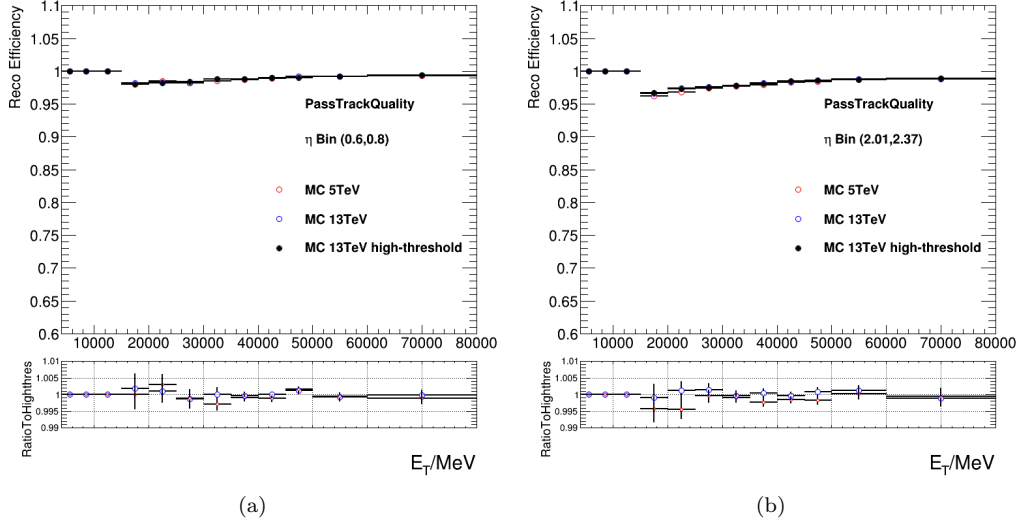


Figure 4.5: The reconstruction efficiency observed in MC simulation as a function of the generator level electron E_T , for electrons reconstructed in (a) the barrel ($0.6 < \eta < 0.8$) and (b) the endcap ($2.01 < \eta < 2.37$). The red open circle is the efficiency measured in $\sqrt{s} = 5.02$ TeV simulation, the blue open circle is low-pileup $\sqrt{s} = 13$ TeV data, and the filled black circle is the efficiency measured in high-pileup $\sqrt{s} = 13$ TeV data. The error bars represent the total uncertainty. The lower panel shows the ratio between the measured efficiency with respect to the high-pileup 13 TeV efficiencies, along with the total uncertainty in the ratio.

Figure 4.6 shows the electron identification scale factors from various algorithms [118], for an electron with p_T between 20 GeV and 25 GeV. The identification efficiency in simulation was found to be $\sim 5\%$ lower $\sqrt{s} = 5.02$ TeV than $\sqrt{s} = 13$ TeV. The cause for this discrepancy was not identified, thus the electron identification efficiencies and uncertainties derived in $\sqrt{s} = 5.02$ TeV data were used for the $\sqrt{s} = 5.02$ TeV analyses discussed in this thesis.

The electron isolation efficiencies at $\sqrt{s} = 5.02$ TeV were measured in the dilepton $\sigma_{t\bar{t}}$ analysis, using the tag and probe method in $Z \rightarrow ee$ events. The efficiency was parameterized as a function of lepton p_T , lepton η , and the I_{trk} variable, which is defined as: $p_{T,\text{cone}}^{\text{var40}}/p_T$ ⁷. Figure 4.7 shows the electron isolation efficiencies measured in $\sqrt{s} = 5.02$ TeV data as a function of the three variables. The scale factors at $\sqrt{s} = 5.02$ TeV are measured to be around unity. However, the simulation is shown to predict a lower efficiency than data for electrons with $p_T < 20$ GeV, electrons in the

⁷ $p_{T,\text{cone}}^{\text{var40}}$ uses a variable radius cone of $\Delta R = \min\left(\frac{10 \text{ GeV}}{p_T[\text{GeV}]}, 0.4\right)$

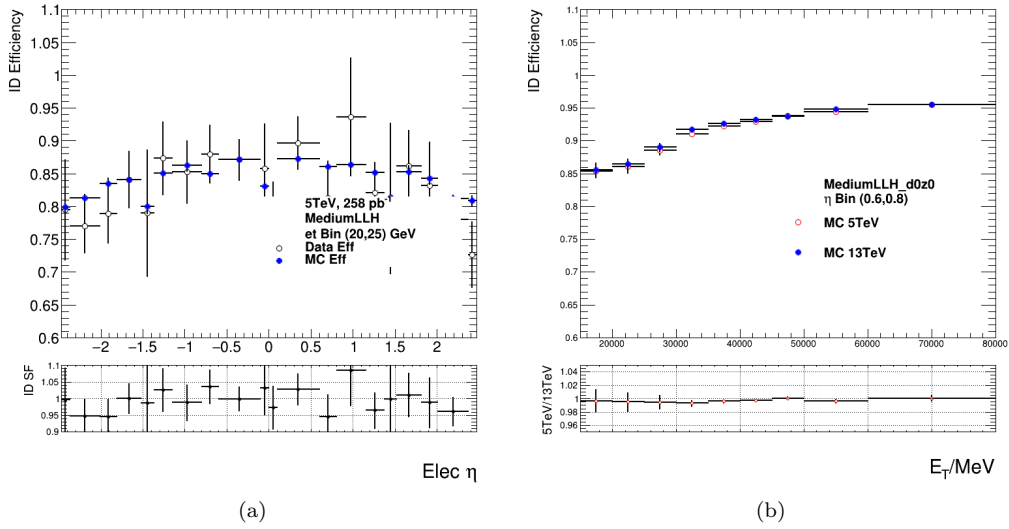


Figure 4.6: The electron identification efficiencies measured in $Z \rightarrow ee$ data events, as a function of the electron (a) η and (b) E_T . (a) shows the efficiency measured in data and simulation as measured with $\sqrt{s} = 5.02$ TeV data, and with a reconstructed electron E_T between 20 GeV and 25 GeV. The lower panel in (a) shows the ratio of the data and the MC simulation (scale factors), along with the uncertainty in the ratio. (b) compares the identification efficiencies in simulation at high-pileup 13 TeV data and $\sqrt{s} = 5.02$ TeV data as a function of E_T , and with a reconstructed electron $0.6 < \eta < 0.8$. The lower panel shows the ratio of the efficiency measured at 5.02 TeV and high-pileup 13 TeV. The error bars in both plots represent the total uncertainty.

transition region, and electrons with large values of I_{trk} . Details on the isolation efficiency calculation for $\sqrt{s} = 5.02$ TeV data are provided in Ref. [119].

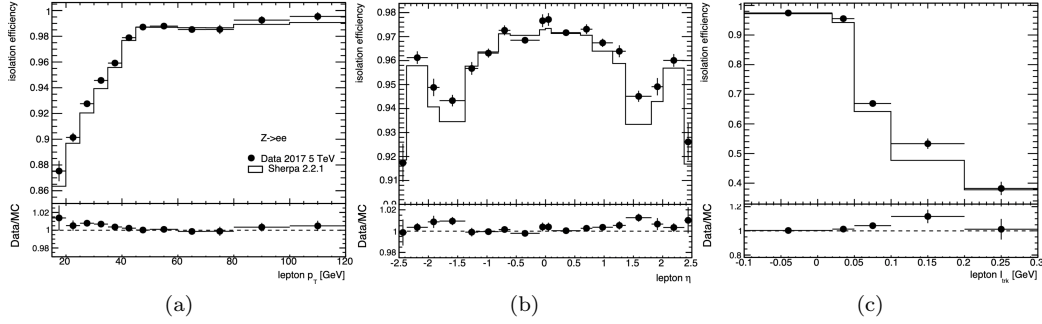


Figure 4.7: Electron isolation efficiency measured in data and MC from tag-and-probe measurements in $Z \rightarrow ee$ events with the 5.02 TeV dataset. The efficiencies are plotted as a function of (a) lepton p_T , (b) lepton η , and (c) the I_{trk} variable. The error bars represent the total uncertainty on the measurement. The lower panel shows the ratio of the data and the MC simulation (scale factors), along with the uncertainty in the ratio.

The electron energy scale and resolution corrections were derived using $\sqrt{s} = 5.02$ TeV data, since the low-pileup data was recorded with a dedicated setting for the calorimeter topological cluster noise thresholds, thus requiring a dedicated energy calibration to be used. The calibrations followed the procedure defined in Ref. [108, 118]. Figure 4.8 shows the correction factors α and c , measured in $\sqrt{s} = 5.02$ TeV data, as a function of η .

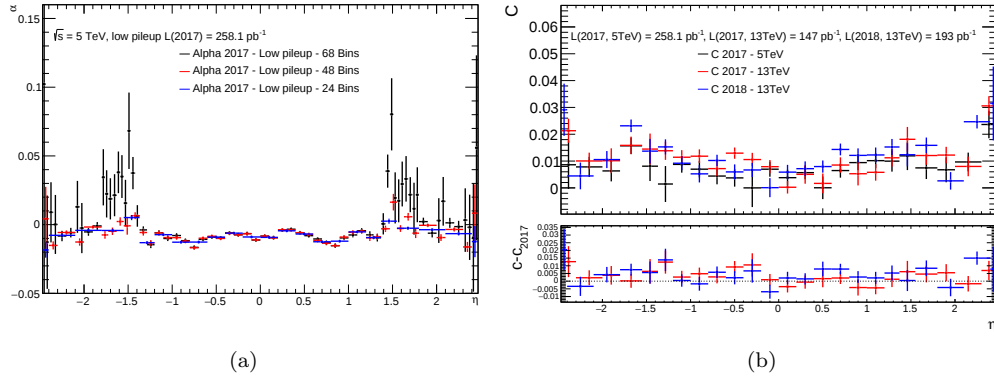


Figure 4.8: The (a) electron energy scale correction factors and (b) electron energy resolution corrections, measured with $\sqrt{s} = 5.02$ TeV data, as a function of the electron η . The bands in (a) show various alternate binning schemes that were used to derive the energy scale corrections whereas the bands in (b) represent the resolution corrections derived in $\sqrt{s} = 5.02$ TeV data (black line), low-pileup 13 TeV data collected in 2017 (red line), and low-pileup 13 TeV data collected in 2018 (blue line). The lower panel in (b) shows the difference in the correction factor for each dataset and the 5.02 TeV dataset. The uncertainties in both plots represent the total uncertainty on these measurements.

4.3 Muon Reconstruction and Calibration

The reconstruction, identification, and isolation algorithms used to select muons are discussed in Section 4.3.1. Corrections for the muon spectra based on $\sqrt{s} = 13$ TeV data are discussed in Section 4.3.2 and Section 4.3.3, while Section 4.3.4 presents additional corrections relevant for measurements using $\sqrt{s} = 5.02$ TeV data. The results of the various muon efficiency and scale factor measurements can be found in Appendix B.3.

4.3.1 Reconstruction, Identification, and Isolation

Reconstruction of muon candidates considered by the analyses discussed in this thesis, is done by combining information from the MS and ID. Tracks from hits in individual MS stations are first reconstructed using a Hough transformation [120]. Track segments in different stations are then combined into preliminary track candidates based on a first-order approximation of a muon in a magnetic field. A global χ^2 fit of the muon trajectory in a magnetic field is then performed, using track candidates in multiple MS detectors, accounting for muon interactions in detector material, and considering possible detector misalignment. The muon trajectory is then corrected for outlier tracks, ambiguities are resolved, and the fit is repeated [121].

“Combined” muons (CB muons) are reconstructed by combining MS tracks with ID tracks in a combined track fit that accounts for energy loss in the calorimeters [121]. A second algorithm (“inside out” or IO muons) is used to slightly increase the reconstruction efficiency by extrapolating ID tracks to the MS, requiring at least three loosely aligned MS hits, and using these as inputs for a combined fit. The second algorithm is used to increase sensitivity in regions of limited MS coverage and to low p_T muons that might not fully cross through the calorimeter. Additional algorithms discussed in Ref. [121] can also be used but are not relevant to this thesis and thus not discussed here.

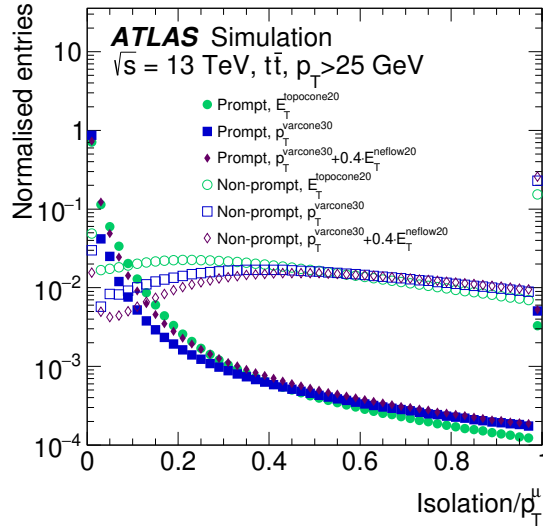
Muon candidates are identified from reconstructed muon tracks by applying cuts on: the number of detector hits, track fit properties, and the compatibility, $\mathcal{C}$ (Equation 4.4), between the ID and MS charge to momentum ratios (q/p^X for detector X) and their uncertainties ($\sigma(q/p^X)$). Multiple identification working points are used in ATLAS. However, this section will focus on the **Medium** identification requirement as that is the one used by the analyses presented in this thesis. The other working points are discussed in Ref. [121].

$$\mathcal{C} = \frac{|q/p^{\text{ID}} - q/p^{\text{MS}}|}{\sqrt{\sigma(q/p^{\text{ID}})^2 + \sigma(q/p^{\text{MS}})^2}} \quad (4.4)$$

The **Medium** working point for muons in the ID acceptance uses only CB and IO muons with $|\eta| < 2.5$. Such muons are required to have at least two MS stations where the muon has at least three hits in the MDT or CSC detectors (denoted as precision stations). In the MS crack region ($|\eta| < 0.1$),

the requirement is relaxed to have only one precision station, provided that there is a maximum of one station where the muon has less than three hits in the MS and is also missing at least three hits that are expected when accounting for detector material and muon trajectory (denoted as precision hole stations). Requirements on the longitudinal and transverse impact parameters are used to reject muons arising from either hadron decays and muons not originating from the hard scatter. This cut is called “muon vertex association” and requires $|z_0|\sin(\theta) < 0.5 \text{ mm}$ and $\frac{d_0}{\sigma(d_0)} < 3$. Finally, $\mathcal{C}$ is required to be less than seven [121].

Similar to the electron isolation discussed in Section 4.2.1, isolated muons arising from the hard scatter are selected, by applying cuts on both a track based and calorimeter based isolation variable. The track based variable is calculated by summing the transverse momenta of all tracks with $p_T > 1 \text{ GeV}$ around a cone in η - ϕ space, and then subtracting the momenta associated with the muon track. For muons with a $p_T < 50 \text{ GeV}$, a variable cone of size $\Delta R = \min\left(\frac{10 \text{ GeV}}{p_T[\text{GeV}]}, 0.3\right)$ is used whereas for muons with $p_T > 50 \text{ GeV}$, a fixed cone of $\Delta R = 0.2$ is used. These two variables are denoted $p_{T,\text{cone}}^{\text{var30}}$ and $p_{T,\text{cone}}^{\text{fixed20}}$, respectively. The calorimeter based isolation variable for muons is complementary to the one used for electrons but with negligible leakage effects. Figure 4.9 shows distributions of various muon isolation variables [121] in $t\bar{t}$ MC. The **FTight.FixedRad** isolation requirement used in this thesis, requires: $E_{T,\text{cone}}^{\text{isol}} < 0.15p_T$ and $p_{T,\text{cone}}^{\text{var30}} < 0.04p_T$ for muons with p_T smaller than 50 GeV. For muons with p_T greater than 50 GeV, $p_{T,\text{cone}}^{\text{fixed20}}$ is used instead of $p_{T,\text{cone}}^{\text{var30}}$. For a muon with p_T between 20 and 100 GeV, this working point is 89% efficient in isolating prompt muons and 1% efficient in misidentifying non-prompt muons from b and c hadron decays. The efficiencies were calculated using $t\bar{t}$ simulation.



(a)

Figure 4.9: Distributions of various muon isolation variables divided by the reconstructed muon p_T , in simulated $t\bar{t}$ events at 13 TeV. The $t\bar{t}$ selection is required to have a $p_T > 25 \text{ GeV}$ and the distributions are normalized to unity. The green circle and blue square are the $p_{T,\text{cone}}^{\text{var30}}$ and the calorimeter based isolation variable, respectively.

4.3.2 Efficiency Measurement

Just like the electrons, the muon efficiencies in MC must be corrected to match those observed in data. This section discusses the reconstruction, identification, and isolation efficiency and scale factor measurements using the tag-and-probe method with $Z \rightarrow \mu\mu$ and $J/\psi \rightarrow \mu^+\mu^-$ events, as seen with the full Run 2 dataset [121].

Due to the multifaceted nature of muon identification, three types of unbiased probes are necessary to extract the efficiency for the **Medium** working point. The ID tracking efficiency is probed using MS tracks that cannot be matched to an ID track, and extrapolating them to the IP (called MS probe). Similarly, ID and calorimeter-tagged (CT) probes are used to determine the efficiencies in the MS. ID probes rely only on only ID tracks, whereas CT probes search for an energy deposit in the calorimeter that matches an ID track [121]. The efficiency for an algorithm X given probe P ($\epsilon(X|P)$) can then be calculated as: $\epsilon(X|P) = \frac{N_P^X}{N_P^{\text{all}}}$. Here, N_P^X is the number of muon candidates with an algorithm X , that fall within $\Delta R < 0.05$ of a probe P , and N_P^{all} is the total number of selected probes.

The identification efficiency can then be written as [121]

$$\epsilon(X) = \epsilon(X|\text{ID and MS})\epsilon(\text{MS}|\text{ID})\epsilon(\text{ID}|\text{MS}) + \epsilon(X \text{ and not MS}|\text{ID})\epsilon(\text{ID}|\text{MS}) \quad (4.5)$$

The first term is the reconstruction efficiency conditional on the combined tracks in the MS and ID, and thus requires two distinct probes to measure. The second term is used to account for muons with partial track information and is sensitive to low p_T muons. The conditional ID probe is approximated with a CT probe since it is difficult to measure efficiencies conditional on ID tracks. Thus, the efficiency is written as

$$\epsilon(X) = (\epsilon(X|\text{ID and MS})\epsilon(\text{MS}|\text{CT}) + \epsilon(X \text{ and not MS}|\text{CT})) \cdot \epsilon(\text{ID}|\text{MS}) \quad (4.6)$$

Details of the exact selection requirements and background treatments used in the efficiency measurements are discussed in Ref. [121]. Systematic uncertainties on the efficiencies and their relevant scale factors are determined by varying: selection requirements, tag-muon requirements, and parameters associated with the background estimate [121].

4.3.3 Muon Momentum Scale Calibrations

Before muon objects can be used for physics analyses, the muon momentum scale must be calibrated in order to correct for: energy loss when traversing the detector, mis-modelling of the detector and magnetic field, and detector misalignment. First, a charge dependent momentum scale correction is measured and applied to data, in order to correct for detector misalignment. This is then followed by a correction applied to the simulated muon momentum scale. The corrections are derived using $J/\psi \rightarrow \mu^+\mu^-$ and $Z \rightarrow \mu\mu$ decays, and additional validations are performed using dimuon events

from $J/\psi \rightarrow \mu^+ \mu^-$, $\Upsilon \rightarrow \mu \mu$, and $Z \rightarrow \mu \mu$ decays.

Although the MS [78, 122] and ID detectors [123] undergo alignment procedures and apply such corrections to data, residual effects can manifest as charge dependent biases on the sagitta⁸ during muon reconstruction. For an uncorrected transverse momentum p_T^{Uncorr} , this bias can be corrected (to first-order) according to

$$\frac{1}{p_T^{\text{Corr}}} = \frac{1}{p_T^{\text{Uncorr}}} + q \cdot \delta_S \Rightarrow p_T^{\text{Corr}} = \frac{p_T^{\text{Uncorr}}}{1 + q \delta_S p_T^{\text{Uncorr}}} \quad (4.7)$$

Here, p_T^{Corr} is the corrected muon transverse momentum, q is the charge of the reconstructed muon, and δ_S is the correction on the sagitta (also called sagitta bias). In a two particle system where the mass of the daughter particles is much smaller than the energy scale (like the dimuon system in $Z \rightarrow \mu \mu$ decays), the invariant mass can be written as: $m_{ab}^2 = 2p_{T,a} p_{T,b} (\cosh(\Delta\eta) + \cos(\Delta\phi))$. For $Z \rightarrow \mu \mu$ decays, $p_{T,a}$ and $p_{T,b}$ can be written based on their charge, as $p_{T,+}$ and $p_{T,-}$. Using this formalism and assuming $\delta_S \ll 1$, the corrected invariant mass in a dimuon system ($m_{\mu\mu}^{2 \text{ Corr}}$) is related to the uncorrected invariant mass ($m_{\mu\mu}^{2 \text{ Uncorr}}$) according to Equation 4.8.

$$m_{\mu\mu}^{2 \text{ Corr}} = \frac{2p_{T,+}^{\text{Uncorr}} p_{T,-}^{\text{Uncorr}} (\cosh(\Delta\eta) + \cos(\Delta\phi))}{\left(1 + \delta_S p_{T,+}^{\text{Uncorr}}\right) \left(1 - \delta_S p_{T,-}^{\text{Uncorr}}\right)} \Rightarrow \frac{m_{\mu\mu}^{2 \text{ Uncorr}}}{\left(1 + \delta_S p_{T,+}^{\text{Uncorr}}\right) \left(1 - \delta_S p_{T,-}^{\text{Uncorr}}\right)} \quad (4.8)$$

$$m_{\mu\mu}^{2 \text{ Corr}} \approx m_{\mu\mu}^{2 \text{ Uncorr}} + m_{\mu\mu}^{2 \text{ Uncorr}} \delta_S \left(p_{T,-}^{\text{Uncorr}} - p_{T,+}^{\text{Uncorr}}\right) + \mathcal{O}(\delta_S^2)$$

The sagitta bias is measured for both data and MC, in bins of η and ϕ by minimizing the variance in the dimuon invariant mass distribution, recomputing the invariant mass distribution, and iterating [124]. The difference in the sagitta bias observed in data and MC is used as a correction on data. Systematic uncertainties arising from the methodology and extrapolations to momenta outside the phase space of $Z \rightarrow \mu \mu$ decays are considered in the bias measurement as discussed in Ref. [124]. Figure 4.10 shows the sagitta bias measured before and after applying the correction on $\sqrt{s} = 13 \text{ TeV}$ data collected in 2017. The bias is measured to be a maximum of 0.4 TeV^{-1} before the correction but decreases by three orders of magnitude to 5 GeV^{-1} , after applying the correction.

The momentum scale in MC is now simultaneously corrected for the ID tracks, MS tracks, and CB tracks. The corrected transverse momentum for a given type of track X ($p_T^{\text{Corr}, X}$) is written as

$$p_T^{\text{Corr}, X} = \frac{p_T^X + s_0^X + s_1^X p_T^X}{1 + r_0^X g_0/p_T^X + r_1^X g_1 + r_2^X g_2 p_T^X} \quad (4.9)$$

In the numerator, p_T^X is the uncorrected transverse momentum using a track X , s_0 , and s_1 are additional $\eta - \phi$ dependent corrections to the muon momentum scale that correct for inaccurate descriptions of energy loss effects and the description of the magnetic field, respectively. The denominator of Equation 4.9 broadens the p_T resolution in MC so that it matches the resolution observed in data. The relative momentum resolution can be described as: $\frac{\sigma(p_T)}{p_T} = r_0/p_T \oplus r_1 \oplus r_2 p_T$.

⁸The sagitta is the distance between the midpoint of an arc and the midpoint of the chord spanned by the arc.

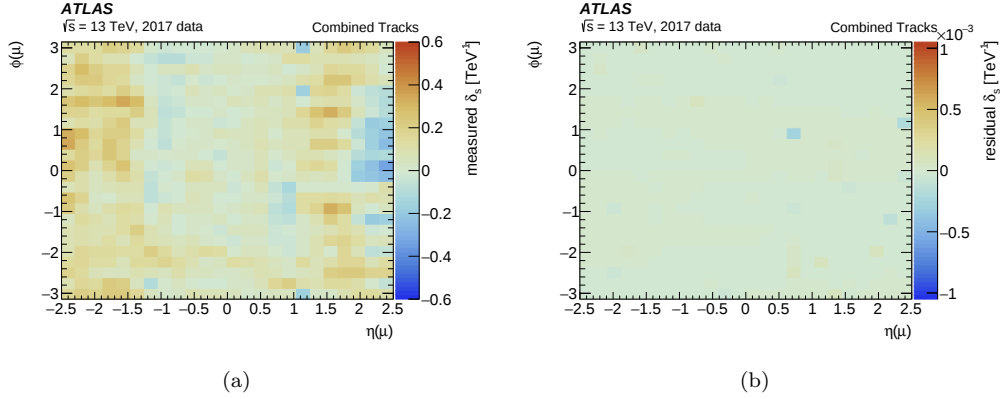


Figure 4.10: Sagitta bias (δ_S) measured using 2017 data for CB muons (a) before and (b) after, applying the bias correction.

The terms r_0 , r_1 , and r_2 are maps in the $\eta - \phi$ space and represent the uncertainties related to: energy loss, magnetic field modelling, and detector misalignment. The g_i terms represent a standard Gaussian distribution. Note that the s_2 term is not used because the effect of misalignment on the momentum scale is corrected in data using the sagitta bias correction.

The s_0^{ID} and r_0^{X} terms are set to zero since these terms were found to have negligible effects on the momentum scale and resolution, respectively [124, 125]. The r_2^{MS} term is determined from: alignment studies using cosmic-ray data, special runs with the toroidal magnet turned off [122], and detector alignment procedures [126]. The rest of the terms are determined by performing an iterative χ^2 fit on the dimuon invariant mass distributions in $Z \rightarrow \mu\mu$ and $J/\psi \rightarrow \mu^+\mu^-$ decays. Major sources of systematic uncertainty include the choice of selection requirements, signal modelling, background modelling, and assumptions and choices made in the algorithm. Further details on the fit procedure and the systematic uncertainties considered, are discussed in Ref. [124].

The scale calibrations are validated in $Z \rightarrow \mu\mu$ and $J/\psi \rightarrow \mu^+\mu^-$ decays with a looser muon selection criteria than the one used to derive the calibrations. $\Upsilon \rightarrow \mu\mu$ decays are used as an additional validation since they provide a statistically independent set of muons. The momentum scale can be probed by examining the average dimuon invariant mass. By assuming that the momentum resolution of the two muons ($\frac{\sigma(p_T)}{p_T}$) is equal, the relative invariant mass resolution can be written as

$$\frac{\sigma(m_{\mu\mu})}{m_{\mu\mu}} = \frac{1}{\sqrt{2}} \frac{\sigma(p_T)}{p_T} \quad (4.10)$$

Both the scale and resolution are then determined by fitting to the dimuon invariant mass spectra, as described in Ref. [124]. Figure 4.11 shows the average dimuon invariant mass and the dimuon invariant mass resolution from $\Upsilon \rightarrow \mu\mu$ decays, as a function of the η of the muon with the largest p_T . The scale and resolution observed in data and simulation agree within the systematic uncertainty. The scale uncertainty increases from 0.05% in the low $|\eta|$ regime to $\sim 0.1\%$ at high $|\eta|$. The resolution

is $\sim 3\% - 4\%$ across the detector. Figure 4.12 shows the relative dimuon invariant mass resolution as a function of p_T , for the $J/\psi \rightarrow \mu^+\mu^-$, $\Upsilon \rightarrow \mu\mu$, and $Z \rightarrow \mu\mu$ decays. For a muon with $p_T = 20 \text{ GeV}$, the dimuon invariant mass resolution is approximately ~ 0.015 , which results in a relative muon momentum resolution of ~ 0.021 . The muon momentum resolution then increases to ~ 0.47 at high p_T . Furthermore, the simulation is observed to agree with data across the muon p_T spectrum.

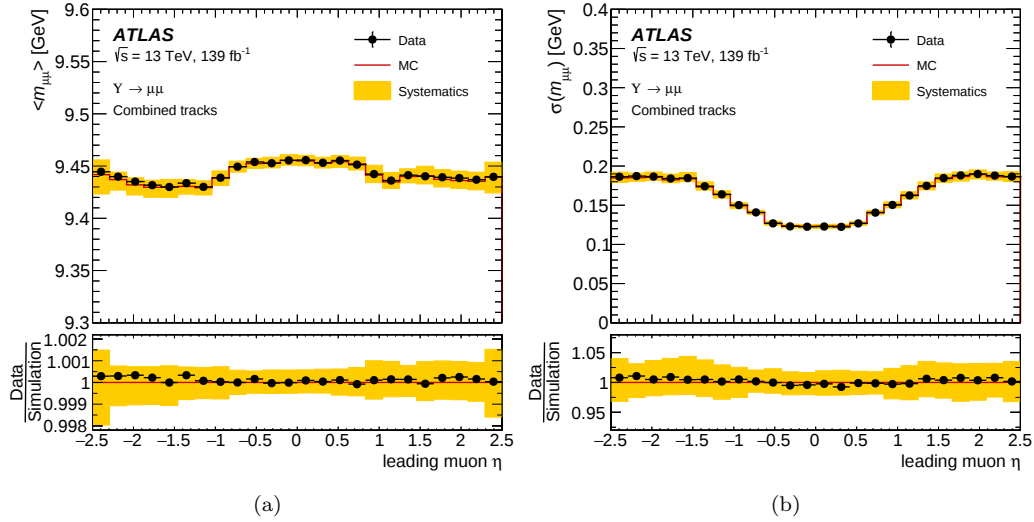


Figure 4.11: Fitted (a) mean mass of the dimuon system and (b) dimuon invariant mass resolution for CB muons measured using $\Upsilon \rightarrow \mu\mu$ events in data and simulation, as a function of the muon η of the highest p_T muon. The upper panels show the results obtained on data and simulation after all corrections. The lower panels show the ratios of the data to the MC simulation. The error bars represent the statistical uncertainty on data. The shaded band represents the systematic uncertainty in the correction and the systematic uncertainty in the extraction method, summed in quadrature.

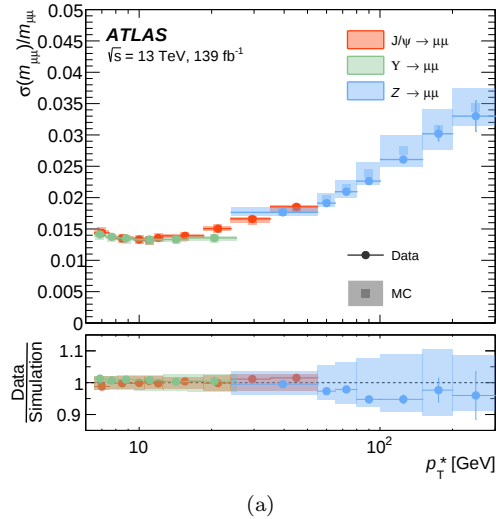


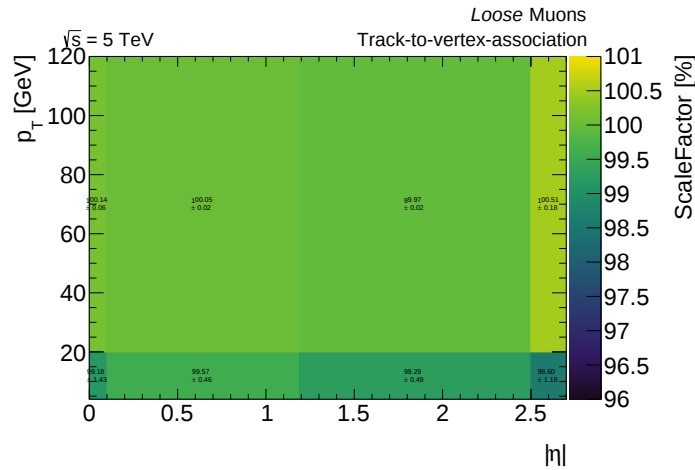
Figure 4.12: The relative dimuon mass resolution measured from $J/\psi \rightarrow \mu^+\mu^-$, $\Upsilon \rightarrow \mu\mu$, and $Z \rightarrow \mu\mu$ data and simulated events, as a function of p_T^* . p_T^* is the p_T of the dimuon system calculated independently of the transverse momenta of the two muons. The lower panel shows the ratio of the data to the MC simulation. The error bars represent the statistical uncertainty while the bands show the systematic uncertainties.

4.3.4 $\sqrt{s} = 5.02$ TeV Corrections

For the muon reconstruction and identification efficiencies, it was observed that the efficiencies measured with high-pileup 13 TeV data showed good agreement with the efficiencies measured at $\sqrt{s} = 5.02$ TeV. An additional extrapolation uncertainty was considered by evaluating the change in scale factors as a function of $\langle\mu\rangle$. The difference in the reconstruction scale factor based on the extrapolation was found to be 0.07% and was used as an additional uncertainty on the high-pileup 13 TeV scale factors [127].

The track to vertex association scale factors and the isolation scale factors were determined in-situ using $\sqrt{s} = 5.02$ TeV data. Figure 4.13 shows the vertex association scale factors measured with 5.02 TeV data, as a function of muon $|\eta|$ and p_T . For muons with p_T greater than 20 GeV, the vertex association scale factors are equal to one [127]. The isolation efficiency for muons was determined using the same method as the electron isolation efficiencies, in the dilepton $\sigma_{t\bar{t}}$ measurement. Figure 4.14 shows the muon isolation efficiencies measured in $\sqrt{s} = 5.02$ TeV data, as a function of the muon p_T , η , and I_{trk} variable. The scale factors at $\sqrt{s} = 5.02$ TeV are measured to be around unity. However, the simulation is shown to predict a higher efficiency than data for muons with $p_T < 50$ GeV.

A dedicated charge dependent sagitta bias correction is derived for the $\sqrt{s} = 5.02$ TeV dataset and used instead of the $\sqrt{s} = 13$ TeV based corrections. Unlike the sagitta bias correction, the muon momentum scale and resolution in data and simulation at $\sqrt{s} = 5.02$ TeV are observed to be well calibrated, even when using the high-pileup 13 TeV calibrations. The residual differences are on a per-mille level and are covered by the existing systematic uncertainties. Thus, the high-pileup muon momentum scale is applied to the low-pileup dataset.



(a)

Figure 4.13: The track to vertex association scale factor determined using $Z \rightarrow \mu\mu$ events at $\sqrt{s} = 5.02$ TeV, as a function of muon $|\eta|$ and p_T .

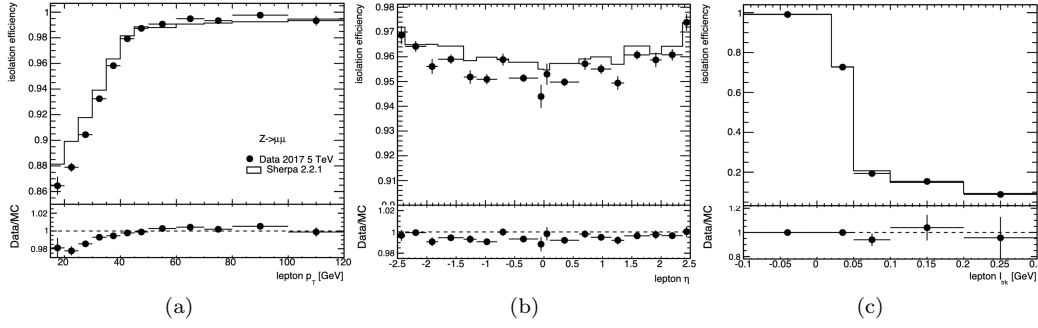


Figure 4.14: Muon isolation efficiency measured in data and MC from tag-and-probe measurements in $Z \rightarrow \mu\mu$ events with the 5.02 TeV dataset. The efficiencies are plotted as a function of (a) lepton p_T , (b) lepton η , and (c) the I_{trk} variable. The error bars represent the total uncertainty on the measurement. The lower panel shows the ratio of the data and the MC simulation (scale factors), along with the uncertainty in the ratio.

4.4 Jet Reconstruction and Calibration

Collimated sprays of hadrons arising from high energy quarks and gluons can be measured by the ATLAS detector. Such sprays are called “jets” and arise due to the colour confinement property of quarks and gluons. Section 4.4.1 describes the jet reconstruction algorithms relevant for the analyses discussed in this thesis whereas Sections 4.4.2 and 4.4.3 describe the standard ATLAS MC based corrections applied to the jets and an in-situ η -intercalibration applied to data. The MC based corrections are used to correct the Jet Energy Scale (JES) for various detector mis-modelling effects whereas the in-situ calibration corrects the JES in data such that it matches the JES observed in MC. Finally, Sections 4.4.4 and 4.4.5 describe the Z +jet balance calibration with $\sqrt{s} = 5.02$ TeV data and the calculation of the Jet Energy Resolution (JER).

4.4.1 Jet Reconstruction

Jets observed by the ATLAS detector are reconstructed by using the anti- k_t algorithm since it is insensitive to soft and collinear gluon emissions [128]. In the anti- k_t algorithm, two measures, d_{ij} and d_{iB}

$$d_{ij} = \min\left(\frac{1}{p_{T,i}^2}, \frac{1}{p_{T,j}^2}\right) \cdot \frac{\Delta R_{ij}}{R} \quad (4.11)$$

$$d_{iB} = \frac{1}{p_{T,i}^2}$$

are used to determine whether the four vector representing particles or pseudo-jets should be clustered or not. The measures depend on $p_{T,i}$, the transverse momenta of the object i , ΔR_{ij} which is the ΔR between objects i and j , and a radius term R that defines the size of the jet. In the anti- k_t algorithm, d_{ij} and d_{iB} are first calculated for all objects in an event, objects with the lowest d_{ij}

are then combined, and object i defined as a jet if d_{iB} is the smallest measure. This algorithm is iterated for all particles in an event. Figure 4.15 shows how the anti- k_t algorithm results in conical distributions in $\eta - \phi$ space of the collection of constituents [128]. Note that the definitions of d_{ij} and d_{iB} ensure that the measures are insensitive to low p_T and collinear emissions of gluons. The anti- k_t algorithm used in ATLAS is implemented in the FASTJET package [129, 130] and uses sets of four vector information measured from the detector as inputs.

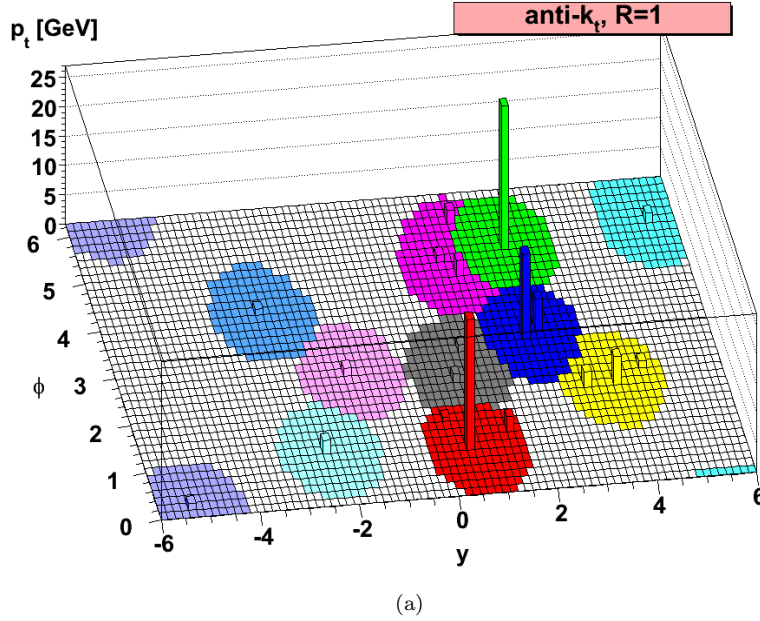


Figure 4.15: A sample parton level event generated with HERWIG [131], together with additional soft p_T “ghosts”, clustered according to the anti- k_t algorithm.

Jets used by the analyses discussed in this thesis are defined using “particle flow” objects. Particle flow jets utilize both calorimeter and track based information, and can thus take advantage of the improved p_T resolution of the ID in the low p_T regime, and the high energy resolution of the calorimeter at higher energies [132]. The first step towards defining a particle flow jet is reconstructing clusters of calorimeter cells using the nearest neighbour algorithm [115]. Jets defined using such clusters are called “EMTopo” jets.

Charged object tracks are then matched with calorimeter clusters using the “ghost matching” algorithm [133]. This algorithm considers tracks as calorimeter inputs with infinitesimally small p_T , before applying the anti- k_t algorithm. Tracks then reconstructed within a certain radius of an anti- k_t jet are considered to be ghost matched. The energy contributions of the ghost matched tracks is then subtracted from the matched calorimeter clusters and additional corrections to the track p_T and calorimeter energy are applied. The p_T of the matched track is then used as a substitute for the charged particle energy, and given as an input to the anti- k_t algorithm alongside the subtracted calorimeter clusters. Particle flow jets discussed in this thesis are constructed using the $R = 0.4$ radius parameter. Details on the particle flow algorithm can be found in Ref. [132, 134].

4.4.2 MC Based Jet Energy Scale Corrections

The JES is a correction factor that is applied and corrects the energy of jets measured by the detector, and brings them to the jet energy at truth level (i.e. the state before any interaction with the detector). This correction is used to account for detector effects and bring the measured jet energy closer to the true jet energy. First, a correction that removes excess energy associated with pileup collisions is applied. This is followed up by the “absolute JES” calibration which corrects the detector level jet energy and direction such that it matches the values seen at the truth level in MC dijet events. A “global sequential calibration” (GSC) is then used to reduce the effects from jet flavour dependence and improve the jet resolution without changing the average jet energy response. The GSC is also derived using dijet MC events. The samples used to determine the MC based corrections, and the various systematic uncertainties considered in the corrections, are described in Ref. [134]. Further details on the three corrections are described in Appendix B.4.

All three corrections are applied to both data and MC before a final in-situ calibration is used to account for any residual differences in the JES determined in MC events and data. The in-situ calibration is determined in well-defined physics processes, and used to correct for any residual differences between data and simulation. This in-situ correction is only applied to data. There are four steps to the in-situ calibration performed at $\sqrt{s} = 13$ TeV: a η -intercalibration, a Z +jet balance calibration, a γ +jet balance calibration, and a multijet balance calibration. For the analyses performed at $\sqrt{s} = 5.02$ TeV, only a dedicated Z +jet balance is applied, in conjunction with a η -intercalibration that is based on $\sqrt{s} = 13$ TeV data. Thus, this section will not discuss the γ +jet balance or the multijet balance techniques that were performed for $\sqrt{s} = 13$ TeV analyses (further details on these can be found in Ref. [134]).

4.4.3 η -intercalibration

The η -intercalibration is used to match the energy scales of jets with $|\eta_{\text{det}}| > 0.8$ to the energy scale of jets with $|\eta_{\text{det}}| < 0.8$. This is done by selecting dijet events back-to-back in ϕ , that have two jets in different η bins, denoted as i and j . The momentum balance between the two jets can then be probed with the asymmetry $\mathcal{A}$

$$\mathcal{A} = \frac{p_{\text{T}}^i - p_{\text{T}}^j}{p_{\text{T}}^{\text{avg}}} \quad (4.12)$$

Here, p_{T}^i and p_{T}^j are the transverse momenta of the jet in η bin i and j , while $p_{\text{T}}^{\text{avg}}$ is the average p_{T} of the two jets. The response is expressed as a function of the asymmetry and a 3-dimensional fit is performed to extract the correction factors. The three dimensions are defined as the two η bins and a bin of $p_{\text{T}}^{\text{avg}}$. Figure 4.16 compares the jet response in data and MC, as a function of jet p_{T} (for a given range of jet η_{det}) and η_{det} (for a given range of jet p_{T}). The response in data is observed to be larger than MC across jet p_{T} and η_{det} . A fractional uncertainty of $\sim 1\% - 2\%$ is observed in the $|\eta_{\text{det}}| > 0.8$ region [134].

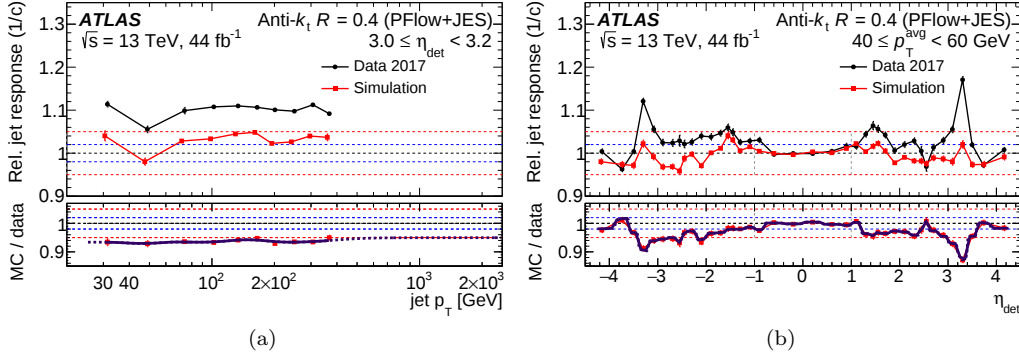


Figure 4.16: The relative jet response measured for $R = 0.4$ particle flow jets in data (black dots) and simulation (red squares), as a function of (a) jet p_T and (b) η_{det} . For (a), the jet is required to have $3.0 < \eta_{\text{det}} < 3.2$ whereas in (b), the average jet p_T must be between 40 GeV and 60 GeV. The lower panel shows the response ratio of simulation to data (red squares) as well as the smoothed in situ calibration factor derived from the ratio (solid curve) which is used to perform the η -intercalibration. Dotted lines show the extrapolation of the in situ calibration to the regions without data points. The dashed red and blue horizontal lines provide reference points for the reader.

4.4.4 $\sqrt{s} = 5.02$ TeV Z +jet Balance

In the $\sqrt{s} = 5.02$ TeV analyses, the Z +jet balance is calculated and applied to the $\sqrt{s} = 5.02$ TeV data, while the MC jets are corrected using $\sqrt{s} = 13$ TeV calibrations discussed above. Such a method accounts for any residual effects from translating the high-pileup calibrations to the low-pileup environment. Using only the Z +jet balance lead to larger uncertainties, but was preferred over the full calibration due to the other corrections being independent of $\sqrt{s}$ ⁹, time constraints, and the low impact of JES uncertainties on the $\sqrt{s} = 5.02$ TeV measurements discussed in this thesis.

The Z -jet balance calibration used $\sqrt{s} = 5.02$ TeV data, $Z \rightarrow ee$, and $Z \rightarrow \mu\mu$ MC events, as described in Section 6.2. The two leptons were required to be a same-flavour opposite-sign lepton pair (e^+e^- or $\mu^+\mu^-$), with $p_T > 20$ GeV, and one lepton must pass a single lepton trigger. The leptons were also required to pass the identification and isolation requirements described in Section 6.3. Selected events must have at least one reconstructed jet (described in Section 6.3) with a p_T greater than 10 GeV and $|\Delta\phi(Z, \text{jet})| > 2.8$ rad. For the $\sigma_{t\bar{t}}$ measurement, only “central jets” (jets with $|\eta| < 2.5$) were considered whereas the t -channel measurement also included “forward jets” (jets with $2.5 < |\eta| < 4.0$) in the calibration. This section will present results from the calibration with forward jets, since they are more recent and approximately a superset of the calibration with only central jets.

To ensure that the dilepton pair most likely comes from a Z boson decay, the dilepton invariant mass ($m_{\ell\ell}$) must fall within the Z -mass window of 81 GeV to 101 GeV. The reference p_T , p_T^{ref} was then defined as the projection of the Z boson transverse momentum along the jet axis: $p_T^{\text{ref}} = p_T^Z \times |\cos \Delta\phi(Z, \text{jet})|$. If a second jet exists in this selection, it is required to have a p_T less than

⁹The pileup dependence was studied in the low-pileup $\sqrt{s} = 5.02$ TeV sample and found to be inconsequential to the jet energy scale.

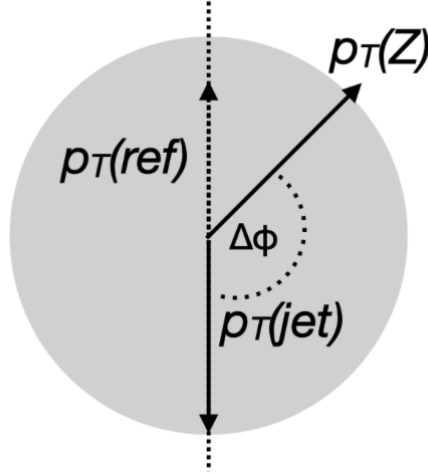


Figure 4.17: A cartoon showing the Z +jet system, the transverse momenta of the Z boson and jet, and p_T^{ref} . The angle $\Delta\phi$ is defined as the azimuthal angle between the momentum direction of the Z boson and the recoiling jet.

Table 4.1: Number of events passing the various selection requirements for the Z +jet balance study in data, nominal SHERPA MC, and the alternate POWHEG+PYTHIA 8 samples. The preselection includes the single lepton trigger, lepton reconstruction, identification, isolation, and p_T cuts.

Cutflow	Data	Nominal simulation	Alternate simulation
Preselection	69703	73693	65561
Z -mass cut	59563	63893	58338
Single jet requirement	33450	33599	36672
Back-to-back topology cut	16208	15708	19979

$\max(10 \text{ GeV}, 0.1 p_T^{\text{ref}})$. Figure 4.17 shows a cartoon of the Z +jet balance system.

The selection described above is applied to data, the nominal $Z \rightarrow ee$ and $Z \rightarrow \mu\mu$ MC samples, and alternative samples. The alternate samples were simulated using the POWHEG v2 [64–67, 135] generator with the CT10 NLO [136] PDF set and employing PYTHIA 8.186 [137] with the AZNLO tune [138] and CTEQ6L1 PDF set at NLO [58], for the parton shower and hadronization model. Table 4.1 presents the yields of events passing the various selection requirements for the aforementioned samples.

The response (r) is determined per-event as the ratio $r = p_T^{\text{jet}} / p_T^{\text{ref}}$. It is then used to calibrate the jets by evaluating the mean value of r , $\langle r \rangle$ in bins of jet p_T and $|\eta|$. Ideally, $\langle r \rangle = 1$ for perfectly calibrated jets but effects such as out-of-cone radiation and the jet p_T^{ref} threshold can bias $\langle r \rangle$ in both data and simulation. The in-situ correction used to correct the JES in data is then derived by evaluating the ratio

$$\mathcal{C}_{\text{in-situ}}^{ij} = \frac{\langle r \rangle_{\text{simulation}}^{ij}}{\langle r \rangle_{\text{data}}^{ij}}$$

Here, $\mathcal{C}_{\text{in-situ}}^{ij}$ is the correction factor that must be applied to data for a given bin i in jet p_T and j in

jet $|\eta|$. The numerator and denominator in the right-hand side are the average response measured in simulation and data, for a given bin i and j .

Due to lower statistics in the forward region, the correction is split into five bins of p_T for central jets and three bins for forward jets. Five bins in jet $|\eta|$ are used across the p_T spectra. Figure 4.18 shows the correction factors when comparing data to the nominal Sherpa sample and the alternate sample. Both the correction and the statistical uncertainty on the correction are observed to be larger in forward jets due to low statistics for forward jets. Figure 4.19 shows the nominal correction factor as a function of p_T for various $|\eta|$ cuts, after a smoothing algorithm was applied [139]. The effects of the in-situ correction are propagated to the E_T^{miss} calculation discussed in Section 4.5.

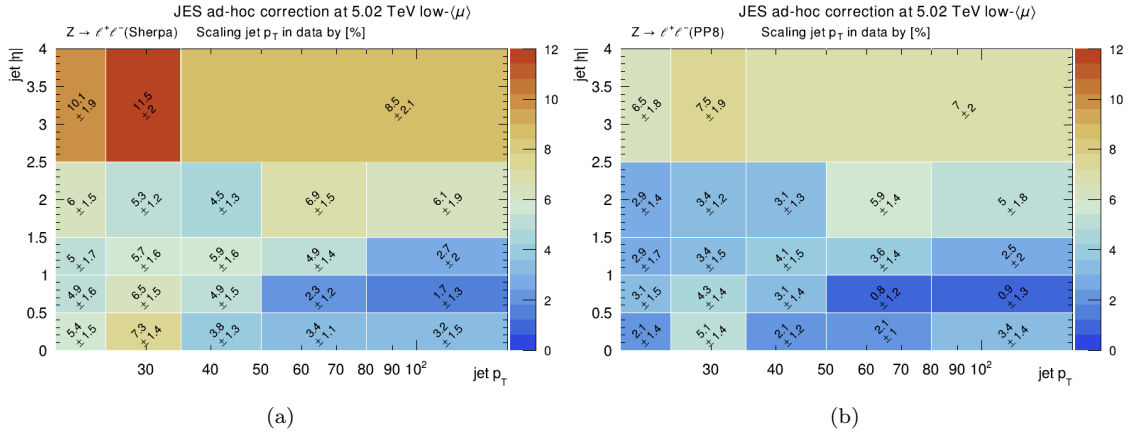


Figure 4.18: The $C_{\text{in-situ}}^{ij}$ correction factors derived by comparing $\sqrt{s} = 5.02$ TeV data to (a) the nominal SHERPA MC and (b) the alternate POWHEG+PYTHIA 8 MC samples. The corrections are shown in bins of jet p_T and $|\eta|$. The errors on the correction include the statistical uncertainty of the data and MC simulated events.

The uncertainty in the correction is decorrelated into a statistical component and a modelling component. MC templates for both components are evaluated by scaling the p_T in the MC and propagating the effects to the missing energy. A template representing the statistical uncertainty is derived by scaling the MC p_T down by the statistical uncertainty from the nominal correction (shown in Figure 4.18). Practically this means that, for a jet falling in the bottom left bin (i.e. jet $p_T = 15$ GeV and $|\eta| = 0.1$), the jet p_T is scaled by 0.985. Correspondingly, the modelling uncertainty is derived by applying the signed difference between the nominal correction and the alternate correction.

In the $\sigma_{t\bar{t}}$ measurement, it was decided to treat the statistical and modelling uncertainties as a single uncertainty, by summing in quadrature the two sources of uncertainty. This led to an overestimate of the uncertainty on the in-situ correction since it double counted the data statistical uncertainty. Thus, the new treatment discussed above was used for the $\sigma(tq + \bar{t}q)$ analysis.

The effect of the SHERPA based correction can be seen by comparing the MC agreement between corrected data and uncorrected data. The normalization and shape effects of the correction are seen

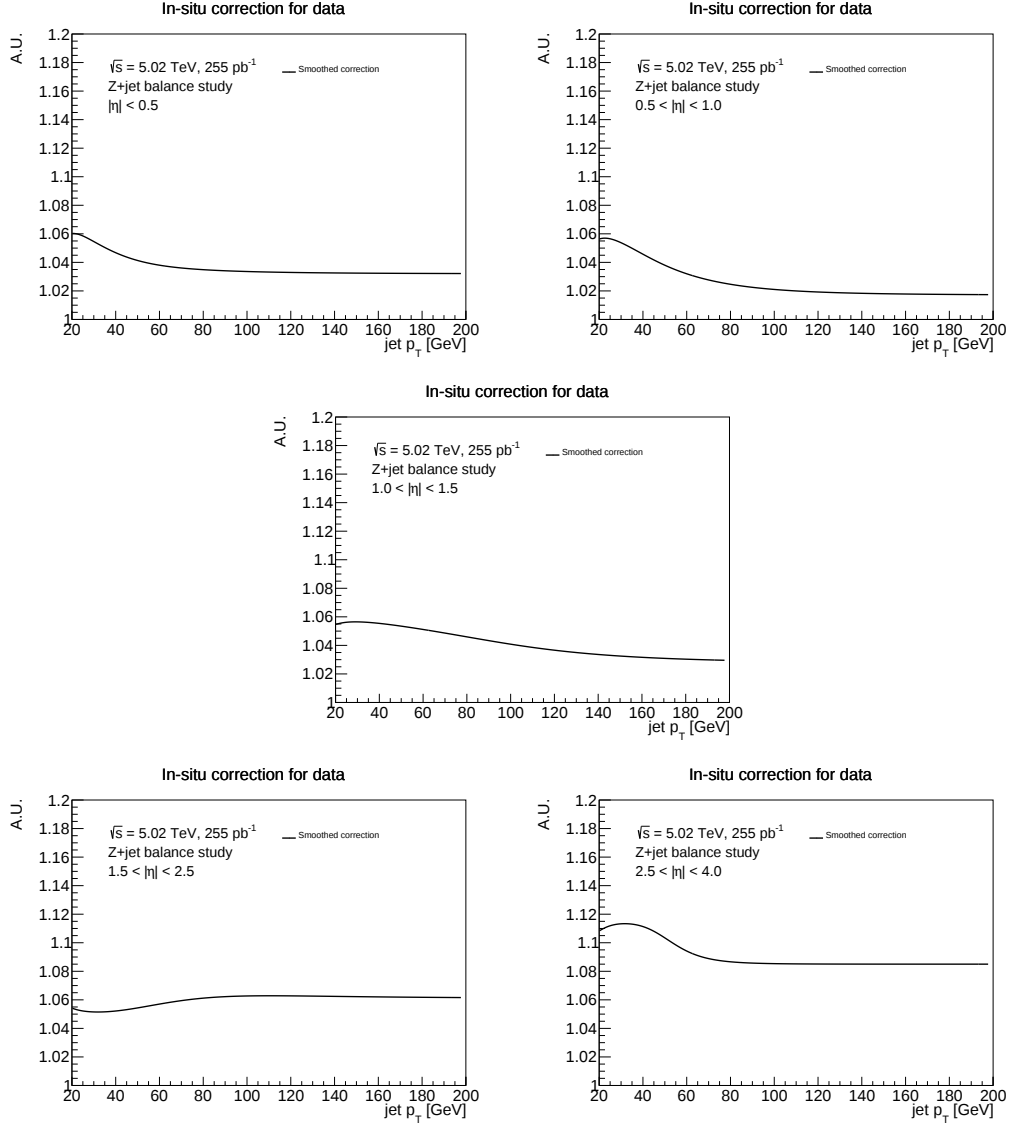


Figure 4.19: The smoothed correction factors that are based on the nominal SHERPA MC samples. The factors are presented as a function of jet p_T for various jet $|\eta|$ values.

in the distribution of $\langle r \rangle$ as a function of p_T^{ref} and the inclusive distribution of the ratio of jet p_T to p_T^{ref} , as seen in Figure 4.20. There is poor normalization and shape agreement pre-correction and excellent agreement post-correction.

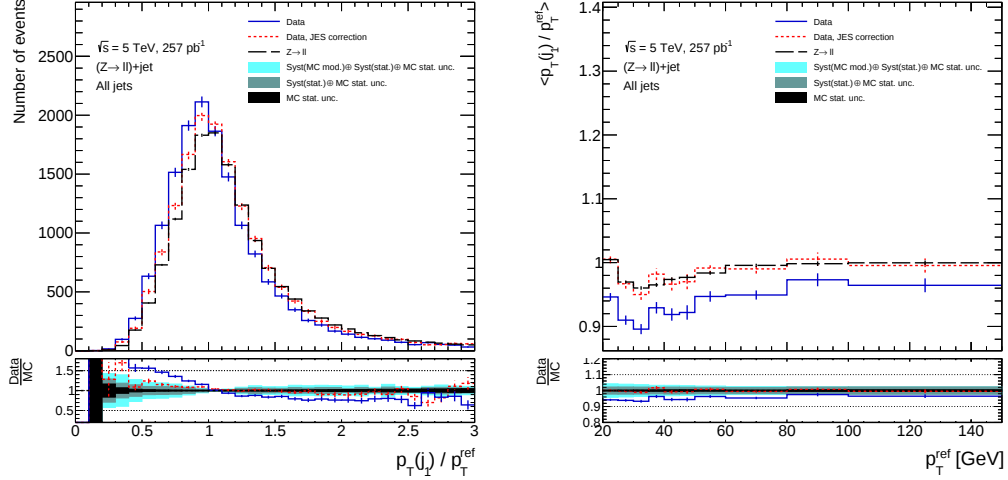


Figure 4.20: The (a) Z-jet balance ($\langle R \rangle$) distribution and (b) $\langle R \rangle$ as a function of p_T^{ref} , for central and forward jets. The unmodified and modified data (based on the SHERPA correction) are shown by solid blue line and dashed red line, respectively. The black, dark cyan, and light cyan bands represent the statistical uncertainty in the MC prediction, the statistical uncertainty from the in-situ correction summed in quadrature with the statistical uncertainty in the MC prediction, and the modelling uncertainty from the in-situ correction summed in quadrature with all other uncertainties, respectively.

4.4.5 Measurement of the Jet Energy Resolution

The relative JER from detector effects is determined by measuring the asymmetry between dijet events, with one jet acting as the probe jet and the other a reference jet. The reference jet is required to fall in the well calibrated detector region of $0.2 < |\eta_{\text{det}}^{\text{ref}}| < 0.8$ whereas the probe jet can have $|\eta_{\text{det}}^{\text{ref}}| < 4.5$. In a given bin of p_T^{avg} and $\eta_{\text{det}}^{\text{probe}}$, the uncertainty on the asymmetry can be expressed using Equation 4.13. Further details on the JER measurement are described in Appendix B.5

$$\sigma_{\mathcal{A}} = \left(\frac{\sigma_{p_T}}{p_T} \right)^{\text{probe}} \oplus \left(\frac{\sigma_{p_T}}{p_T} \right)^{\text{ref}} \quad (4.13)$$

The relative resolution of the probe jet can then be measured by subtracting the relative resolution of the reference jet from the uncertainty found in the asymmetry. Note that $\sigma_{\mathcal{A}}$ can be further broken into two components that are summed in quadrature, one representing the truth jet resolution and the other representing the detector level resolution. Since we are interested in the detector resolution, we can extract it by deconvoluting the truth level effects.

First, the truth level asymmetry ($\mathcal{A}^{\text{truth}}$) and detector level asymmetry distributions are measured

and fit to ad-hoc functions in simulation and data, respectively. The detector level asymmetry distribution can then be parametrized as a convolution of: $\sigma_{\mathcal{A}}^{\text{truth}} \otimes \mathcal{G}(\mu, \sigma_{\mathcal{A}}^{\text{det}})$. Here, $\mathcal{G}(\mu, \sigma_{\mathcal{A}}^{\text{det}})$ is a Gaussian distribution with a mean and standard deviation μ and $\sigma_{\mathcal{A}}^{\text{det}}$, respectively. An iterative fit is then used to extract $\sigma_{\mathcal{A}}^{\text{det}}$ and thus the relative jet energy resolution. Details on the fitting procedure and sources of uncertainties are further discussed in Ref. [134]. Figure 4.21 shows the relative jet energy resolution measured in data and simulation, and the absolute uncertainty on the relative JER, as a function of jet p_T . The relative JER is found to be underestimated by MC for jets in the $0.2 < |\eta_{\text{det}}^{\text{ref}}| < 0.7$ region with $p_T > 90$ GeV. The uncertainties on the JER are typically a few percent.

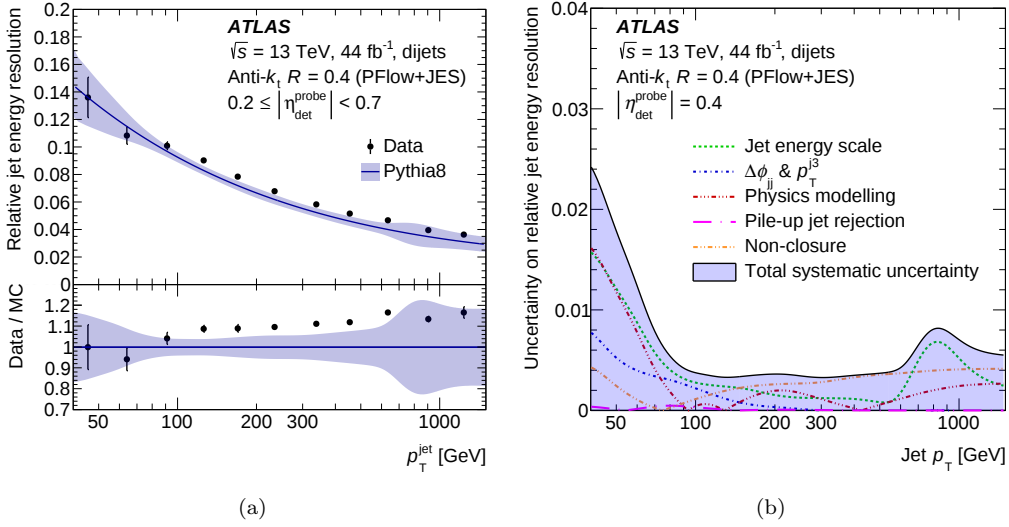


Figure 4.21: The (a) relative jet energy resolution and (b) absolute uncertainty in the relative resolution as a function of p_T , for particle flow jets with $0.2 < \eta_{\text{det}} < 0.7$. The resolution in data is shown using black dots, with the error bars indicating the statistical uncertainty on the data. The detector level resolution measured in simulation is shown by the solid black curve, with the blue band representing the total systematic uncertainty. The systematic uncertainty is dominated by terms propagated from the JES uncertainty, while additional terms arise from the analysis selection, pile-up rejection (JVT), physics modelling (comparison with alternative generator), and non-closure effects.

The relative JER can be parametrized using Equation 4.14, where the first term N represents contributions from pileup and electronic noise, S represents statistical fluctuations in the deposited energy, and C represents uncertainties in the calorimeter response and from energy deposits in passive material [134].

$$\frac{\sigma(p_T)}{p_T} = \frac{N}{p_T} \oplus \frac{S}{\sqrt{p_T}} \oplus C \quad (4.14)$$

The noise contribution from pileup can be extracted from data by measuring the p_T difference between random cones of jets that pass a set of unbiased triggers [134]. The electronic noise term is measured by comparing the JER measured in simulation with pileup, and the JER where the simulation does not consider pileup.

The final JER measurement is extracted by performing a χ^2 fit between the two measurements discussed above. Details on the combination procedure and the treatment of systematic uncertainties in the combination can be found in Ref. [134]. Figure 4.22 compares the final relative JER curve and its absolute uncertainty, for particle flow and EMTopo $R = 0.4$ jets, as a function of jet p_T . Particle flow jets provide a $\sim 25\%$ smaller relative resolution for low p_T jets. However, particle flow jets with a $p_T > 100$ GeV have a larger relative resolution than EMTopo jets. The absolute uncertainty across the p_T spectrum in particle flow jets is measured to be lower or approximately equal to EMTopo jets.

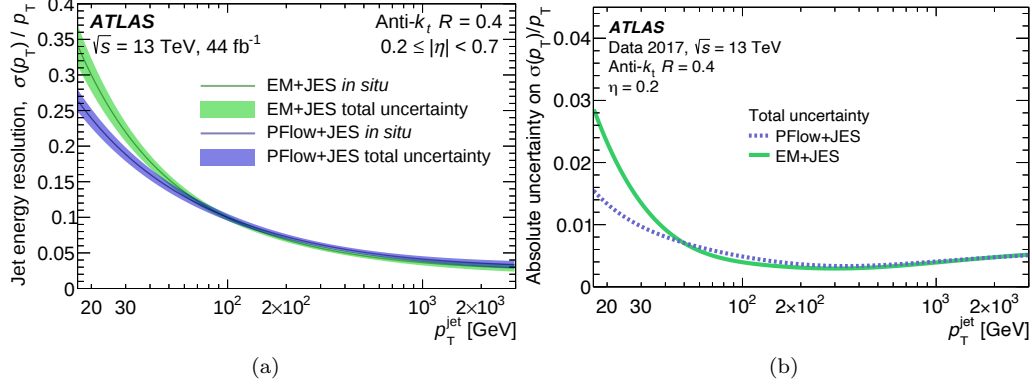


Figure 4.22: The (a) relative jet energy resolution and (b) absolute uncertainty on the relative jet energy resolution, for fully calibrated particle flow (green curve) and EMTopo (blue curve) jets, as a function of jet p_T . The blue and green bands in (a) represent the total uncertainty on the measured relative jet energy resolution. For both plots, only jets with $0.2 < |\eta| < 0.7$ are considered.

4.5 Missing Transverse Energy Reconstruction and Calibration

The missing transverse energy is a variable that allows one to determine the presence of a neutrino in collider experiments. Since the transverse momenta of all particles should sum to 0, conservation of momentum dictates that the sum of the transverse momentum for all final state objects observed by the detector, should also equal 0 as well. Small deviations from zero can arise from inefficient object reconstruction due to detector resolution effects. Large deviations on the other hand are associated with the presence of objects that cannot be detected - such as neutrinos¹⁰. Section 4.5.1 discusses the reconstruction algorithm for E_T^{miss} . Section 4.5.2 presents the E_T^{miss} calibration using $\sqrt{s} = 13$ TeV data. The $\sqrt{s} = 5.02$ TeV analyses discussed in this thesis used the E_T^{miss} uncertainties based on $\sqrt{s} = 13$ TeV data, since no significant deviation was observed when using calibrations based on $\sqrt{s} = 13$ TeV data.

¹⁰In such a case, the missing transverse momentum is equal to the missing transverse energy since neutrinos are effectively massless at the LHC scale. Thus, missing transverse energy and missing transverse momentum are used interchangeably when discussing LHC physics.

4.5.1 E_T^{miss} Reconstruction

The x and y components of the missing transverse energy are first determined by applying the conservation of momentum on both axes independently. This can be written as

$$E_i^{\text{miss}} = - \sum_h p_{ih} - \sum_s p_{is} \quad (4.15)$$

Here, the index i runs over the two axes, p_{ih} is the momentum in axis i for a “hard object” h , and p_{is} is the momentum in axis i for a “soft object” s . Hard objects refer to the selected: electrons, muons, photons, τ leptons, and jets and Soft objects refer to the set of tracks that are not associated with any of the hard objects. The first and second terms are referred to as the “hard term” and “soft term”, respectively. The selection requirements for the hard term are based on standard ATLAS definitions while removing overlapping contributions. Details on the selection for the **Tight** E_T^{miss} working point (used in the $\sqrt{s} = 5.02$ TeV analyses) are presented in Ref. [140].

From Equation 4.15, it is possible to compute E_T^{miss} and the angle of the E_T^{miss} vector ϕ^{miss} by: summing E_x^{miss} and E_y^{miss} in quadrature, and taking the arctan of the ratio $\frac{E_y^{\text{miss}}}{E_x^{\text{miss}}}$, respectively.

4.5.2 E_T^{miss} Uncertainties

Uncertainties in the E_T^{miss} response and resolution are approximately $\sqrt{E_T^{\text{miss}}}$ and determined by examining the balance between the soft term and hard term in events with no expected neutrinos (i.e. $Z \rightarrow \mu\mu$ decays). With a perfect detector, such events should give a soft term that is equal yet opposite (in the transverse plane) to the hard term since there is no neutrino. The parallel and perpendicular projections ($\mathcal{P}_{\parallel}$ and $\mathcal{P}_{\perp}$, respectively) of the soft term on the hard term are then used to determine the uncertainty on the E_T^{miss} scale and resolution.

The average value of $\mathcal{P}_{\parallel}$, the root mean square deviation of $\mathcal{P}_{\parallel}$, and the root mean square deviation of $\mathcal{P}_{\perp}$ are defined as the “parallel scale”, “parallel resolution”, and “transverse resolution”, respectively. The three quantities are plotted as functions of the hard term’s transverse momentum p_T^{hard} . The predicted distributions from various MC generators are then compared with data collected in Run 2, and the largest deviations between data and simulation are used to define a systematic uncertainty for each variable. The transverse resolution is not considered since it is consistent with 0 in both data and simulation [140, 141]

Figure 4.23 compares the parallel scale, parallel resolution, and transverse resolution distributions in data and MC, using particle flow jets and the **Loose** E_T^{miss} definition, as a function of p_T^{hard} . Both the scale and resolutions observed in simulation are found to underpredict the results seen in data. The two resolution uncertainties are determined to be ~ 2 GeV for a p_T^{hard} between 0 GeV and 40 GeV. In the same p_T^{hard} range, the scale uncertainty increases from ~ 0.2 GeV to ~ 1 GeV [140].

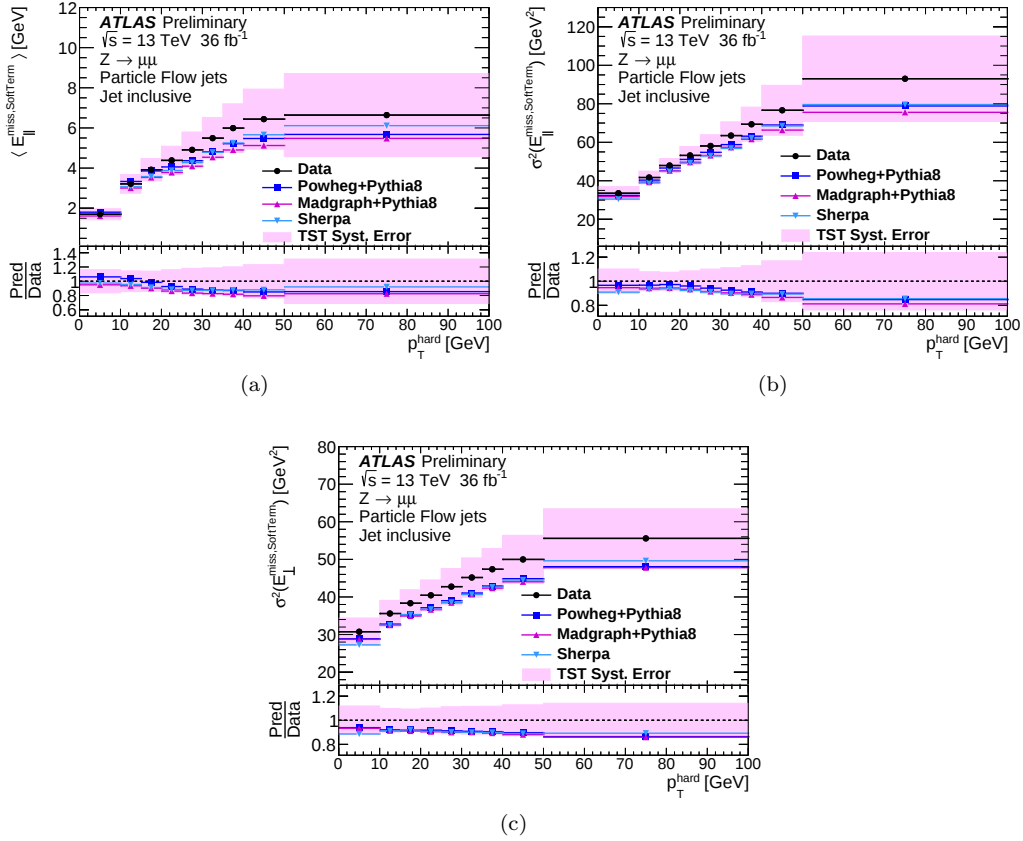


Figure 4.23: The (a) parallel scale, (b) parallel resolution, and (c) transverse resolution distributions for data (dots) in $Z \rightarrow \mu\mu$ events, as a function of p_T^{hard} . Various MC simulations are represented by dots of different colours. The error bars on the dots represent the statistical uncertainty on the data or the statistical uncertainty on prediction. The pink band corresponds to the systematic uncertainties applied to the simulation. The lower panels show the ratio of the data and predicted distributions, along with the uncertainty in the ratio.

Chapter 5

Flavour Tagging

Due to the existence of a b -quark in virtually all top quark decays, an algorithm to select for jets arising from b -quark decays (b -jets) is used to select for top quarks. Section 5.1 discusses the b -jet identification (also denoted as “ b -tagging”) algorithms in ATLAS whereas Section 5.2 presents the efficiency measurements and scale factor measurements for b -tagging.

5.1 b -jet Identification and Tagging

Jets that contain b -hadron decays can be identified by examining the jets for the features unique to the decay of b -hadrons. Typically, b -hadrons have a lifetime of $\mathcal{O}(1\text{ ps})$ which means that a b -hadron travelling near the speed of light will move $\sim 300\text{ }\mu\text{m}$. Thus, b -hadrons arising from the hard scatter will be displaced from the primary vertex by a few hundred microns or more. Tracks associated with the b -hadron decay will result in a “secondary vertex” that can be identified using the charged tracks from the decay. High level algorithms used for b -jet tagging include the: IP2D, IP3D [142], a track based recurrent neural network (RNNIP) [143], the SV1 [144], and JetFitter [145] secondary vertex tagging algorithms.

The IP2D algorithm is constructed using probability distributions of the transverse impact parameter significance $d_0/\sigma(d_0)$, as seen in simulated b -jets, charm quark associated jets (c -jets), and light quark associated jets (light-jets). Similar to the electron identification discussed in Section 4.2.1, the likelihood ratio of the IP2D distributions for the various flavour hypothesis is constructed and then used to determine the flavour of a given jet. The IP3D variable is an extension of the IP2D algorithm, that also takes into account the longitudinal impact parameter significance $z_0/\sigma(z_0)$, in the likelihood ratios. The RNNIP neural network is trained to discriminate between jets arising from a b -quark, c -quark, or light quark decay. It takes as an input the parameters of all tracks in a jet, the transverse and longitudinal significance of the track, the fractional jet p_T carried by a track, the

ΔR between the track and jet, and the number of hits in the ID.

The **SV1** algorithm looks for the existence of a displaced secondary vertex in a jet. First, two track vertices are identified from all the tracks associated in a jet, an iterative χ^2 fit is performed in order to match tracks to a single secondary vertex, and tracks are removed from the fit until quality control criteria are satisfied [144]. The **JetFitter** algorithm attempts to find a secondary vertex by reconstructing the full b - and c -hadron decay chains. In both cases, low level variables of the secondary vertex can be used to identify b -jets.

The analyses discussed in this thesis use the **DL1r** feed-forward neural network [146] to identify b -jets. Similar to **RNNIP**, **DL1r** is trained to output variables that discriminate based on the jet flavour, and takes as input: kinematic variables, **IP2D** and **IP3D** likelihood ratios, **RNNIP** probabilities, and secondary vertex kinematic variables from both the **SV1** and **JetFitter** algorithms. A full list of input variables and training parameters can be found in Ref. [146]. A discriminant used to identify b -jets (D_b) is then constructed from the **DL1r** probabilities, as shown in Equation 5.1. Similar discriminants can be constructed to select for c -jets or light flavoured jets.

$$D_b = \ln \left(\frac{p_b}{f_c p_c + (1 - f_c) p_{\text{light}}} \right) \quad (5.1)$$

Here, p_b , p_c , and p_{light} represent the output score of the **DL1r** algorithm for a jet while assuming a b -jet, c -jet, and light-jet hypothesis, and f_c is the fraction of c -jets in the background. f_c can be modified for each individual analysis and is considered to be 0.018 for both analyses discussed in this thesis. Figure 5.1 shows the p_b distribution from the **DL1r** algorithm as well as the D_b distribution for b -jets, c -jets, and light flavoured jets seen in $t\bar{t}$ MC. Various working points are defined by determining the cut on D_b where a select fraction of b -jets, as seen in $t\bar{t}$ MC are kept. Figure 5.2 shows the b -jet identification efficiency versus the c -jet, and light-jet rejection¹. For a b -tagging efficiency of 60% (70%), the c -jet rejection is ~ 30 (~ 10), and light-jet rejection is $\sim 2000\%$ (~ 417).

5.2 Efficiency and Scale Factor Measurements

Similar to the lepton selection, efficiencies and scale factors from b -tagging must be measured when using a b -tagging algorithm in an analysis. The b -tagging scale factor correction to an MC event is the product of multiplicative scale factors of all jets in an event, that depend on the flavour and kinematics of a jet, and whether it passes the b -tagging algorithm. The scale factors are determined by measuring the b -tagging efficiency [147], c -jet misidentification efficiency [148, 149] in $t\bar{t}$ decays, and light-jet misidentification efficiency [150, 151] in Z +jets decays.

Figure 5.3 shows the b -jet identification, and the c - and light-jet misidentification scale factors for the 70% **DL1r** working point in particle flow jets, as functions of jet p_T . The b -jet tagging scale factor is 0.95 for jets with p_T of 20 GeV and has an uncertainty of $\sim 6\%$. At ~ 150 GeV, the scale

¹The rejection is defined as the inverse of the efficiency of tagging c -jets or light-jets as b -tagged jets.

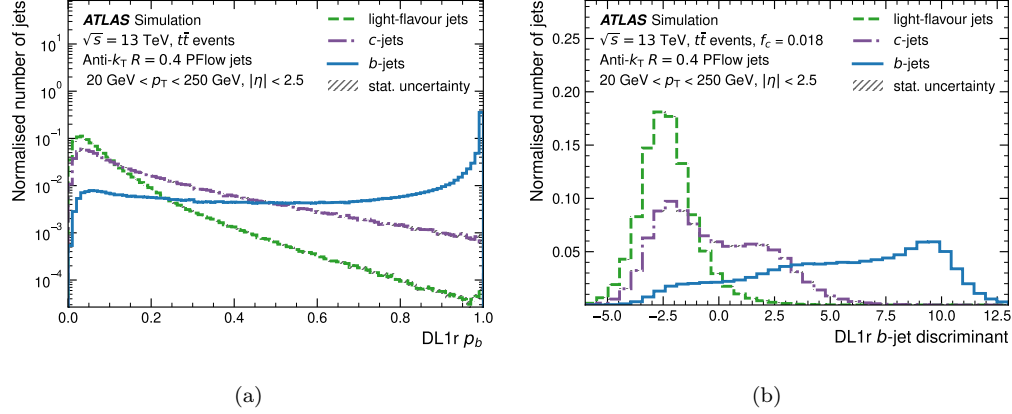


Figure 5.1: Distributions of the (a) p_b output from the DL1r algorithm and (b) D_b discriminant constructed from the three DL1r output score while assuming $f_c = 0.018$. The green, purple, and blue curves are all normalized to unity and represent the distributions for light flavour jets, c -jets, and b -jets, respectively. All distributions are determined using $t\bar{t}$ MC, with $R = 0.4$ particle flow jets with $20 \text{ GeV} < p_T < 250 \text{ GeV}$, and $|\eta| < 2.5$. The hashed band represents the statistical uncertainty on the MC.

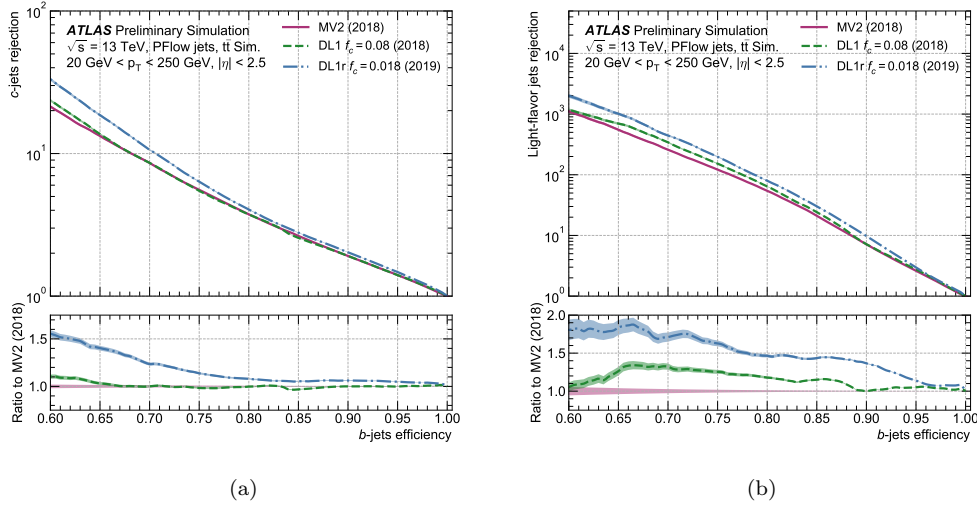


Figure 5.2: Distributions of the (a) c -jet rejection and (b) light-jet rejection as a function of the b -jet tagging efficiency using the MV2 (solid red curve), DL1 (dashed green curve), and DL1r (dashed blue curve) algorithms. The DL1 and DL1r algorithms use an f_c of 0.08 and 0.018, respectively. The performance is determined using a simulated $t\bar{t}$ with $R = 0.4$ particle flow jets with $|\eta| < 2.5$ and p_T between 20 GeV and 250 GeV. The shaded bands represent the statistical uncertainty. The lower panels show the ratio of the rejection of various algorithms to the rejection observed using the MV2 algorithm.

factor trends towards unity and the uncertainties decrease to a few percent whereas for p_T near 400 GeV, the scale factor is smaller than unity and the uncertainties increase again. The c -jet and light-jet mistagging efficiencies have much larger uncertainties of $\mathcal{O}(10\%)$ and vary as a function of p_T . Sources of systematic uncertainties in the scale factors include: the statistical uncertainties in data and MC, jet energy scale and resolution uncertainties, signal-modelling uncertainties, and background-modelling uncertainties. To reduce complexity in analyses, a principal component analysis is used to keep only the largest sources of uncertainties, and additional extrapolation uncertainties are considered since the efficiencies are not measured for jets with $p_T > 400$ GeV.

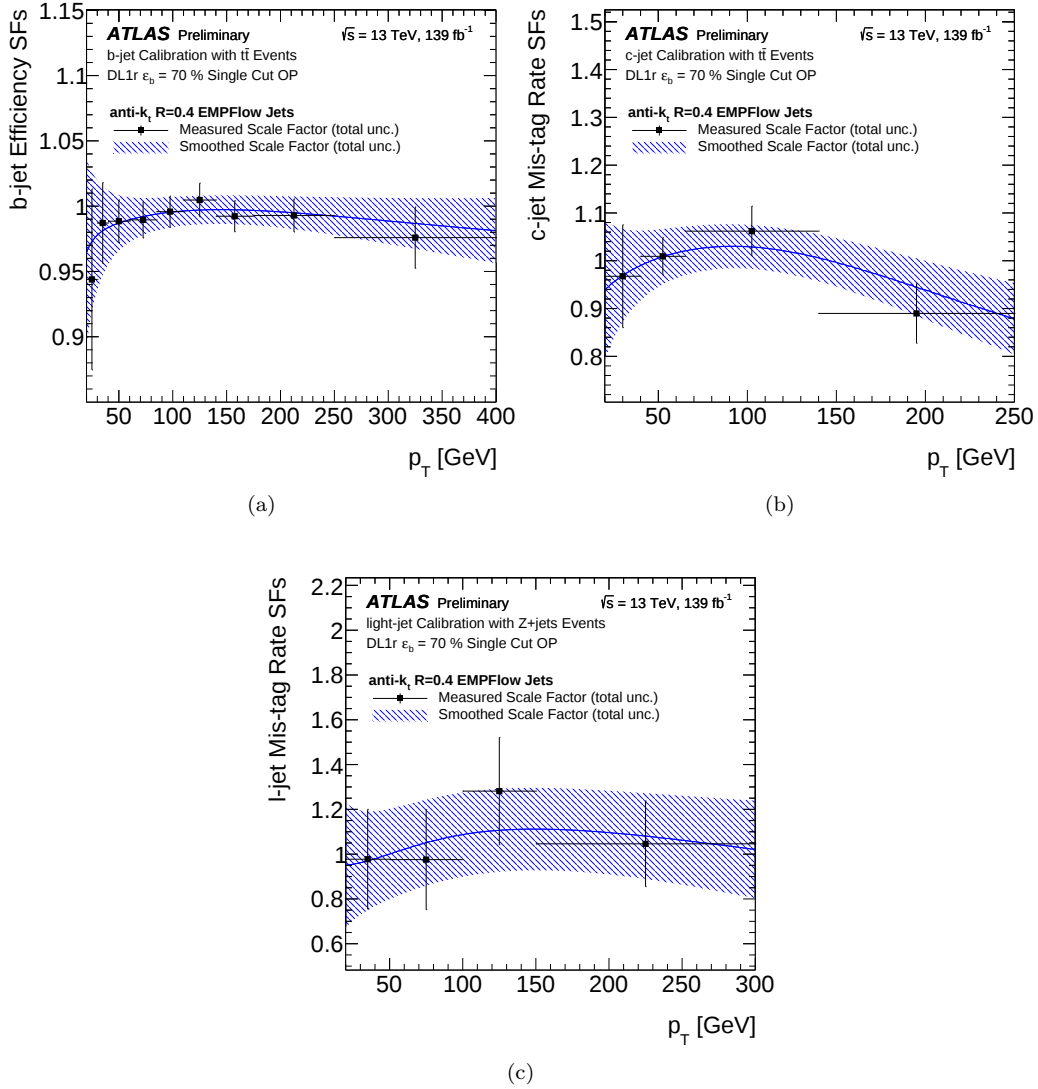


Figure 5.3: Scale factors for the (a) b -jet tagging efficiency, (b) c -jet mistagging efficiency, and (c) light-jet mistagging efficiency, as a function of p_T . All scale factors are measured for $R = 0.4$ particle flow jets using the DL1r algorithm at the 70% working point. The black dots are the measured scale factors with the total uncertainty whereas the blue band and curves are the smoothed sale factors and uncertainties.

Chapter 6

$t\bar{t}$ Pair-production Cross-Section at $\sqrt{s} = 5.02$ TeV

6.1 Introduction

This chapter presents a measurement of the $t\bar{t}$ pair-production cross-section in pp collisions at a centre-of-mass energy of 5.02 TeV. This was the first ATLAS measurement of $\sigma_{t\bar{t}}$ at this energy and used 257 pb^{-1} worth of data collected by the ATLAS detector from pp collisions at the LHC in 2017.

The pair-production process has been observed and measured at the Tevatron [152–155] in 1.80 TeV and 1.96 TeV $p\bar{p}$ collisions and at the LHC in 7 TeV, 8 TeV, 13 TeV, and 13.6 TeV pp collisions by the ATLAS [156–159], CMS [160–163], and LHCb [164, 165] Collaborations. The CMS Collaboration has previously measured the $t\bar{t}$ cross-section in the single-lepton and dilepton channels at $\sqrt{s} = 5.02$ TeV using data collected in 2017 [166]. A similar approach to the CMS measurement is taken in this analysis.

Section 6.2 describes the data and simulated samples used in this analysis. This is followed by Section 6.3 that describes the objects used in this analysis while Section 6.4 describes the misidentified lepton background estimate. Section 6.5 and Section 6.6 describe the event selection and the separation of signal and background using a Boosted Decision Tree (BDT), respectively. Systematic uncertainties are presented in Section 6.7 and Section 6.8 discusses the results of the statistical analysis to measure the cross-section. Finally, the combination of the cross-section measurements in the two channels and the effect of this measurement on the proton PDFs are discussed in Section 6.9 and Section 6.10, respectively.

6.2 Data and MC Samples

This analysis is performed using the dataset described in Section 3. The data was collected by the ATLAS detector during the 2017 LHC pp collision run at $\sqrt{s} = 5.02$ TeV and corresponds to a total integrated luminosity of 257 pb^{-1} .

The background processes in this analysis arise from the SM production of W +jets, single-top-quark production, the presence of non-prompt or misidentified leptons (also denoted as the fake lepton background), Z +jets, and diboson (WW , WZ , ZZ) production. The misidentified lepton background contains events with non-prompt electrons, non-prompt muons, jets misidentified as electrons, and photons misidentified as electrons. The fake lepton background is estimated via a data-driven method while all other SM backgrounds are estimated using MC simulation.

Dedicated MC samples were generated at $\sqrt{s} = 5.02$ TeV based on the generator scheme used for $\sqrt{s} = 13$ TeV analyses [167]. All simulated samples were normalized according to the most accurate theoretical cross-sections and k -factor calculations available at the time. The MC samples were processed through the full ATLAS detector simulation [168] based on the GEANT4 framework [76]. All simulated samples were processed through the same reconstruction algorithms and analysis chain as the data. Heavy flavour decays were modelled using the EVTGEN-1.6.0 [75] program, except for processes modelled using the SHERPA generator [169].

The nominal $t\bar{t}$ sample was produced using the POWHEG BOX v2 [64–67] NLO matrix element calculation with the NNPDF3.0NLO PDF set [54] and employed the PYTHIA 8.210 model with the NNPDF2.3LO PDF set and the A14 tune [170] for the parton shower, hadronization, and underlying-event modelling. In the POWHEG configuration, the cut-off scale for the first gluon emission (represented by the h_{damp} parameter) was set to $\frac{3}{2}m_t$ and the factorization (μ_f) and renormalization (μ_r) scales were set to $\mu_f = \mu_r = \sqrt{m_t^2 + p_{T,t}^2}$, where the top-quark transverse momentum ($p_{T,t}$) is evaluated before simulating extra radiation [171].

The $t\bar{t}$ and single-top-quark MC samples were normalised to their total inclusive cross-section multiplied by the branching ratio for a top-quark decay in the lepton+jets channel. The inclusive cross-section for $t\bar{t}$ was calculated for a centre-of-mass energy of $\sqrt{s} = 5.02$ TeV at NNLO in the strong coupling constant α_s including resummation of the next-to-next-to-leading logarithmic (NNLL) soft-gluon terms by the TOP++ program [172] while assuming a top-quark mass of $m_t = 172.5$ GeV. The inclusive cross-section with its uncertainties is: $\sigma_{t\bar{t}} = 68.2_{-2.3}^{+1.9}$ (QCD scale) ± 4.8 (PDF and α_s) pb. The PDF and α_s uncertainties were calculated using the PDF4LHC prescription with the MSTW2008, CT10 NNLO and NNPDF2.3 5f FFN PDF sets. The scale uncertainties were calculated from the envelope of predictions with the μ_r and μ_f scales varied independently up or down by a factor of two from their default values of $\mu_r = \mu_f = m_t$, whilst never letting them differ by more than a factor of two. The calculation is documented in Ref. [173].

Alternative $t\bar{t}$ simulation samples were generated in order to assess systematic uncertainties.

One sample used the POWHEG MC generator with the HERWIG 7.1.6 parton shower and hadronization model [73, 74] employing the H7UE tune [74]. Another sample was generated using the MADGRAPH5_AMC@NLO v2.3.3.p1 generator (referred to hereafter as AMC@NLO) [68] with the NNPDF3.0NLO PDF set while using the PYTHIA 8 parton shower and hadronization model. Uncertainties in the amount of parton shower radiation were evaluated by reweighting the nominal $t\bar{t}$ sample to effectively change QCD scales and shower parameters, and by generating an additional POWHEG+PYTHIA 8 sample with $h_{\text{damp}} = 3m_t$. The top-quark mass was set to $m_t = 172.5$ GeV in all top-quark samples, and the EVTGEN program [75] was used to handle the decays of b - and c -flavoured hadrons. All samples were normalised using the NNLO+NNLL $t\bar{t}$ cross-section prediction discussed above.

The effects of initial- and final-state radiation (ISR/FSR) and missing higher-order QCD corrections are estimated by independently varying the renormalization scale, factorisation scale, and the effective values of strong coupling constant that controls the amounts of ISR and FSR radiation. Further details about the sample settings can be found in Ref. [174].

The t -channel, Wt associated production and s -channel processes for single-top-quarks were simulated using the POWHEG v2 [175, 176] generator with the NNPDF3.0NLO PDF set and employing PYTHIA 8 with the A14 tune as the parton shower and hadronization model. The diagram-removal scheme [177] was used to handle the interference between the $t\bar{t}$ and Wt final states.

The Wt sample was normalised to a cross-section of 6.05 ± 0.57 pb obtained by extrapolating [178] the approximate NNLO calculation [179, 180] using the MSTW2008 NNLO PDF set [181, 182] to $\sqrt{s} = 5.02$ TeV, while taking into account PDF and QCD scale uncertainties. The t - and s -channel samples were normalised to the cross-section predictions from their MC generator (9.8 pb and 0.815 pb, respectively) and the uncertainties were conservatively taken to be 9.5% for both processes.

Two alternative Wt samples were generated: one using the POWHEG+PYTHIA 8 MC generator but with the diagram subtraction scheme [176, 183] and the other using the POWHEG MC generator with the HERWIG 7.1.6 parton shower and hadronization model employing the H7UE tune. Furthermore, alternate t -channel and s -channel samples using the POWHEG+HERWIG 7.1.6 scheme were also generated. All alternate samples are normalized to their respective nominal cross-sections described above.

The V +jets ($V = W, Z$) backgrounds were simulated with the SHERPA-2.2.5 [70] generator using NLO-accurate MEs for up to two jets, and MEs accurate to LO for up to four jets calculated with the Comix [184] and OpenLoops [185, 186] libraries. They were matched with the SHERPA parton shower [72] using the MEPS@NLO prescription [187] and the tune developed by the SHERPA authors with NNPDF3.0 PDF set. The samples were normalised using a NNLO cross-section prediction of 739.2 pb (7259.0 pb) for the Z (W) boson samples.

The W +jets simulated event samples are split into three categories via a $\Delta R < 0.3$ truth matching

cut. This cut can be used to determine if a jet is associated with a b -hadron decay, c -hadron decay, or a τ decay. The three W +jets categories are defined as: $W+ \geq 1b$, $W+ \geq 1c$ and $W+l$ jets where b, c, l refer to a b quark, c quark, and light-flavour jet, respectively. As described in Section 6.7, the modelling uncertainty on W +jets uses the three categories of W +jets as individual components whereas all other uncertainties are treated as a single background component denoted by W +jets.

Diboson production was generated using SHERPA-2.1.1 with MEs computed at NLO accuracy in QCD for up to one additional parton and at LO accuracy for up to three additional partons. The CT10 PDF set was used for the diboson samples.

Table 6.1 provides a summary of the MC samples used in this measurement.

Table 6.1: Signal and background processes with their corresponding generators, parton shower model, and generator level PDFs. The sample highlighted in blue and bolded is a sample that is only used for the t -channel cross-section measurement.

PROCESS	ME GENERATOR	PS MODEL	ME PDF
$t\bar{t}$ non-all-hadronic decay channel	POWHEG	PYTHIA8	NNPDF3.0 NLO
$t\bar{t}$ alternate PS	POWHEG	HERWIG7	NNPDF3.0 NLO
$t\bar{t}$ alternate generator	AMC@NLO	PYTHIA8	NNPDF3.0 NLO
$t\bar{t}$ alternate $h_{\text{damp}} = 3m_t$	POWHEG	PYTHIA8	NNPDF3.0 NLO
Single (anti)top t -channel	POWHEG	PYTHIA8	NNPDF3.0 NLO
Single (anti)top t -channel alternate PS	POWHEG	HERWIG7	NNPDF3.0 NLO
Single (anti)top t-channel pTHard variation	POWHEG	PYTHIA8	NNPDF3.0 NLO
Single (anti)top s -channel	POWHEG	PYTHIA8	NNPDF3.0 NLO
Single (anti)top tW DR scheme	POWHEG	PYTHIA8	NNPDF3.0 NLO
Single (anti)top s -channel alternate PS	POWHEG	HERWIG7	NNPDF3.0 NLO
Single (anti)top tW alternate PS	POWHEG	HERWIG7	NNPDF3.0 NLO
Single (anti)top tW DS scheme	POWHEG	PYTHIA8	NNPDF3.0 NLO
$Z \rightarrow ee$	SHERPA-2.2.5	SHERPA-2.2.5	NNPDF3.0 NLO
$Z \rightarrow \mu\mu$	SHERPA-2.2.5	SHERPA-2.2.5	NNPDF3.0 NLO
$Z \rightarrow \tau\tau$	SHERPA-2.2.5	SHERPA-2.2.5	NNPDF3.0 NLO
$W \rightarrow e\nu$	SHERPA-2.2.5	SHERPA-2.2.5	NNPDF3.0 NLO
$W \rightarrow \mu\nu$	SHERPA-2.2.5	SHERPA-2.2.5	NNPDF3.0 NLO
$W \rightarrow \tau\nu$	SHERPA-2.2.5	SHERPA-2.2.5	NNPDF3.0 NLO
$XY \rightarrow llll$	SHERPA-2.1.1	SHERPA-2.1.1	CT10
$XY \rightarrow lll\nu$	SHERPA-2.1.1	SHERPA-2.1.1	CT10
$XY \rightarrow ll\nu\nu$	SHERPA-2.1.1	SHERPA-2.1.1	CT10
$XY \rightarrow ll\nu$	SHERPA-2.1.1	SHERPA-2.1.1	CT10
$XY \rightarrow ll\nu\nu$	SHERPA-2.1.1	SHERPA-2.1.1	CT10
$XY \rightarrow ll\nu$	SHERPA-2.1.1	SHERPA-2.1.1	CT10
$XY \rightarrow ll\nu\nu$	SHERPA-2.1.1	SHERPA-2.1.1	CT10
$W^+ \rightarrow l\nu + W^- \rightarrow qq$	SHERPA-2.1.1	SHERPA-2.1.1	CT10
$W^+ \rightarrow qq + W^- \rightarrow l\nu$	SHERPA-2.1.1	SHERPA-2.1.1	CT10
$W \rightarrow l\nu + Z \rightarrow qq$	SHERPA-2.1.1	SHERPA-2.1.1	CT10
$W \rightarrow qq + Z \rightarrow ll$	SHERPA-2.1.1	SHERPA-2.1.1	CT10
$Z \rightarrow ll + Z \rightarrow qq$	SHERPA-2.1.1	SHERPA-2.1.1	CT10

6.3 Objects

The final states used in this measurement require the presence of exactly one charged lepton candidate (electron or muon), at least two hadronic jets, and missing transverse momentum. In order to satisfy this topology requirement, events were required to pass a single electron

(HLT_e15_lhloose_nod0_L1EM12) or a single muon trigger (HLT_mu14) and the lepton candidate is required to have a $p_T > 18$ GeV since both triggers are fully efficient above this p_T requirement [118, 127]. The reconstruction algorithms and calibrations for the electron candidates, muon candidates, jets, and E_T^{miss} are described in Sections 4.2, 4.3, 4.4, and 4.5, respectively.

Events are also required to be consistent with the beam-collision region in the $x - y$ plane and to have at least one reconstructed vertex with at least two associated tracks that have a $p_T > 0.5$ GeV. For the final states considered in this analysis, the vertex reconstruction and selection efficiency is close to 100% [107].

Electron candidates are required to pass the medium likelihood (LHMedium) identification criteria within the fiducial region of $|\eta_{\text{cluster}}| < 2.47$, where η_{cluster} is the pseudorapidity of the calorimeter energy deposit associated with the electron candidate. Candidates within the transition region between the barrel and end-cap electromagnetic calorimeters ($1.37 < |\eta_{\text{cluster}}| < 1.52$) are excluded. Electron candidates are then required to be isolated in order to reduce the background from non-prompt leptons, electron conversions, and hadrons. This is achieved by applying the FixedCutTight isolation requirement discussed in Section 4.2.1. Muon candidates after reconstruction are required to pass the Medium selection criteria and have $|\eta| < 2.5$. The FCTight_FixedRad muon isolation selection is used to select prompt isolated muons as discussed in Section 4.3.1. b -jets are identified using the DL1r b -tagging algorithm with the 70% working point. The b -tagging algorithm is only applied to jets with $|\eta| \leq 2.5$. The b -tagging efficiencies were previously measured at $\sqrt{s} = 5.02$ TeV in the dilepton channel measurement that was released before the ℓ +jets measurement [119]. The efficiencies were found to match the $\sqrt{s} = 13$ TeV efficiencies within statistical uncertainty. Thus, the MC b -tagging efficiency scale factors were taken directly from those provided for the $\sqrt{s} = 13$ TeV dataset.

6.4 Misidentified Lepton Background

Non-prompt leptons, hadrons, and photons may also satisfy the selection criteria, thus giving rise to the “non-prompt and fake lepton” background that must be accounted for. In this measurement, the fake lepton background normalization and shape were estimated using the data driven “matrix method” [188].

The matrix method exploits differences in lepton-identification-related properties between prompt, isolated leptons from W and Z boson decays (referred to as “real leptons” below) and fake leptons. For this purpose, two samples are defined after imposing the final kinematic selection requirements but differing in the lepton identification criteria: “tight” sample and a “loose” sample. The tight selection employs the complete set of lepton identification criteria used in the analysis and is a subset of the loose selection, where the lepton identification and isolation criteria are relaxed. The identification, isolation, and selection of leptons in loose and tight selections are summarized in Table 6.2. The method assumes that the total number of selected events in each sample (N^{tight} and

N^{loose}) can be expressed as a linear combination of the number of events with real and fake leptons as defined in Equation 6.1

$$\begin{aligned} N^{\text{tight}} &= N_{\text{real}}^{\text{tight}} + N_{\text{fake}}^{\text{tight}} \\ N^{\text{loose}} &= N_{\text{real}}^{\text{loose}} + N_{\text{fake}}^{\text{loose}} \end{aligned} \quad (6.1)$$

Now, if one defines ϵ_{real} (ϵ_{fake}) as the probability that a real (fake) lepton satisfies both the loose and tight criteria, one can write 6.1 as

$$\begin{aligned} N^{\text{tight}} &= \epsilon_{\text{real}} N_{\text{real}}^{\text{loose}} + \epsilon_{\text{fake}} N_{\text{fake}}^{\text{loose}} \\ \epsilon_{\text{real}} &= \frac{N_{\text{real}}^{\text{tight}}}{N_{\text{real}}^{\text{loose}}} \\ \epsilon_{\text{fake}} &= \frac{N_{\text{fake}}^{\text{tight}}}{N_{\text{fake}}^{\text{loose}}} \end{aligned} \quad (6.2)$$

Note that this system of equations can be written as Equation 6.3, hence the name of “matrix method”.

$$\begin{pmatrix} N^{\text{tight}} \\ N^{\text{loose}} \end{pmatrix} = \begin{bmatrix} \epsilon_{\text{real}} & \epsilon_{\text{fake}} \\ 1 & 1 \end{bmatrix} \cdot \begin{pmatrix} N_{\text{real}}^{\text{loose}} \\ N_{\text{fake}}^{\text{loose}} \end{pmatrix} \quad (6.3)$$

This system can then be inverted to find the number of fake lepton events passing the loose lepton criteria

$$N_{\text{fake}}^{\text{loose}} = \frac{1}{\epsilon_{\text{real}} - \epsilon_{\text{fake}}} (\epsilon_{\text{real}} N^{\text{loose}} - N^{\text{tight}}), \quad (6.4)$$

From this, it is possible to find the number of fake lepton events passing the tight lepton criteria, by multiplying Equation 6.4 by ϵ_{fake} . To estimate the fake background contribution in data, each data event passing the loose lepton selection is weighted with

$$w = \frac{\epsilon_{\text{fake}}}{\epsilon_{\text{real}} - \epsilon_{\text{fake}}} (\epsilon_{\text{real}} - \delta) \quad (6.5)$$

where $\delta = 1$ if the event passes the tight lepton criteria, and 0 otherwise.

Table 6.2: Lepton identification, isolation, and selection for the loose and tight lepton regions.

	Loose selection	Tight selection
Electron identification level	LooseAndBLayerLH	MediumLH
Electron isolation requirement	None	ECTight
Muon identification level	Medium	Medium
Muon isolation requirement	None	ECTight_FixedRad
Electrons trigger	HLT_e15_lhloose_nod0_L1EM12	
Muon trigger	HLT_mu14	
Electrons selection	$p_T > 18 \text{ GeV}, d0 < 5, z0 < 0.5$	
Muon selection	$p_T > 18 \text{ GeV}, d0 < 7, z0 < 0.5$ $p_T > 18 \text{ GeV}, d0 < 3, z0 < 0.5$	

A requirement on the number of jets and b -tagged jets is applied to the regions used to measure the real and fake efficiencies. Both efficiencies were measured after requiring at least one jet and ≥ 1 b -jet ($\geq 1j, \geq 1b$). The 85% b -tagging efficiency working point with the DL1r tagger, which gives a rejection factor of ~ 38 against light-quark jets and ~ 2 against jets originating from charm quarks,

is used to identify said b -jets. An additional alternate region, without a requirement on the number of b -jets ($\geq 1j$) is used to assess the effect of systematic uncertainties in the fake lepton background.

The real efficiencies are measured in the two same-flavour opposite-sign (SFOS) regions dominated by the $Z \rightarrow \ell^+ \ell^-$ and $t\bar{t}$ production. Real leptons are identified by selecting for either isolated electrons with a correctly identified charge or prompt muons. To further increase the purity of real lepton events, the invariant mass of the two leptons is required to fall within 80 GeV and 100 GeV.

The fake efficiencies are calculated from the W +jets, Z +jets, $t\bar{t}$, single-top, and diboson MC events failing the truth cuts used to select for real leptons. Although the fake efficiencies are typically calculated in data, this was not possible for this analysis due to limited statistics. The electron fake efficiencies are measured by selecting two opposite-flavour same-sign (OFSS) electron-muon ($e^\pm \mu^\pm$) pairs while the muon fake efficiencies are measured using same-flavour same-sign (SFSS) muon-muon ($\mu^\pm \mu^\pm$) pairs.

Figure 6.1 shows the distributions of the number of MC events from each process as a function of the lepton p_T . This plot shows the events selected by requiring $\geq 1j$ and a $E_T^{\text{miss}} \leq 20$ GeV cut that is not included in the nominal calculation. Light-flavour decays from hadrons containing u , d , and c quarks are the dominant source of misidentified electrons across the p_T range. There are also slight contributions from heavy-flavour decays from b and c hadrons, and τ -lepton decays at lower p_T . Heavy-flavour decays and τ lepton decays are the dominant sources of misidentified muons at low p_T and high p_T , respectively.

The regions used for the efficiency measurements are summarized in Table 6.3.

Table 6.3: Summary of the different regions used for the real and fake efficiency measurements. The term “inclusive” is used to indicate that no requirements on the number of b -jets are applied.

REGION USED FOR	N_l ($l = e, \mu$)	NUMBER OF JETS	NUMBER OF b -JETS
$\epsilon_{\text{real}}(e)$ extraction	$2 (e^\pm e^\mp)$, 80 GeV ; $m(e^\pm e^\mp)$; 100 GeV	$\geq 1j$	inclusive, $\geq 1b$
$\epsilon_{\text{real}}(\mu)$ extraction	$2 (\mu^\pm \mu^\mp)$, 80 GeV ; $m(\mu^\pm \mu^\mp)$; 100 GeV	$\geq 1j$	inclusive, $\geq 1b$
$\epsilon_{\text{fake}}(e)$ extraction	$2 (e^\pm \mu^\pm)$	$\geq 1j$	inclusive, $\geq 1b$
$\epsilon_{\text{fake}}(\mu)$ extraction	$2 (\mu^\pm \mu^\pm)$	$\geq 1j$	inclusive, $\geq 1b$

When applying the matrix-method estimate, the real and fake efficiencies are applied separately for electrons and muons and parametrized in bins of lepton $|\eta|$ and $|\phi|$ as shown in Figure 6.2. After investigating various combinations of parameterizations and selection regions, the parametrization using lepton $|\phi|$ in the $\geq 1j, \geq 1b$ region is used as the nominal fake lepton background. The lepton $|\phi|$ parametrization in the $\geq 1j$ region and the lepton $|\eta|$ parametrization in the $\geq 1j, \geq 1b$ region are used to determine systematic uncertainties in the fake lepton background.

Plots comparing the predicted and observed distributions in fake lepton enriched control regions were used to evaluate various combinations of kinematic variables and selection regions. Only combinations which showed good agreement in the control regions were considered. Such plots can be found in Appendix D for the nominal parametrization and Ref. [189] for all combinations considered.

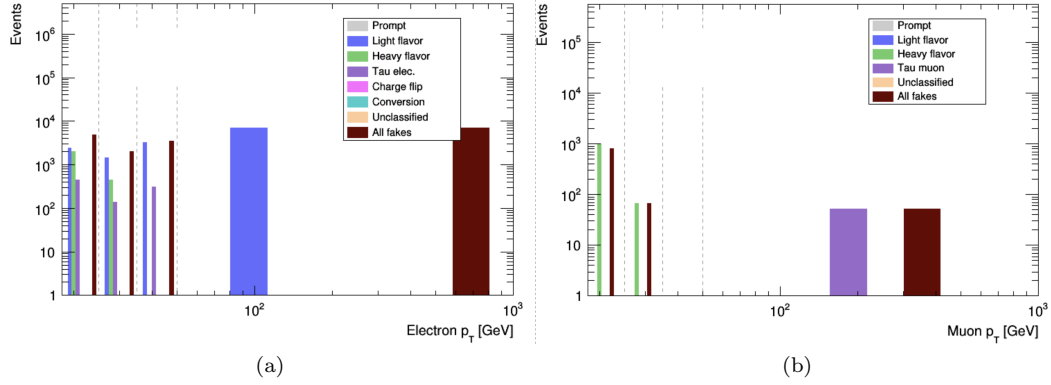


Figure 6.1: Number and type of fake/non-prompt (a) electrons and (b) muons in the $\geq 1j$ region, as a function of lepton p_T .

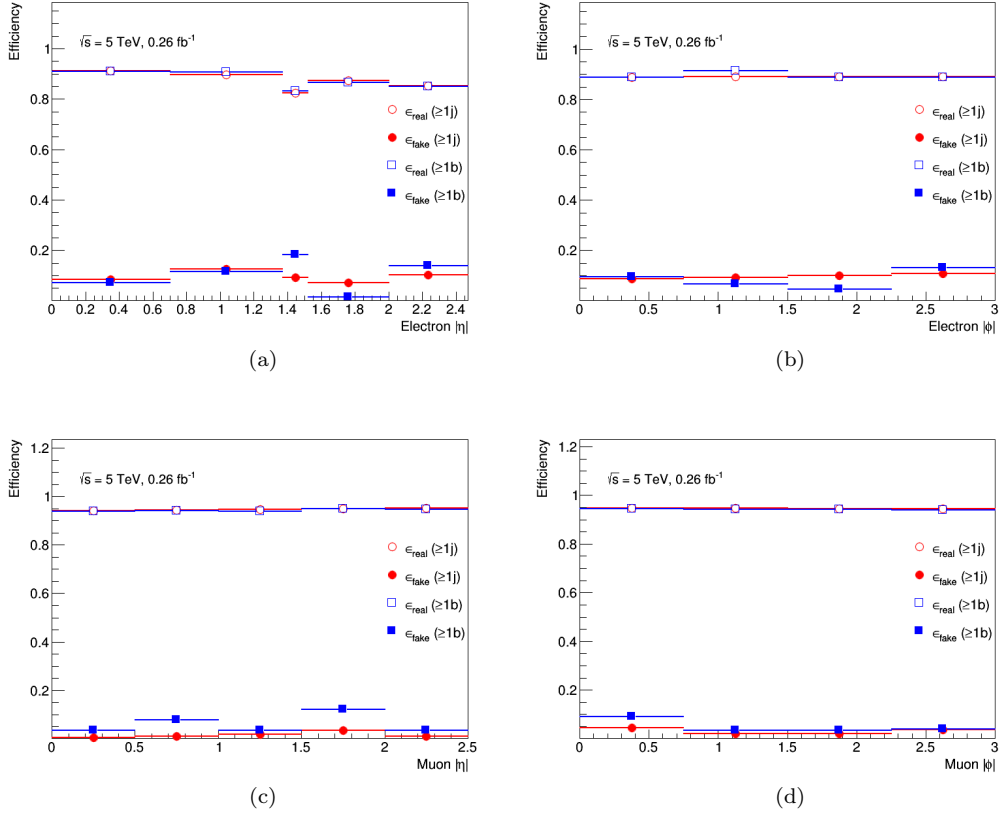


Figure 6.2: ϵ_{real} and ϵ_{fake} for (a, b) electrons and (c, d) muons as a function of (a, c) the lepton $|\eta|$ and (b, d) lepton $|\phi|$. The efficiencies are shown separately for two selection requirements. The uncertainties are smaller than the marker sizes.

6.5 Event Selection and Classification

Signal events from top-quark-pair production with the ℓ +jets decay topology are characterized by the presence of four high- p_T jets. Out of the four jets, two jets arise from a W -boson decay and the other two are b -quark jets coming from the top-quark decay. Furthermore, the event has exactly one charged lepton and some missing transverse momentum from the escaping neutrino.

Following this signature, events are required to have exactly one reconstructed electron or muon candidate with $p_T > 25$ GeV, at least two jets with $p_T > 20$ GeV, of which at least one must be b -tagged. Orthogonality is maintained with a dedicated measurement in the dilepton channel [119] by ensuring true dilepton events with a single-lepton in the crack region (used by the dilepton channel analysis) do not pass the single-lepton selection.

Since the misidentified lepton background is difficult to model precisely, its contribution is reduced with dedicated cuts. Events containing a misidentified lepton tend to have low E_T^{miss} and low m_T^W ¹ relative to single-top-quark events. Thus, a cut on the m_T^W and the “triangular”² variable is an effective way to reduce this background. A cut of $E_T^{\text{miss}} > 30$ GeV and $m_T^W > 30$ GeV is applied to reduce the misidentified lepton background. In the region with at least five jets, of which at least two must be b -tagged, the requirement is loosened to $E_T^{\text{miss}} > 30$ GeV and $E_T^{\text{miss}} + m_T^W > 60$ GeV.

After the event selection, the events are split into two orthogonal regions according to the lepton flavour: the “electron+jets” and “muon+jets” regions for validation and applying the fake lepton background. For the final results, both lepton channels are summed together and fit to data. Events passing the selection are further split into six non-overlapping regions according to the number of jets and b -tagged jets as summarized in Table 6.4.

Table 6.4: Definitions of the six non-overlapping analysis regions based on jet and b -jet multiplicity. The label in the brackets is used to represent the region in the fitting plots.

REGION (NAME IN THE FIT)	JET MULTIPLICITY	b -JET MULTIPLICITY
$\ell+2j \geq 1b$ (CR0)	2	≥ 1
$\ell+3j$ 1b (CR1)	3	1
$\ell+3j$ 2b (CR2)	3	2
$\ell+\geq 4j$ 1b (SR1)	≥ 4	1
$\ell+4j$ 2b (SR2)	4	2
$\ell+\geq 5j$ 2b (SR3)	≥ 5	2

Figure 6.3 shows the expected proportions of different backgrounds in each of the six regions. In the six regions, the $W + \geq 1b$ jet and $W + \geq 1c$ jet contributions altogether constitute the majority of the W +jets background. The event yields prior to the fit are summarized in Table 6.5 and comparisons between data and prediction for kinematic properties in all regions prior to the fit are documented in Appendix E.

¹ m_T^W is the W transverse mass defined as: $m_T^W = \sqrt{2p_T^\ell E_T^{\text{miss}} (1 - \cos \phi)}$, where p_T^ℓ is the transverse momentum of the charged lepton and ϕ is the opening azimuthal angle between the charged lepton and missing transverse momenta.

² The triangular variable is defined as the sum of missing transverse momentum and transverse mass of W ($E_T^{\text{miss}} + m_T^W$)

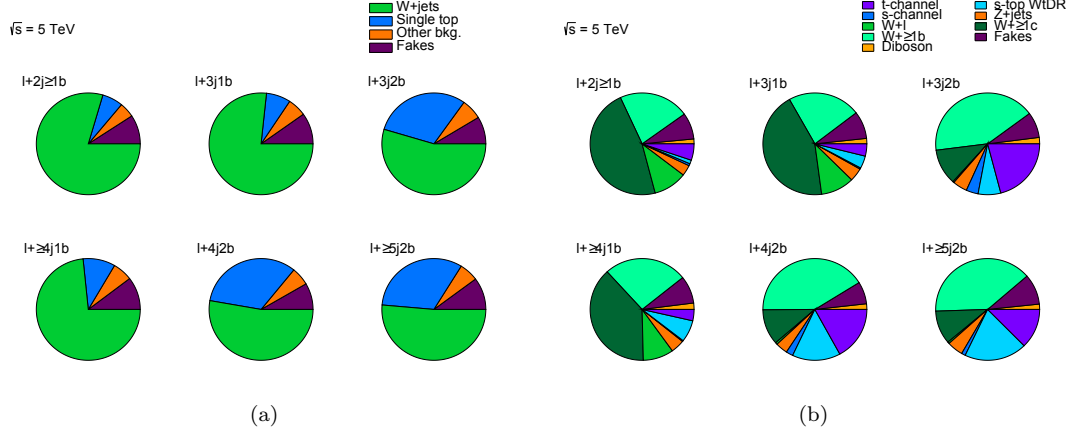


Figure 6.3: Fractional contributions of the various backgrounds to the total background prediction in each of the six regions with the $W+jets$ and single-top-quark backgrounds treated as (a) single backgrounds and (b) split into their components.

Table 6.5: Number of pre-fit signal, background and observed data events in the six analysis regions passing the selection. The ‘Other backgrounds’ category contains $Z+jets$ and diboson contributions. The uncertainties in the signal and background yields combine the statistical uncertainty and systematic uncertainties discussed in Section 6.7.

	$\ell+2j \geq 1b$	$\ell+3j 1b$	$\ell+3j 2b$	$\ell+\geq 4j 1b$	$\ell+4j 2b$	$\ell+\geq 5j 2b$
$t\bar{t}$	194 ± 27	310 ± 33	199 ± 24	690 ± 60	318 ± 32	380 ± 60
Single-top	195 ± 22	98 ± 12	38 ± 5	67 ± 9	22 ± 4	15.9 ± 2.7
$W+jets$	1700 ± 400	690 ± 210	58 ± 23	350 ± 120	30 ± 14	19 ± 10
Other backgrounds	110 ± 40	55 ± 23	7.2 ± 3.0	29 ± 12	3.5 ± 1.5	3.7 ± 1.7
Misidentified leptons	250 ± 130	110 ± 60	10 ± 5	60 ± 30	6 ± 3	8 ± 5
Total	2500 ± 400	1260 ± 210	312 ± 34	1200 ± 160	380 ± 40	430 ± 70
Data	2411	1214	293	1135	375	444

6.6 Signal Discrimination

A Boosted Decision Tree algorithm (BDT) is used to further separate the signal events from background events. A BDT is an algorithm trained to classify events using outputs from a collection of decision trees. The decision trees are based on features from a set of input variables, thus enhancing their separation power by accounting for correlations between input parameters. The BDT used in this analysis are implemented using the Toolkit for Multivariate Analysis (TMVA) framework [190].

6.6.1 BDT Training

During the “training step”, the BDT is provided with the truth MC classification information, so it can learn how to separate the signal $t\bar{t}$ events from the SM background. The BDT is trained using gradient boosting, where a loss function³ to be minimized is defined, and decision trees are sequentially added to an ensemble in order to minimize the loss function of the ensemble. The final discriminant of the BDT (denoted as the BDT response) is produced by taking the average output of the ensemble.

Only simulated MC events (W +jets, single-top, Z +jets and diboson production) with positive weights⁴ were used for the training set.

Due to the low MC background statistics available for the model training, only two BDTs were trained in two separate non-overlapping regions. One BDT is trained inclusively in the first three regions: $(\ell+2j \geq 1b)$, $(\ell+3j \text{ } 1b)$ and $(\ell+3j \text{ } 2b)$. This training region is denoted as $\ell + (2, 3)j, (1, 2)b$. The second BDT is trained in the last three regions: $(\ell+\geq 4j \text{ } 1b)$, $(\ell+4j \text{ } 2b)$ and $(\ell+\geq 5j \text{ } 2b)$. This training region is denoted as $\ell + (4, \geq 5)j, (1, 2)b$. This training configuration was found to perform as well as dedicated trainings in each specific region.

The list of input variables for the BDT was chosen from a large number (~ 100) of potential variables that were studied for their separation⁵ between signal and background and the agreement between data and prediction. The set of chosen input variables was also required to have low correlations, which is optimal for the BDT training even though the variables were preprocessed⁶ before training.

Four of the variables are common to both BDTs while the other two variables in each of the

³A function that compares the output from the model with the “truth” values it is trained against. The loss function is minimal when the model successfully predicts events.

⁴Certain MC generators and showers have only positive weighted events (the weight representing the frequency of a given event in a phase-space) whereas others can have negative weights if the phase-space is too tight.

⁵The separation quoted in these plots is defined as: $\frac{1}{2} \sum_i \frac{(S_i - B_i)^2}{(S_i + B_i)}$ where i is the bin and S_i (B_i) is the number of signal (background) events in the i -th bin. The separation is zero for identical signal and background shapes, and it is one for shapes with no overlap.

⁶The data preprocessing is done prior to presenting the input variables to the multivariate method. The preprocessing implemented in TMVA is useful to reduce correlations among the variables, to transform their shapes into more appropriate forms, and to accelerate the response time of the chosen method.

BDTs are unique. The variables used in the BDT training are listed in Table 6.6. Comparisons

Table 6.6: Input variables used to train the two BDTs in the single-lepton channel.

VARIABLE	DEFINITION	$\ell + (2, 3)\text{j}, (1, 2)\text{b}$	$\ell + (4, \geq 5)\text{j}, (1, 2)\text{b}$
H_T^{had}	Scalar sum of all jet transverse momenta	✓	✓
FW2 (l+j)	Second Fox-Wolfram moment computed using all jets and the lepton	✓	✓
Lepton η	Lepton pseudorapidity	✓	✓
ΔR_{bl} (med.)	Median ΔR between the lepton and b -jets	✓	✓
ΔR_{jj} (med.)	Median ΔR between any two jets	✓	–
$m(jj)^{\text{min}, \Delta R}$	Mass of the combination of any two jets with the smallest ΔR	✓	–
ΔR_{uu} (med.)	Median ΔR between any two untagged jets	–	✓
$m(uu)^{\text{min}, \Delta R}$	Mass of the combination of any two untagged jets with the smallest ΔR	–	✓

between the data and predicted histograms for the BDT input variables using events passing the preselection in the lepton+jets final state are shown in Appendix F

The Pearson correlation coefficients between the input variables were validated in both data and MC simulation. Figure 6.4 shows the correlation coefficients between the input variables extracted from data, the sum of the MC background sample, and the difference in correlations between the two, respectively. Some moderate correlations between variables built using only jets in the region with exactly two jets are observed. However, this does not influence the performance of the training due to the decorrelation step performed before the training. Moreover, the differences between the correlation matrices are found to be consistent between data and MC simulation indicating good MC modelling of the data and providing confidence in the overall training procedure.

6.6.2 BDT Testing and Validation

A test for over-training (when a BDT learns to mimic the training data response, including noise, instead of learning the general patterns in the training data) is performed during the “testing step” where the discriminant constructed from the training is applied to an orthogonal sample that has not been used in the training step using the “k-fold cross-validation” algorithm. The training set is split into three equal-sized partitions (folds). One of the three folds is designated as the “test set” and the other two as the “training set” and the BDT is then trained and tested with this scheme. This procedure is repeated until each fold has been used as the test set exactly once. This ensures an orthogonal test set for each training and data efficiency is gained at the cost of an increased computational burden. A visual representation of the k-fold cross-validation algorithm used is depicted in Figure 6.5. The background rejection versus signal efficiency curves (ROC curves) for the testing samples are shown in Figure 6.6 for each of the folds and their average.

Figure 6.7 shows the cross-validation test of the BDT response distributions, where the signal and background distributions for the testing and training samples are superimposed. The shape differences between the training and testing samples are typically due to reduced statistics of the samples.

Proper training and validation requires three statistically independent data sets: one for the

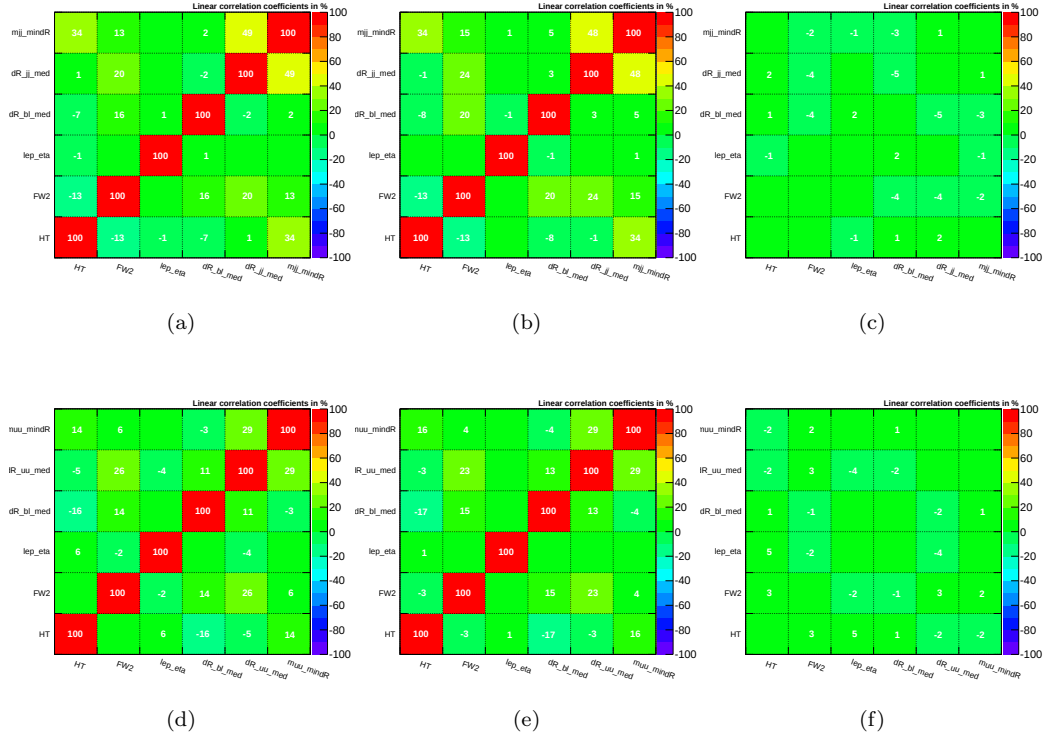


Figure 6.4: Linear correlation matrices of the input variables in the (a-c) $\ell + (2, 3)j, (1, 2)b$ training region and (d-f) $\ell + (4, \geq 5)j, (1, 2)b$ training region extracted from the (a, d) data sample, (b, e) the sum of MC background samples, and (c, f) the difference between the two.

The data set is split into equal sized folds

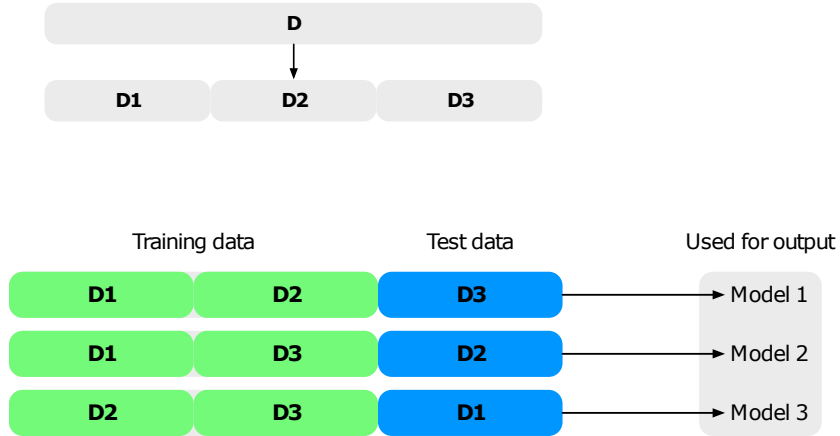


Figure 6.5: Visual representation of the k-fold cross-validation.

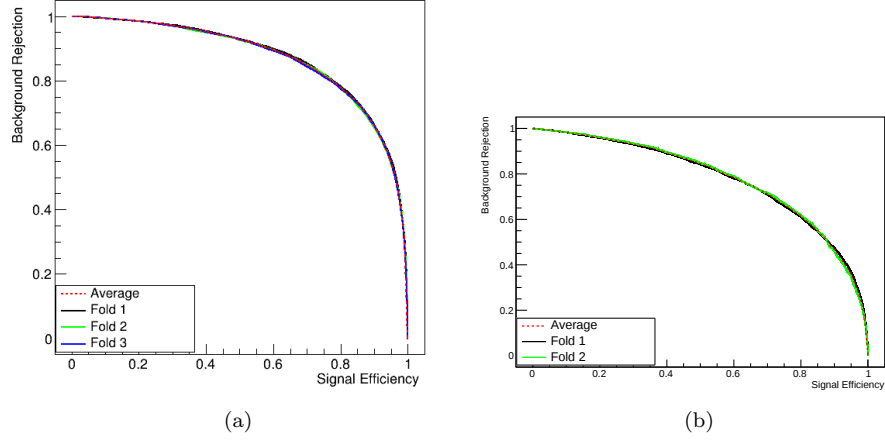


Figure 6.6: Background rejection versus signal efficiency obtained by varying the requirement on the BDT response distribution for the events of the test sample showing (a) the 3 folds for $\ell + (2, 3)j, (1, 2)b$ training region and (b) 2 folds for $\ell + (4, \geq 5)j, (1, 2)b$ training region. The average ROC curve of each of the individual folds is shown as dotted red line.

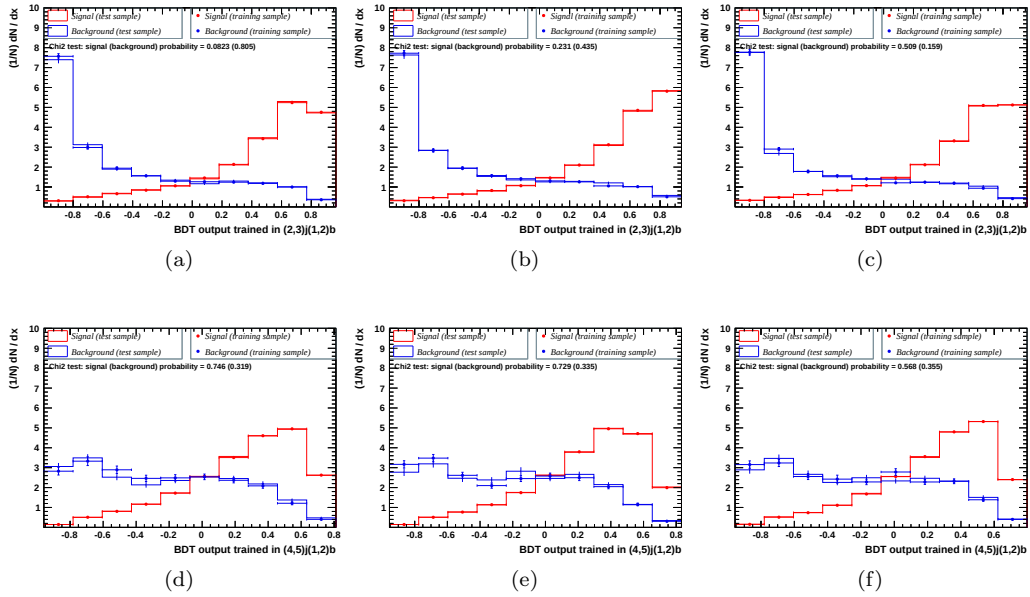


Figure 6.7: The over-training tests of the three BDT folds in the (a-c) $\ell + (2, 3)j, (1, 2)b$ training region and (d-f) two folds in $\ell + (4, \geq 5)j, (1, 2)b$ training region. The errors shown are statistical only.

parameter optimization, one to check for over-training, and the last one to validate the performance. A “validation step” is performed in order to validate our model performance with completely orthogonal data.

The average of the folds BDT response obtained while training in $\ell + (2, 3)j, (1, 2)b$ region is evaluated in the three regions that have never been used for training: $(\ell + \geq 4j \text{ } 1b)$, $(\ell + 4j \text{ } 2b)$ and $(\ell + \geq 5j \text{ } 2b)$. Similarly, the average of the folds BDT response obtained while training in $\ell + (4, \geq 5)j, (1, 2)b$ region is evaluated in the three regions that have never been used for training: $(\ell + 2j \geq 1b)$, $(\ell + 3j \text{ } 1b)$ and $(\ell + 3j \text{ } 2b)$. Figure 6.8 shows the comparison between data and prediction of this validation study. The BDT response distribution does not use the information of the variables $\Delta R_{uu}(\text{med.})$ and $m(uu)^{\text{min.}\Delta R}$ in regions where they are not defined.

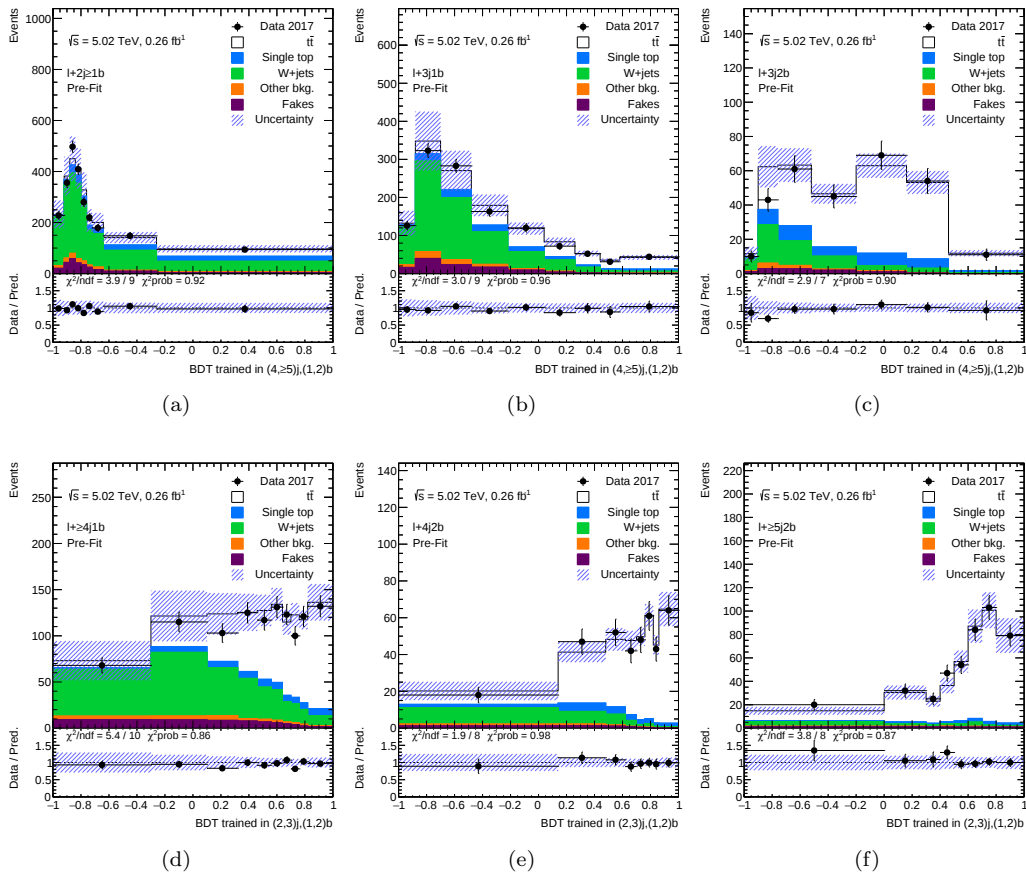


Figure 6.8: Comparison between data and prediction of the BDT distributions with training done in (a-c) $\ell + (4, \geq 5)j, (1, 2)b$ region and in (d-f) $\ell + (2, 3)j, (1, 2)b$ regions in the lepton+jets final state in all six regions. The data and predicted distributions are shown for (a) $\ell + 2j \geq 1b$, (b) $\ell + 3j \text{ } 1b$, (c) $\ell + 3j \text{ } 2b$, (d) $\ell + \geq 4j \text{ } 1b$, (e) $\ell + 4j \text{ } 2b$, and (f) $\ell + \geq 5j \text{ } 2b$. The average of the 3-folds BDT response is used. The last bin contains the overflow and the bottom panel displays the ratio of data to the total prediction. The hashed area represents the total uncertainty on the background.

6.6.3 BDT Application

The trained BDT model is used for the classification of data samples with unknown signal and background composition. The fold assignment is done by evaluating a deterministic expression with a uniformly distributed random number identifier that is independent of the content of an event as an input [190]. Hence, the “cross-evaluation” is used during the application phase: it allows one to use all the three models generated by the 3-folds cross-validation procedure. In this way, the final BDT response distribution, used to perform the likelihood fit described in Section 6.8, is evaluated on events which were not used to train the particular model. The cross-evaluation procedure ensures that the analysis does not suffer from a bias by applying the BDT to events used in training.

The BDT trained in the $\ell + (2, 3)\text{j}, (1, 2)\text{b}$ region is applied in its three corresponding regions: $(\ell+2\text{j}\geq 1\text{b})$, $(\ell+3\text{j} \geq 1\text{b})$ and $(\ell+3\text{j} \geq 2\text{b})$ and the BDT trained in the $\ell + (4, \geq 5)\text{j}, (1, 2)\text{b}$ region is applied to its three corresponding regions: $(\ell+\geq 4\text{j} \geq 1\text{b})$, $(\ell+4\text{j} \geq 2\text{b})$ and $(\ell+\geq 5\text{j} \geq 2\text{b})$. Figure 6.9 compares the expected shapes of the BDT response distributions between the $t\bar{t}$ signal and the total predicted background. The BDT response distribution clearly provides a better discrimination between events from the signal hypotheses and the background, than any single input variable. Figure 6.10 shows the comparison between data and prediction of the BDT response distribution after the preselection in the lepton+jets final state in all six regions. Good agreement between the observed data and predicted distributions is observed for all the regions.

6.7 Systematic Uncertainties

Several sources of systematic uncertainties that can affect the normalization and shape of the signal and background BDT response distributions are considered.

6.7.1 Luminosity, Pileup and Beam Energy Uncertainties

The luminosity scale for the low-pileup pp collision data was measured by ATLAS at $\sqrt{s} = 5.02$ TeV using dedicated Van der Meer scans. These scans allow for calibrations of luminosity-sensitive detectors with a known luminosity and thus allow one to estimate the luminosity in other pp collisions [191]. The LUCID-2 detector [192] was used for the primary luminosity measurements and the results were complemented by measurements using the inner detector and calorimeters. The uncertainty in the integrated luminosity was calculated to be 1.6% following the methodology discussed in Ref. [88].

The LHC beam energy is known to be within 0.1% of the nominal value based on the LHC magnetic model and comparisons of the revolution frequencies of proton and lead-ion beams. According to the NNLO+NNLL predictions of Top++ program [172], a 0.1% variation in $\sqrt{s}$ corresponds to a 0.3%

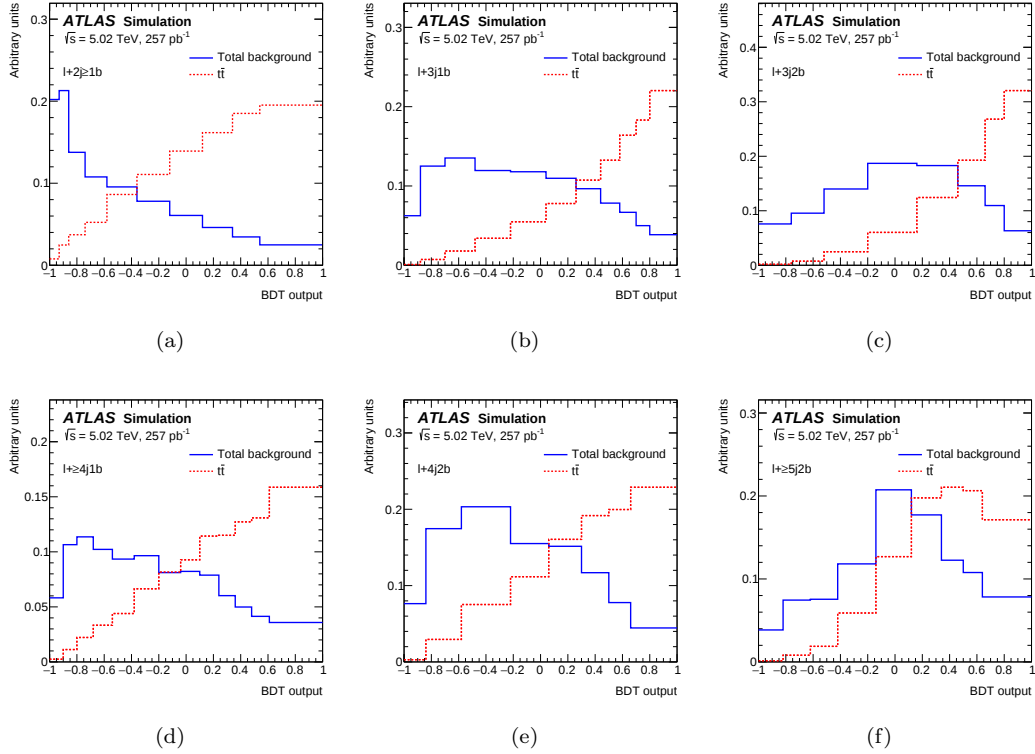


Figure 6.9: Comparison between the shapes of the BDT response for the $t\bar{t}$ signal (red) and total background (blue) in (a) $\ell+2j \geq 1b$, (b) $\ell+3j 1b$, (c) $\ell+3j 2b$, (d) $\ell+4j 1b$, (e) $\ell+4j 2b$, and (f) $\ell+5j 2b$. The distributions are normalised to unit area in order to visualize the separation in the BDT response between the two samples.

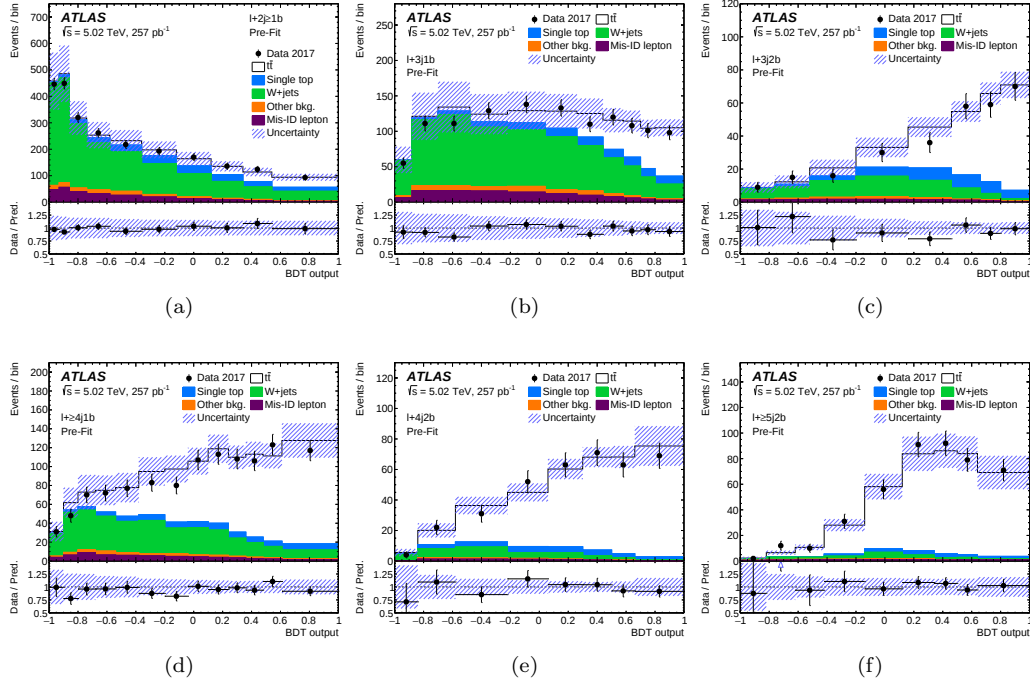


Figure 6.10: The BDT response distribution for data (dots) in (a) $\ell+2j \geq 1b$, (b) $\ell+3j \geq 1b$, (c) $\ell+3j \geq 2b$, (d) $\ell+4j \geq 1b$, (e) $\ell+4j \geq 2b$, and (f) $\ell+5j \geq 2b$. The MC simulation of the signal (white histograms) and various backgrounds (represented by histograms of different colours) are also included. The error bars on the dots represent the statistical uncertainty on the data while the blue cross-hatched lines correspond to the total uncertainties on the prediction as described in Section 6.7. The lower panels show the ratio of the data and predicted distributions, along with the uncertainty in the ratio.

variation in the predicted $t\bar{t}$ cross-section. This uncertainty is included in the experimental uncertainty on $\sigma_{t\bar{t}}$ and allows the measurement to be compared to theoretical predictions at $\sqrt{s} = 5.02$ TeV.

6.7.2 Uncertainties on Reconstructed Objects

Uncertainties associated with leptons arise from the reconstruction, identification, trigger and, isolation efficiencies. These uncertainties have been studied using the $Z \rightarrow e^+e^-$ and $Z \rightarrow \mu^+\mu^-$ decays in data and simulation at $\sqrt{s} = 5.02$ TeV [118, 119, 127]. The electron reconstruction efficiency SFs and their corresponding uncertainties were taken unchanged from the high-pileup $\sqrt{s} = 13$ TeV data.

The electron identification efficiencies were determined using the $\sqrt{s} = 5.02$ TeV data. The trigger efficiencies were similarly determined in-situ using a combination of both $\sqrt{s} = 5.02$ TeV and $\sqrt{s} = 13$ TeV data whereas the electron energy calibration was derived using $Z \rightarrow e^+e^-$ events from the $\sqrt{s} = 5.02$ TeV dataset.

The muon reconstruction, identification and trigger efficiencies were found consistent between $\sqrt{s} = 5.02$ TeV and $\sqrt{s} = 13$ TeV, thus their corresponding SFs and uncertainties were taken from $\sqrt{s} = 13$ TeV data. Minor discrepancies between data and simulation for the muon momentum scale and resolution were corrected by applying the recommended corrections from $\sqrt{s} = 5.02$ TeV and $\sqrt{s} = 13$ TeV, respectively.

The lepton isolation efficiency SFs were derived using $\sqrt{s} = 5.02$ TeV data with the tag-and-probe method using $Z \rightarrow ll$ samples, as described in Ref. [119]. In total there are six (twelve) components of uncertainties associated with electrons (muons).

Except for jet flavour composition uncertainties, the JES calibrations and uncertainties derived using $\sqrt{s} = 13$ TeV data were applied unchanged to the $\sqrt{s} = 5.02$ TeV dataset. The nominal ATLAS JES calibration has jet flavour uncertainties based on a quark-gluon fraction of 50%. However, in this analysis, the quark-gluon fractions were calculated using MC samples and this calculated value was used to derive the jet flavour composition uncertainties. This is further discussed in Appendix G. In ATLAS, the JES uncertainty used for measurements at $\sqrt{s} = 13$ TeV is typically decomposed into a set of 29 uncorrelated components with contributions from pileup, jet flavour composition, single-particle response, and effects of jets not contained within the calorimeter. The uncertainty of the Jet Energy Resolution (JER) is represented by eight components that account for jet- p_T and η -dependent differences between simulation and data [134]. The uncertainty in the efficiency to pass the Jet Vertex Tagger (JVT) requirement for pileup suppression is also considered [193]. The JVT is a high-level discriminant used to identify and suppress pileup jets using tracking information. Further details on the JVT are discussed in Ref [193].

Due to the lower levels of pileup and modified calorimeter cluster noise thresholds, a potentially different JES between data and simulation is observed at $\sqrt{s} = 5.02$ TeV. The response was studied

using the Z +jet p_T balance technique (further described in Section 4.4.4), an in-situ correction was applied to the jets in data, and an additional non-closure systematic uncertainty on the JES was introduced.

The uncertainty in E_T^{miss} due to a possible mis-calibration of its soft-track component was derived from comparisons of the p_T balance between the hard and soft components in data and simulation [194]. The performance of E_T^{miss} reconstruction at low-pileup probed in this analysis is completely dominated by the real and instrumental missing energy in the hard-scattering event. Thus, the corresponding uncertainties derived using $\sqrt{s} = 13$ TeV data are applied unchanged to the $\sqrt{s} = 5.02$ TeV dataset. The JES in-situ correction is also propagated to the missing transverse momentum calculation as appropriate.

The uncertainties in the b -tagging calibration are determined separately for b -jets, c -jets and light-flavour-jets [147, 148, 150] using a 19-component breakdown (11 for b -jets, 4 for c -jets and 4 for light-flavour jets) to account for differences between data and simulation. For light-flavour jets they depend on p_T and η whereas for b - and c -jets they are only p_T dependent. The uncertainties derived with high-pileup data are applied unchanged to the $\sqrt{s} = 5.02$ TeV dataset since the efficiencies were found to match the $\sqrt{s} = 13$ TeV efficiencies within statistical uncertainty [119].

6.7.3 Uncertainties on Signal Modelling

The uncertainty due to missing higher-order QCD corrections in the ME computation is estimated by independently varying the renormalization (μ_R) and factorization (μ_F) scales by factors of 2.0 and 0.5.

Uncertainties in the amounts of ISR from the parton shower are assessed by varying the corresponding parameter of the A14 parton shower tune (Var3c) [170]. The uncertainty in the FSR is evaluated by varying the nominal value of scale μ_R^{FSR} by factors of 2.0 and 0.5.

Uncertainties due to the choice of parton shower and hadronization model are estimated by comparing the nominal sample from POWHEG BOX interfaced to PYTHIA-8 with an alternative sample generated using POWHEG BOX but using the HERWIG-7.1.3 [195] parton shower model.

The uncertainty from the choice of NLO matrix element generator was evaluated by comparing the predictions of the baseline POWHEG BOX interfaced to PYTHIA-8 and an alternative sample generated using AMC@NLO interfaced to PYTHIA-8. The latter generator predicts a slightly softer lepton p_T spectrum and hence a lower acceptance at both $\sqrt{s} = 5.02$ TeV and $\sqrt{s} = 13$ TeV. This is found to model the lepton p_T spectrum seen in $\sqrt{s} = 13$ TeV data slightly better than the nominal sample [158].

PDF uncertainties are evaluated for the signal following the PDF4LHC15 prescription [196] and a set of 30 Hessian eigenvectors corresponding to independent PDF variations were included in

the fit. Internal reweighting in the nominal sample is used to reweigh to the PDF4LHC15 PDF and its uncertainty set, after which the symmetrized uncertainties are propagated to the fit. The uncertainties due to the PDF choice are only estimated for the $t\bar{t}$ signal since uncertainties due to the PDF choice are found to be negligible for the background samples.

Both the parton shower uncertainty and the uncertainty arising from generator choice follow a dedicated decorrelation scheme similar to the one used in Ref. [159]. Both uncertainties are first split into their shape and normalization components and the effect on the shape is decorrelated between all six regions, and described by six separate nuisance parameters (NPs, further discussed in Appendix C). The effect on the normalization is further split in a pure acceptance uncertainty and a component which reflects migrations between the six analysis regions, while keeping overall normalization constant. Thus, the uncertainty between the nominal and alternative models is split into eight NPs each. The “acceptance” represents the difference in the yields after the pre-selection and amounts to 0.83% for the parton shower uncertainty and -1.05% for the generator uncertainty. The migration component on the other hand is sensitive to the $t\bar{t}$ yield difference in the individual regions. The $t\bar{t}$ acceptance component of all regions is subtracted from the migration components to avoid double counting the uncertainty. The resulting overall, acceptance and migration normalization uncertainties can be seen in Table 6.7.

Table 6.7: Normalization uncertainties due to the $t\bar{t}$ parton shower and NLO matrix element generator. The first two rows show the overall normalization effect due to these two uncertainties in each region. The last two rows show the effect of the migration component between the six analysis regions, while not changing the overall normalization. The last column reflects the inclusive acceptance uncertainty (calculated by multiplying the uncertainty in the first six columns by the respective $t\bar{t}$ yield in each region) and in the bottom two rows is equal to 0.0%, reflecting that the migration component has no impact on the total yields, and hence the acceptance and migration components are completely orthogonal.

	$\ell+2j \geq 1b$	$\ell+3j \ 1b$	$\ell+3j \ 2b$	$\ell+\geq 4j \ 1b$	$\ell+4j \ 2b$	$\ell+\geq 5j \ 2b$	Inclusive
$t\bar{t}$ PS norm. overall	-6.1%	-7.7%	-5.5%	4.5%	-4.9%	12.8%	-1.05%
$t\bar{t}$ Gen. norm. overall	-7.9%	-2.8%	-8.2%	4.8%	-6.4%	1.5%	0.83%
$t\bar{t}$ PS norm. migration	-6.8%	-8.5%	-6.3%	3.6%	-5.7%	11.8%	0.0%
$t\bar{t}$ Gen. norm. migration	-6.9%	-1.8%	-7.2%	5.9%	-5.5%	2.6%	0.0%

6.7.4 Uncertainties on Background Modelling

Uncertainties on the fake background estimate are considered separately for fake e +jets and fake μ +jets events. A 50% normalization uncertainty was found to cover the differences between the data and predicted distributions in various control regions enriched in fake lepton events. As discussed in Appendix D, This uncertainty was found to overestimate the mis-modelling between the data and prediction in the control regions. This uncertainty is treated as being further uncorrelated amongst all six analysis regions due to the regions having different compositions of the fake lepton

background. The shape uncertainty in the fake lepton background is evaluated by using the envelope of the two alternate variations discussed in Section 6.4 and follows the same decorrelation scheme as the normalization uncertainty.

A normalization uncertainty of 9.5% corresponding to the extrapolated theoretical uncertainty of the cross-section [197] is applied to the three single-top-quark production backgrounds as independent nuisance parameters. The effects of the ME, μ_r , μ_f , ISR, and FSR is evaluated for all three types of single-top-quark backgrounds as fully correlated shape and normalization nuisance parameters. An additional uncertainty arising from the parton shower choice is considered for the t -channel and tW associated productions. The tW simulated sample that uses the diagram-subtraction method [176] was also compared with a nominal one based on the diagram-removal technique [177] and the difference between the two methods is treated as an uncertainty.

The W +jets modelling uncertainties are evaluated by first splitting the MC-generated W +jets background into three categories $W + \geq 1b$, $W + \geq 1c$, and $W + \geq 1l$ (light quarks or gluons) based on the flavour of additional jets in the event. The uncertainty in each fraction is calculated by adding a 4% uncertainty in quadrature with a 24% uncertainty for each successive jet in the event using Berends scaling [198]. The uncertainties are further decorrelated based on the number of jets, for a total of four normalization NPs per subcategory of W + jets. This conservative approach was taken in lieu of generator comparisons since alternate MC event samples were not available at $\sqrt{s} = 5.02$ TeV. The μ_r and μ_f scales were varied by factors of 1/2 and 2, whilst never allowing them to differ by a factor greater than two from each other, and an envelope is used to estimate additional shape uncertainties for the three subcategories of W +jets background.

The normalization uncertainty in the Z +jets and diboson backgrounds is conservatively taken to be 50%, accounting both for uncertainties in the cross-sections and acceptance uncertainties evaluated at $\sqrt{s} = 13$ TeV by changing the QCD factorisation, renormalization, resummation and CKKW matching scales in the Sherpa generator.

Uncertainties on the background normalizations are summarized in Table 6.8.

Table 6.8: Summary of normalization uncertainties considered. The normalization uncertainty on W +jets events is decorrelated between the number of jets (2, 3, 4, and ≥ 5) in the region. The uncertainty on the fake background estimation is uncorrelated between all six regions and between the e +jets and the μ +jets events. The uncertainty on single-top-quark production is split into three separate nuisance parameters based on the type of single-top-quark production.

BACKGROUND	NORMALIZATION UNCERTAINTY
W +light-quark jets	$4\% \oplus 24\%$ per additional jet
$W + \geq 1c$ jets	$4\% \oplus 24\%$ per additional jet
$W + \geq 1b$ jets	$4\% \oplus 24\%$ per additional jet
Single-top	9.5%
Diboson	50%
Z +jets	50%
Fakes	50%

6.8 Single-lepton Results

Following the statistical method detailed in Section C.1, $\sigma_{t\bar{t}}$ is measured by performing a binned profile likelihood fit to the BDT distributions simultaneously in six analysis regions.

All experimental uncertainties described in Section 6.7 are taken into account. However, systematic uncertainties with an effect less than 0.01% are removed (pruned) in order to improve the stability of the fit. The `COMMONTOOLSMOOTHPARABOLIC` smoothing algorithm [199] in the `TRExFitter` package is used to smooth the shape effects which arise from statistical fluctuations. All uncertainties except one of the NPs representing the JER uncertainty and the three W +jets shape uncertainties are smoothed.

Uncertainties on the PS and ME for all single-top-quark and $t\bar{t}$ samples, W +jets modelling uncertainties, uncertainties on the generator and h_{damp} variations for the $t\bar{t}$ sample, tW diagram-subtraction diagram-removal uncertainty, PDF uncertainties, JER uncertainties, MET resolution uncertainties, JES in-situ non-closure uncertainty, and lepton isolation uncertainties are symmetrized as “one-sided” variations. Since this set of uncertainties only has one variation, the template is constructed such that the other variation is equal but in the opposite direction. All other uncertainties have an “up” and “down” variations (σ_{up} and σ_{down} , respectively) that are symmetrized as: $\frac{\sigma_{\text{up}} - \sigma_{\text{down}}}{2}$.

Prior to the fit to data, a study to evaluate the contribution of each of the six regions to the total sensitivity was performed by fitting to a model dataset that is defined by the predicted cross-section, backgrounds and nominal values of the nuisance parameters rates known as an Asimov sample. An Asimov sample is pseudo-data that is exactly equal to the prediction and can be used to understand the fit behaviour. The effect of a given region on the overall sensitivity can be quantified by comparing the total uncertainty in a fit to an Asimov sample with all regions and a fit done after removing a region. Tab. 6.9 summarizes this study and shows that $\ell+\geq 4j$ 1b is the most influential region in this analysis. A similar study wherein regions are added one after the other is shown in Table 6.10. The uncertainty is broken into its statistical only component and the effects of adding $\ell+2j\geq 1b$, $\ell+3j$ 1b, and $\ell+3j$ 2b is seen. Note that $\ell+3j$ 2b ($\ell+2j\geq 1b$) primarily reduces the systematic (statistical) uncertainty whereas $\ell+3j$ 1b reduces both the statistical and systematic component.

Table 6.9: The effect of removing different regions in a fit to an Asimov sample with the BDT response distribution.

REGION REMOVED	—	$\ell+2j\geq 1b$	$\ell+3j$ 1b	$\ell+3j$ 2b	$\ell+\geq 4j$ 1b	$\ell+4j$ 2b	$\ell+\geq 5j$ 2b
TOTAL UNCERTAINTY (%)	± 4.5	± 4.7	± 4.8	± 4.7	± 5.4	± 4.7	± 4.8

Table 6.10: The effect of adding different regions in a fit to an Asimov sample with the BDT response distribution. Regions are added one after another hence the last column represents all the six regions.

REGIONS	$(\ell+\geq 4j$ 1b), $(\ell+4j$ 2b), $(\ell+\geq 5j$ 2b)	Adding $(\ell+3j$ 2b)	Adding $(\ell+3j$ 1b)	Adding $(\ell+2j\geq 1b)$
STAT. ONLY (%)	± 2.2	± 2.1	± 1.7	± 1.3
STAT. $\oplus$ SYST. (%)	± 6.0	± 5.2	± 4.7	± 4.5

The inclusive $t\bar{t}$ cross-section in the ℓ +jets channel at $\sqrt{s} = 5.02$ TeV is measured to be

$$\sigma_{t\bar{t}} = 68.2 \pm 0.9 \text{ (stat.)} \pm 2.9 \text{ (syst.)} \pm 1.1 \text{ (lumi.)} \pm 0.2 \text{ (beam) pb} \quad (6.6)$$

The measured cross-section is shown with four uncertainties which reflect the: limited size of the data sample, experimental and theoretical systematic effects, the integrated luminosity, and the LHC beam energy. The total relative uncertainty on the cross-section (which reflects the uncertainty on the limited size of the data sample, experimental and theoretical systematic effects and the integrated luminosity) is found to be 4.5%, of which 1.3% is the data statistical uncertainty. Figure 6.11 shows the BDT response distributions after the fit to data in the six analysis regions and the event yields post-fit (NPs are set to their best-fit values, as discussed in Appendix C) are shown in Table 6.11.

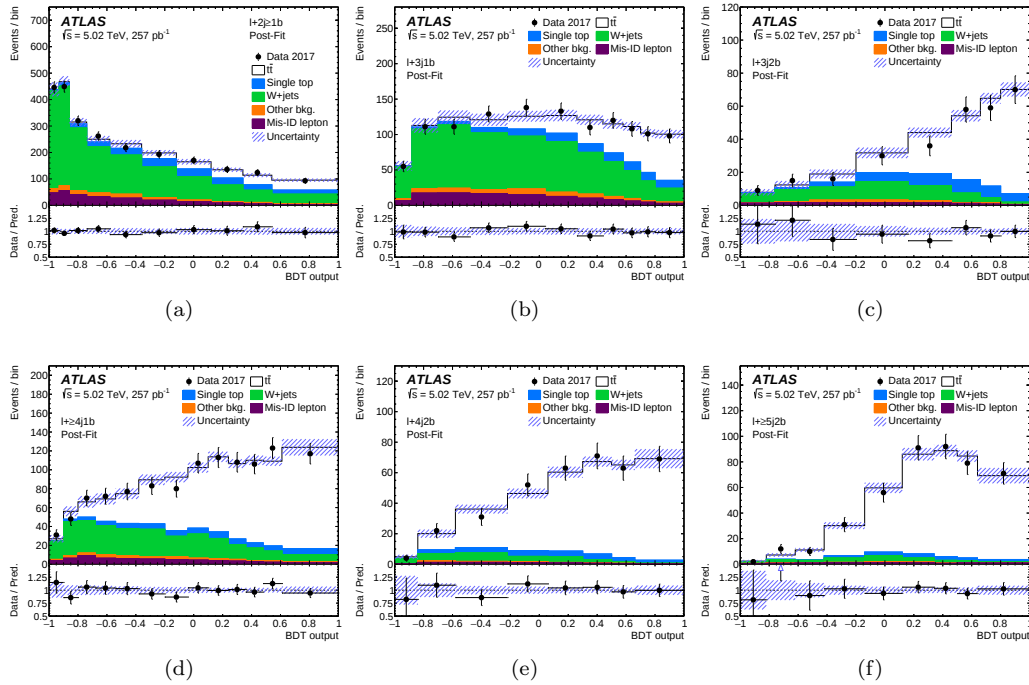


Figure 6.11: The post-fit BDT response distribution for data (dots) in (a) $\ell+2j \geq 1b$, (b) $\ell+3j$ 1b, (c) $\ell+3j$ 2b, (d) $\ell+\geq 4j$ 1b, (e) $\ell+4j$ 2b, and (f) $\ell+\geq 5j$ 2b. The MC simulation of the signal (white histograms) and various backgrounds (represented by histograms of different colours) are also included. The error bars on the dots represent the statistical uncertainty on the data while the blue cross-hatched lines correspond to the total uncertainties on the prediction. The lower panels show the ratio of the data and predicted distributions, along with the uncertainty in the ratio.

Table 6.11: Number of post-fit signal, background and observed data events in the six analysis regions. The ‘Other backgrounds’ category contains Z +jets and diboson contributions. The uncertainties in the signal and background yields include the statistical uncertainty, all systematic uncertainties, and the correlations between them. The uncertainty in the total prediction includes correlations between all systematic uncertainties and thus does not equal the sum in quadrature from the individual components.

	$\ell+2j \geq 1b$	$\ell+3j \ 1b$	$\ell+3j \ 2b$	$\ell+\geq 4j \ 1b$	$\ell+4j \ 2b$	$\ell+\geq 5j \ 2b$
$t\bar{t}$	197 ± 13	309 ± 19	199 ± 11	693 ± 35	314 ± 16	391 ± 20
Single-top	198 ± 18	98 ± 9	38 ± 4	65 ± 6	22.1 ± 3.1	15.2 ± 1.8
W+jets	1660 ± 140	640 ± 70	50 ± 11	290 ± 40	24 ± 8	21 ± 9
Other backgrounds	110 ± 40	54 ± 20	7.3 ± 2.7	28 ± 10	3.4 ± 1.3	3.6 ± 1.5
Misidentified leptons	250 ± 120	120 ± 50	10 ± 5	60 ± 30	6 ± 3	8 ± 5
Total	2410 ± 70	1220 ± 40	304 ± 14	1140 ± 35	369 ± 16	439 ± 20
Data	2411	1214	293	1135	375	444

Figure 6.12 shows the pulls and constraints for the fitted nuisance parameter pulls after the fit to data. The pulls of all nuisance parameters are found to be within 0.45 standard deviations from their pre-fit value and all constraints are smaller than 46% of their initial uncertainty. It should be noted that most of the pulls seen in the jet related NPs arise due to numerical instability in the fit.

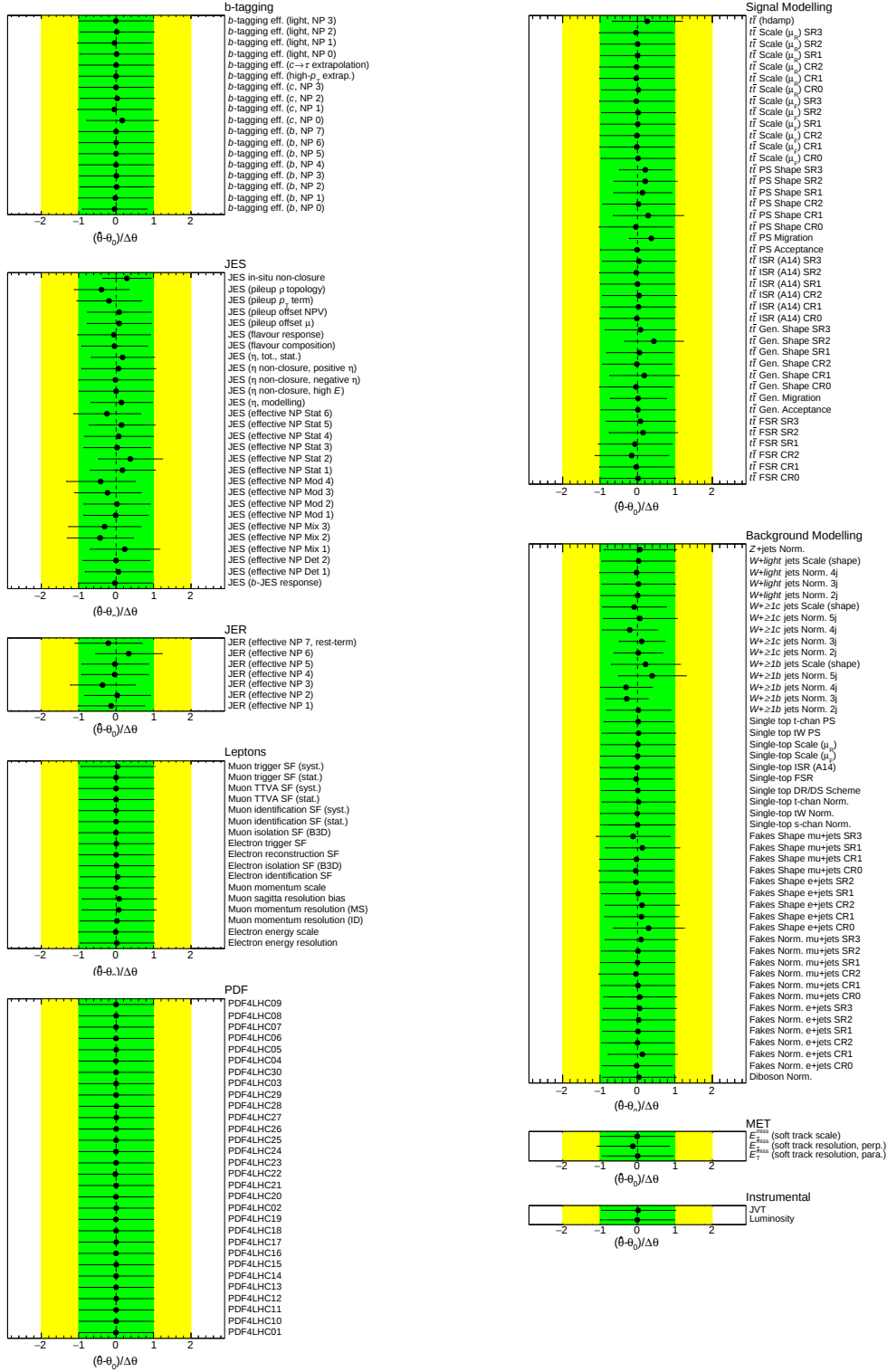


Figure 6.12: Nuisance parameter pulls after a fit to data using the BDT response distributions. The NPs are arranged in different groups.

Figure 6.13 is the “ranking plot” for the fit to data, that shows the pre-fit and post-fit effect of the most significant NPs on the parameter of interest (POI, the ratio of the observed cross-section to the predicted cross-section). The post-fit effect on the POI (denoted as μ in the plots) is shown according to the top horizontal scale. It is calculated by fixing the corresponding nuisance parameter at $\hat{\theta} \pm \sigma_{\theta}$ and redoing the fit. Note that for the post-fit effect, the $\hat{\theta} \pm \sigma_{\theta}$ use post-fit values whereas for the pre-fit effect, they use pre-fit values. $\Delta\mu$ is the difference between the default and modified μ and represents the effect of the nuisance parameter in question. The nuisance parameters are sorted in descending order according to the post-fit effect of each on μ (hashed blue area).

From Figure 6.13, the largest uncertainty arises from the uncertainty in the luminosity followed by uncertainties in electron identification. These uncertainties are then followed by W +jets normalization uncertainties in the various categories of jet flavour and number of jets. The W +jets normalization uncertainties are slightly constrained by the data which is expected since the Berends scaling approach is a significant overestimate. This is then followed by an uncertainty in the b -tagging efficiencies which arises from the requirement of at least one b -tagged jet in this analysis. Uncertainties in the muon identification also show up in the largest uncertainties. However, it is not pulled or constrained. Note that the JES non-closure uncertainty appears near the end and is moderately constrained since it is also an overestimate (discussed in Section 4.4.4).

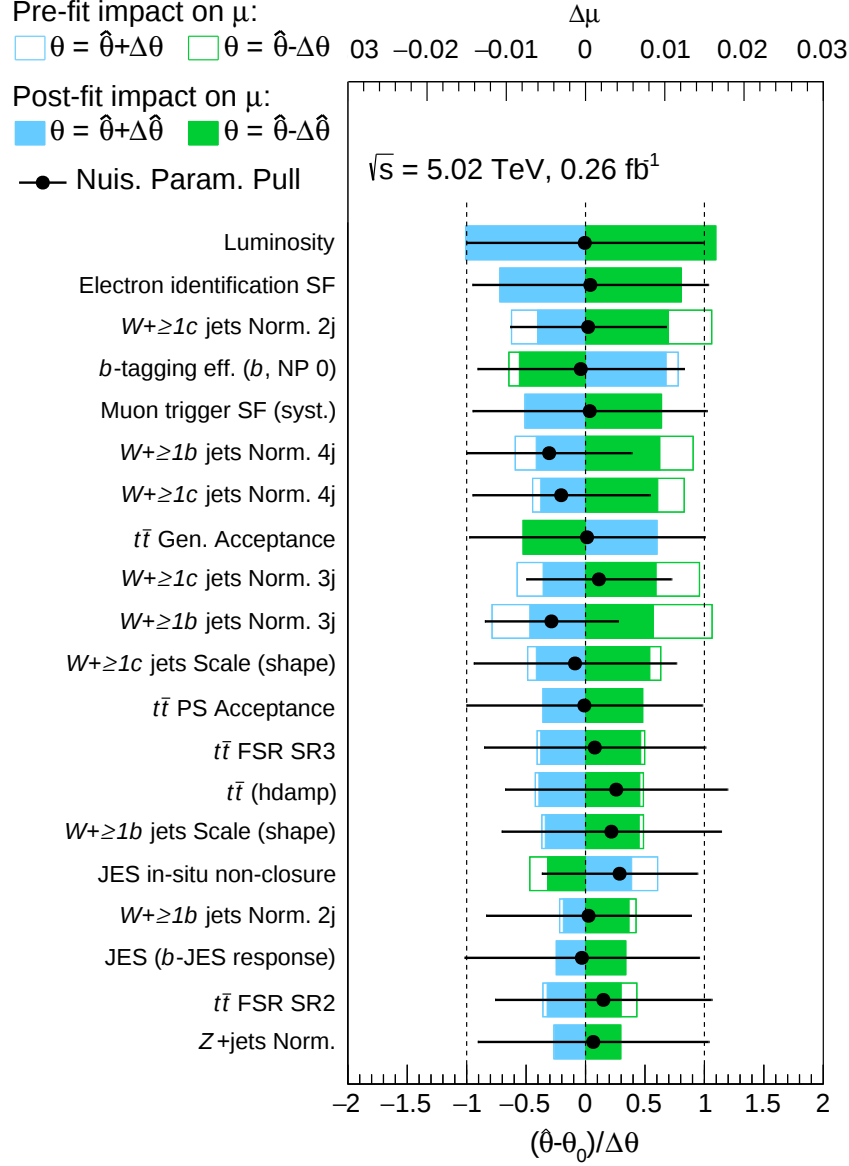


Figure 6.13: Ranking plot showing the effect of each systematic uncertainty on the signal strength (μ) in a fit to data. The black point shows the pulls of various NPs (along the bottom x -axis) whereas the shaded coloured bands show the difference in the POI (along the top x -axis) when varying a NP by $+1\sigma$ (blue) and -1σ (green). The shaded bands represent the post-fit uncertainties whereas the band with an outline is based on the pre-fit uncertainties.

6.8.1 Top-Quark Mass Dependence

The dependence of the inclusive $\sigma_{t\bar{t}}$ cross-section measurement on the assumed value of the top-quark mass m_t is evaluated by quantifying the sensitivity of the cross-section on alternative $t\bar{t}$ MC samples. The four alternate samples use the same settings as the nominal samples but vary the top-quark mass, as described in Table 6.12. The samples were generated with the CT10 PDF set instead of the NNPDF3.0 set used for the nominal samples.

Table 6.12: Summary of the settings used to generate the alternate mass $t\bar{t}$ samples.

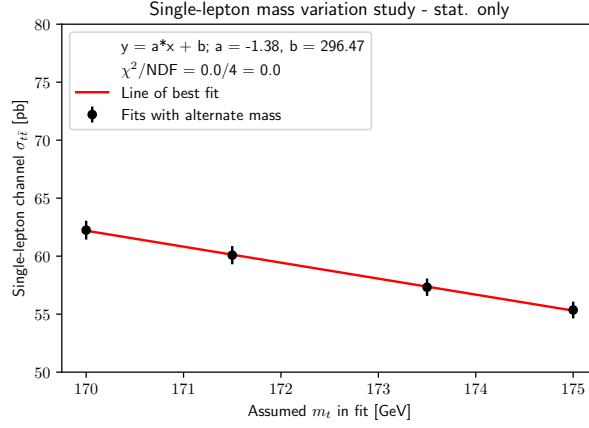
m_t [GeV]	Top-quark width (Γ_t) [GeV]	h_{damp} [GeV]
170	1.254	255
171.5	1.293	257.25
173.5	1.347	260.25
175	1.388	262.50

The BDT distributions for the four alternative top-quark mass variations are used in a fit to data without modifying the fit structure for the NPs since the effects of the top-quark mass on the systematic uncertainties is assumed to be a second-order effect that is negligible. Thus, all the uncertainties are effectively evaluated on the nominal $m_t = 172.5$ GeV sample and the relative difference is propagated to the alternative top-quark mass variations. The measured signal strength in each fit is then used to extract the cross-section for the respective top-quark mass.

Figure 6.14 shows the dependency of the measured inclusive cross-section on the top-quark mass for the single-lepton measurement. The dependence of the measured cross-section on the assumed top-quark mass from the slope is found to be

$$\sigma_{t\bar{t}}[\text{pb}](m_t[\text{GeV}]) = -1.38 \times m_t + 296.47$$

This corresponds to a change of ∓ 1.38 pb for a ± 1 GeV change in m_t ($\mp 2.0\%$ for a ± 1 GeV change).



(a)

Figure 6.14: Dependence of the measured top-quark pair-production cross-section on the top-quark mass assumed in the MC generation. A fit is performed in the mass range around the expected top-quark mass. The uncertainties shown here are statistical only. The central mass sample with $m_t = 172.5$ GeV was not used in this study, as the mass variation samples were generated with a different PDF set.

6.9 Combination

In order to increase the precision on $\sigma_{t\bar{t}}$, the measurement of $\sigma_{t\bar{t}}$ in the single-lepton channel is combined with a corresponding measurement in the dilepton channel [119].

6.9.1 Dilepton Results

The $t\bar{t}$ cross-section was measured in Ref. [119] by performing a counting experiment on opposite-sign dilepton events with exactly one ($N_{1,m}^{ll}$) or two ($N_{2,m}^{ll}$) b -tagged events. This scheme is further extended to the same-flavour channels in bins of the lepton invariant mass (indexed by m), as shown

below

$$\begin{aligned} N_{1,m}^{ll} &= L\sigma_{t\bar{t}}\epsilon_{ll}2\epsilon_b^{ll}(1 - C_b^{ll}\epsilon_b^{ll})f_{1,m}^{ll,t\bar{t}} + \sum_{k=\text{bkg}} s_1^k f_{1,m}^{ll,k} N_1^{ll,k} \\ N_{2,m}^{ll} &= L\sigma_{t\bar{t}}\epsilon_{ll}C_b^{ll}(\epsilon_b^{ll})^2 f_{2,m}^{ll,t\bar{t}} + \sum_{k=\text{bkg}} s_2^k f_{2,m}^{ll,k} N_2^{ll,k} \end{aligned} \quad (6.7)$$

Here, L is the integrated luminosity and ϵ_{ll} is the selection efficiency of the dilepton pair. ϵ_b^{ll} represents the probability for a b -jet from a top-quark decay to fall within the acceptance of the detector, be reconstructed as a jet with $p_T > 25$ GeV, $|\eta| < 2.5$, pass the JVT selection cut and be tagged as a b -jet. The b -tagging correlation is represented by C_b^{ll} . The fractions $f_{1,m}^{ll,k}$ and $f_{2,m}^{ll,k}$ are the fractions of events k ($t\bar{t}$ signal or other backgrounds) in the dilepton mass distribution in bin m for a single and two observed b -jets, respectively. Finally, s_1^k and s_2^k represent scaling factors for the various background samples.

The system of equations is solved for both $\sigma_{t\bar{t}}$ and ϵ_b^{ll} in order to extract the $t\bar{t}$ cross-section and the b -tagging efficiency simultaneously. The effect of various uncertainties is evaluated by solving the system of equations (6.7), where all inputs have been changed to their $\pm 1\sigma$ variations. Note that this method does not take into account any correlations between the various systematic uncertainties unlike the profile likelihood method employed in the single-lepton analysis. Further details of the dilepton analysis can be found in Ref. [119]. The cross-section from the dilepton channel at $\sqrt{s} = 5.02$ TeV is measured to be

$$\sigma_{t\bar{t}} = 65.7 \pm 4.5 \text{ (stat.)} \pm 1.6 \text{ (syst.)} \pm 1.2 \text{ (lumi.)} \pm 0.2 \text{ (beam) pb} \quad (6.8)$$

The four uncertainties correspond to the statistical uncertainty in the data, systematic uncertainties in the detector, signal modelling, and background modelling, uncertainty in the integrated luminosity, and the LHC beam energy uncertainty.

6.9.2 Combination Method

The binned profile likelihood used in the single-lepton analysis leads to a reduction in systematic uncertainties when compared with the cut-and-count method employed in the dilepton measurement due to post-fit correlations between nuisance parameters. In such a case, the post-fit correlations between nuisance parameters are significant and must be considered in any combination attempt. This requirement invalidates the use of the commonly used Best Linear Unbiased Estimator (BLUE) algorithm [200, 201] typically used in combinations. Instead, the dedicated combination tool ‘‘Convino’’ [202, 203] that was designed for such combinations is used.

Convino uses information encoded in the post-likelihood-fit covariance matrix to emulate the likelihood function from the profile likelihood fit. This can then be combined with an emulated likelihood function from the orthogonal measurement in a χ^2 fit. The χ^2 consists of three terms, the first term represents the central values and statistical uncertainty for each measurement following

a χ^2 definition where it is fixed for each measurement. The second term is used to describe the covariance between systematic uncertainties in the same measurement. The final term represents a Gaussian penalty term for systematic uncertainties and encodes assumed covariance between systematic uncertainties in the different measurements that are required as an input.

The χ^2 that is used for the combination can be expressed with the covariance matrix C , written as

$$C = \begin{pmatrix} D & O^T \\ O & S \end{pmatrix} \quad (6.9)$$

Here, the sub-matrix D is the identity matrix representing the covariance between NPs in the dilepton measurement. The sub-matrix S is the post-likelihood-fit covariance matrix for the single-lepton measurement. Information on the measured cross-sections and their statistical uncertainties are encoded in sub-matrices S and D . Finally, sub-matrix O contains the assumed covariance values (denoted as “input correlation values”) between the single-lepton and dilepton systematic NPs that are entered by hand.

The systematics in this combination can be categorized into one of the following three types of uncertainties: “unique”, “one-to-one”, and “one-to-many”. Unique uncertainties are ones which exist only in a single measurement, such as the effect of extra b -hadronization uncertainty in the dilepton channel only. One-to-one uncertainties are systematic uncertainties which are exactly the same in both measurements; like the JVT uncertainty that is the same in both measurements. Finally, one-to-many uncertainties denote the set of uncertainties represented by a single NP in one measurement and multiple NPs in the other measurement, such as the matrix element uncertainty which is a single NP in the dilepton measurement and 8 NPs in single-lepton measurement. Sub-matrix O can be constructed based on the three categories and using the following principles:

1. To first-order, unique systematics in one measurement are uncorrelated with all other systematics in a different measurement.
2. One-to-one systematics are correlated only with the complementary systematic between the two measurements.
3. One-to-many systematics are uncorrelated with all other systematics in a different measurement.

Principles 1 and 2 arise from the definition of correlation amongst two systematic uncertainties whereas principle 3 arises from the insensitivity of the combined uncertainty to the assumed correlation between one-to-many uncertainties as studied in [Appendix H](#).

6.9.3 Combination Results

The combination is performed with the fit to data from both the ℓ +jets and dilepton measurements. The $t\bar{t}$ cross-section at $\sqrt{s} = 5.02$ TeV after combining the single-lepton and dilepton measurements

is

$$\sigma_{t\bar{t}} = 67.5 \pm 0.9(\text{stat.}) \pm 2.3(\text{syst.}) \pm 1.1(\text{lumi.}) \pm 0.2(\text{beam energy})$$

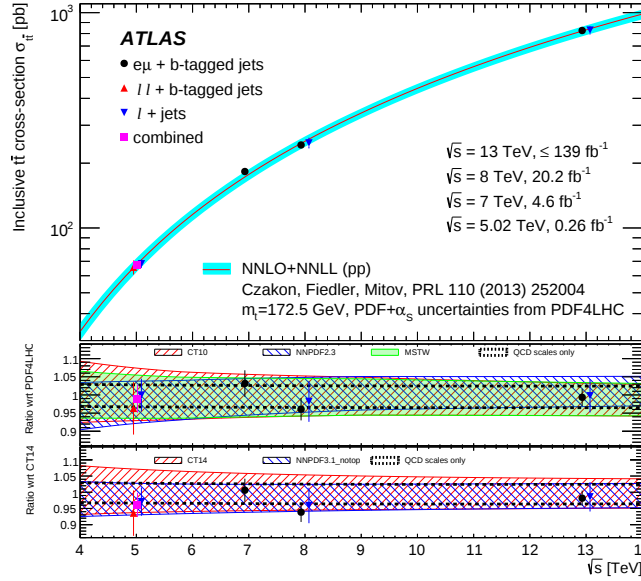
The combined result is consistent with the NNLO+NNLL QCD prediction of $\sigma_{t\bar{t}} = 68.2^{+5.2}_{-5.3}$ pb discussed in Section 6.2, and with the CMS Collaboration measurement [166].

Table 6.13 shows the effect, by groups of uncertainties, on the individual measurements and the combined results. The squared uncertainties quoted for the single-lepton channel and combination measurement are calculated by fixing the set of nuisance parameters corresponding to a category, repeating the fit, and taking a difference between the squares of the resulting uncertainty and the total uncertainty of the nominal fit. The total uncertainty is the sum in quadrature of the total systematic uncertainty and the data’s statistical uncertainty. The total uncertainty on the single-lepton measurement is dominated by the uncertainty in the modelling of W +jets, integrated luminosity, and lepton uncertainties. In the dilepton channel, the total uncertainty is dominated by the statistical uncertainty in data, integrated luminosity, and $t\bar{t}$ modelling uncertainties. The combination obtains a lower uncertainty due to reductions in the signal modelling, electron reconstruction, flavour tagging, and JES uncertainties. The post-Convino-fit correlation matrix can be found as an interactive plot in Ref. [204].

Table 6.13: Breakdown of uncertainties in the dilepton, single-lepton, and combined measurements of the inclusive $t\bar{t}$ cross-section at $\sqrt{s} = 5.02$ TeV. For each category, the dilepton uncertainties are calculated by summing all the contributing uncertainties in quadrature. The squared single-lepton and combination uncertainties are calculated by fixing the set of nuisance parameters corresponding to a category, repeating the fit, and taking a difference between the squares of the resulting uncertainty and the total uncertainty of the nominal fit. Categories that include unique uncertainties, uncorrelated between dilepton and single-lepton measurements, are denoted by *, and those with one-to-many uncertainties by † (see text). Other categories include only one-to-one uncertainty sources, correlated between channels. A signal-modelling uncertainty simulating the effect of extra b -hadronization in the dilepton channel is included in the “ $t\bar{t}$ h_{damp} and scale variations”. The total uncertainty is the sum in quadrature of the total systematic uncertainty, the statistical uncertainty, and the effects of the uncertainties in the integrated luminosity and beam energy. The systematic uncertainties for the single-lepton and combination measurements do not add up in quadrature to the total systematic uncertainty because of their correlations in the fit.

Category	$\delta\sigma_{t\bar{t}}$ [%]		
	Dilepton	single-lepton	Combination
$t\bar{t}$ generator †	1.2	1.0	0.8
$t\bar{t}$ parton shower/hadronization *,†	0.3	0.9	0.7
$t\bar{t}$ h_{damp} and scale variations †	1.0	1.1	0.8
$t\bar{t}$ parton distribution functions †	0.2	0.2	0.2
Single-top-quark background	1.1	0.8	0.6
W/Z + jets background*	0.8	2.4	1.8
Diboson background	0.3	0.1	< 0.1
Misidentified leptons*	0.7	0.3	0.3
Electron identification/isolation	0.8	1.2	0.8
Electron energy scale/resolution	0.1	0.1	< 0.1
Muon identification/isolation	0.6	0.2	0.3
Muon momentum scale/resolution	0.1	0.1	0.1
Lepton-trigger efficiency	0.2	0.9	0.7
Jet-energy scale/resolution	0.1	1.1	0.8
$\sqrt{s} = 5.02$ TeV JES correction	0.1	0.6	0.5
Jet-vertex tagging	< 0.1	0.2	0.2
Flavour tagging	0.1	1.1	0.8
E_T^{miss}	0.1	0.4	0.3
Simulation statistical uncertainty*	0.2	0.6	0.5
Data statistical uncertainty*	6.8	1.3	1.3
Total systematic uncertainty	2.5	4.2	3.4
Integrated luminosity	1.8	1.6	1.6
Beam energy	0.3	0.3	0.3
Total uncertainty	7.5	4.5	3.9

In Figure 6.15, the individual and combined ATLAS Collaboration results are compared with measurements in the dilepton and ℓ +jets channels at other $\sqrt{s}$ values. Predictions using the CT10 [136], NNPDF2.3 [53], MSTW2008 [181, 182], CT14 [205], and NNPDF3.1_NOTOP [55] PDF sets are also shown. The first three PDF sets do not incorporate any constraints from LHC data, while the last two are PDF sets that use some LHC data but no $t\bar{t}$ cross-section measurements.



(a)

Figure 6.15: The upper panel shows $\sigma_{t\bar{t}}$ as a function of centre-of-mass energy $\sqrt{s}$. The points are measurements from the ATLAS Collaboration from including: this analysis, the $e\mu$ plus b -tagged-jets final state at $\sqrt{s} = 7, 8$, and 13 TeV, and from the single-lepton final state at $\sqrt{s} = 8$ and 13 TeV. The blue curve is the predicted NNLO+NNLL theoretical cross-section [206] calculated using TOP++ [172] with the PDF4LHC prescription for PDF and α_s uncertainties [196, 207], and $m_t = 172.5$ GeV. The middle panel shows the ratios of the measurements and predictions to the central value of the prediction using PDF4LHC PDFs. The total uncertainties when using the individual NNPDF2.3, MSTW2008 and CT10 PDFs are shown as overlapping hatched or coloured bands, and the dotted lines show only the QCD scale uncertainties. The lower panel shows the ratios of the measurements and predictions from the CT14 and NNPDF3.1_NOTOP PDFs to the central value from CT14. Measurements made at the same $\sqrt{s}$ are slightly offset for clarity. The $\sqrt{s} = 7$ and 8 TeV results are taken from Refs. [156, 157], with the LHC beam energy uncertainties reduced according to Ref. [208]. The $\sqrt{s} = 13$ TeV results are taken from Refs. [158, 159].

6.10 Effect on Proton PDF

Figure 6.16 compares the measured cross-section at $\sqrt{s} = 5.02$ TeV with the predictions obtained using various PDF sets and shows the effect of the cross-section measurement on the ATLASpdf21 set. For the comparison, the MSHT20 [209], NNPDF4.0 [56], ABMP16 [210], CT18 [59] and CT18A [59] PDFs, and the combination of the CT10 [136], MSTW2008 [181, 182], NNPDF2.3 [53] PDFs using the PDF4LHC recipe, and the recent ATLASpdf21 PDF fit [60] are used. The measured

value is compatible with the predictions from all the PDF sets considered, except for ABMP16, which has a softer gluon distribution and predicts a $\sigma_{t\bar{t}}$ value 2.2 standard deviations lower than measured.

The effect of the $t\bar{t}$ cross-section measurement at $\sqrt{s} = 5.02$ TeV on the proton PDF is studied using the `xFitter` framework [211]. The combined cross-section is included in the ATLASpdf21 set [60] in order to assess the effects of this measurement on the PDF. Figure 6.16 shows the ATLASpdf21 gluon PDF (g) multiplied by the Bjorken- x (denoted as xg) as a function of the Bjorken- x and, a fit including the combined cross-section at $\sqrt{s} = 5.02$ TeV for a scale $Q^2 = 10^4$ GeV². Correlations of systematic uncertainties between data sets are considered in the fit and the hashed bands represent only the experimental uncertainties evaluated at 68% CL with the $\Delta\chi^2 = 1$ criterion. The details of the fit are further discussed in Ref. [60].

At $Q^2 = 10^4$ GeV², the addition of the new data reduces the gluon PDF uncertainty in the region of Bjorken- x above $x \approx 0.05$ and gives e.g. a 5% reduction at $x = 0.1$. The uncertainties in the valance and sea-quark PDFs are unaffected. The inclusion of $\sqrt{s} = 5.02$ TeV data also seems to prefer a harder gluon for $x > 0.1$ as xg increases by $\mathcal{O}(1\%)$. It should be noted that the inclusion of 8 TeV and 13 TeV differential $t\bar{t}$ cross-section data gives a similar effect at high Bjorken- x .

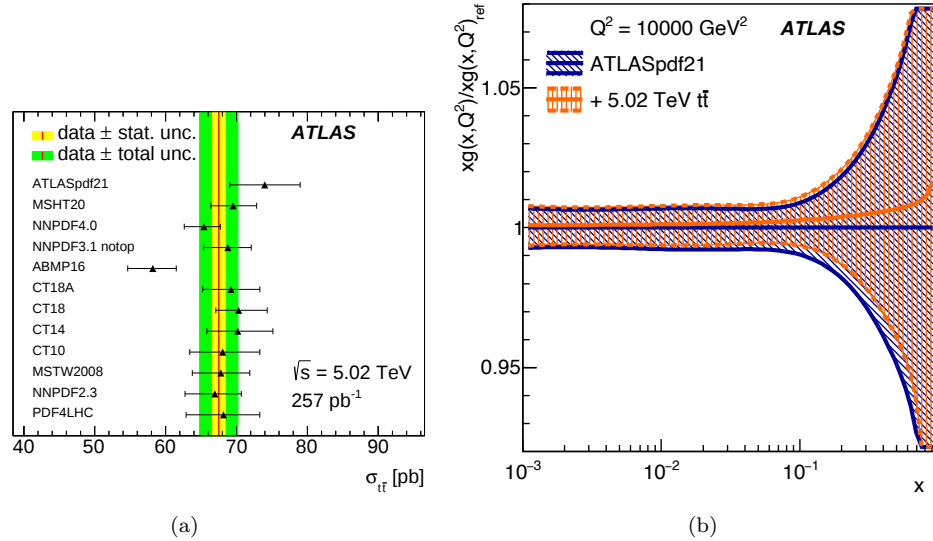


Figure 6.16: The (a) measurement of $\sigma_{t\bar{t}}$ at $\sqrt{s} = 5.02$ TeV in the combined dilepton and single-lepton channels compared with predictions from various NNLO PDF sets and (b) ATLASpdf21 xg PDF compared to the nominal fit and a fit including the $\sqrt{s} = 5.02$ TeV $t\bar{t}$ cross-section measurement at $Q^2 = 10^4$ GeV². The bands in (a) show the experimental measurement, with the statistical (inner yellow band) and total (outer green band) uncertainties shown separately. The last entry shows the prediction using the PDF4LHC recipe which encompasses predictions from the CT10, MSTW2008 and NNPDF2.3 PDF sets. The hatched bands in (b) show the nominal fit (blue band) and the ATLASpdf21 fit with the combined cross-section measurement (orange band). The y-axis in (b) shows the ratio of the fit in question (i.e. the blue or orange band) and the nominal ATLASpdf21 PDF. Thus, the blue band is centred at unity.

Chapter 7

Single-top-quark Production Cross-Section in the t -channel at $\sqrt{s} = 5.02$ TeV

7.1 Introduction

This chapter summarizes the first measurement of $\sigma(tq + \bar{t}q)$, $\sigma(tq)$, $\sigma(\bar{t}q)$, the ratio R_t , and the $|V_{tb}|$ term of the CKM matrix at $\sqrt{s} = 5.02$ TeV. The single-top-quark t -channel process has been observed and measured at the Tevatron [212, 213] in 1.96 TeV $p\bar{p}$ collisions and at the LHC in 7 TeV [214–217] and 8 TeV pp collisions [218, 219]. Measurements using the full Run 2 dataset at 13 TeV have been performed by the ATLAS Collaboration [220] whereas the CMS Collaboration [221] has measured the process using 35.9 fb^{-1} of Run 2 data.

The Feynman diagram of t -channel single-top-quark production with a subsequent leptonic decay of the W boson is shown in Figure 7.1. The final state of the signal events are characterized by a single isolated charged lepton (electron or muon) candidate arising from the decay of the W boson, missing transverse momentum from the escaping neutrino, and exactly two hadronic jets. Out of the two hadronic jets, exactly one must arise from a b -quark decay. The other jet (also denoted as the “untagged jet”) is typically produced with a higher jet $|\eta|$.

Using 255 pb^{-1} worth of events collected by ATLAS in 2017, this analysis applies a series of selection criteria to isolate the t -channel topology by exploiting the kinematic differences between the single-top-quark signal and the other SM background. The backgrounds in this analysis arise from the production of W bosons in association with jets (W +jets), the misidentification of non-prompt leptons, $t\bar{t}$ pair production, the two other single-top-quark processes, the production of Z bosons in

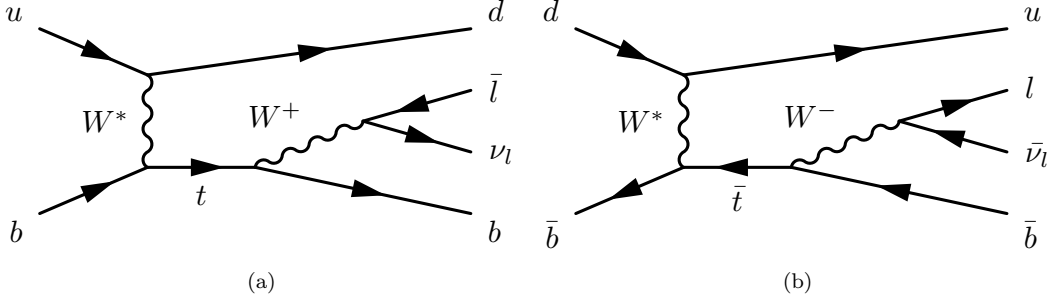


Figure 7.1: Feynman diagrams at leading-order in the strong coupling constant α_s for (a) single-top-quark production and (b) single-antitop-quark production via the t -channel exchange of a virtual W boson (W^*). The diagrams include the semi-leptonic decay of the top quark and the top antiquark.

association with jets (Z +jets), and diboson production. A boosted decision tree is then trained to separate t -channel signal from the other SM backgrounds that pass the selection criteria. Finally, the t -channel cross-section is extracted by performing a binned profile-likelihood fit to the BDT response distributions. The analysis leveraged experience gained by the measurement of the $t\bar{t}$ cross-section at $\sqrt{s} = 5.02$ TeV [222] described in Chapter 6.

Section 7.2 describes the dataset and simulated samples used in this analysis and is followed by Section 7.3 discussing the objects and the event selection. Section 7.4 describes the separation of signal and background using a BDT. Systematic uncertainties that differ in this analysis with respect to the $\sigma_{t\bar{t}}$ measurement are discussed in Section 7.5. Section 7.6 describes the fit structure used in this measurement and is followed by Section 7.7 which presents the results of this measurement.

7.2 Data and MC Samples

7.2.1 Data Samples

This analysis is performed using the same dataset described in Section 6.2. However, the integrated luminosity is slightly different due to an updated luminosity calibration released after the publication of the $\sigma_{t\bar{t}}$ measurement. Thus, this analysis uses an integrated luminosity value of $254.9 \pm 2.6 \text{ pb}^{-1}$.

7.2.2 MC Samples

The same nominal and alternate parton shower MC samples were used for the t -channel as described in Section 6.2. An additional alternate sample with respect to the nominal sample was produced for the t -channel signal, in order to assess the matching uncertainty more accurately and avoid double counting it. This sample was generated using the same settings as the nominal sample but with the

pTHard parameter in PYTHIA 8 generator changed from a nominal of 0 to 1. The **pTHard** parameter controls the definition of the p_T scale used to determine sections of phase-space that POWHEG BOX already covered. A value of 0 corresponds to a p_T scale from POWHEG BOX whereas a value of 1 uses the minimum p_T from the POWHEG BOX emission, the incoming partons, and the outgoing partons [223, 224].

Due to updated theoretical calculations provided after the publication of the $t\bar{t}$ measurement, the MCFM program [225–227] employing the NNPDF3.0NLO PDFs [53] was used to calculate predictions for the single-top-quark (tq) and single-antitop-quark ($\bar{t}q$) production cross-sections in the t -channel at next-to-next-to-leading-order (NNLO) in the strong coupling constant α_s for pp collisions at $\sqrt{s} = 5.02$ TeV. The predicted values are $\sigma(tq) = 20.3^{+0.5}_{-0.4}$ pb, $\sigma(\bar{t}q) = 10.0^{+0.2}_{-0.3}$ pb, $\sigma(tq + \bar{t}q) = 30.3^{+0.7}_{-0.5}$ pb. The ratio R_t is predicted to be $R_t = 2.03^{+0.06}_{-0.07}$. All predictions are assuming a top-quark mass of 172.5 GeV. The quoted uncertainties include the uncertainties from the choice of renormalization scale μ_r , the factorization scale μ_f , the uncertainty in the parton distribution functions (PDFs), and the uncertainty in the value of the strong coupling constant α_s . The scale uncertainties are determined by varying μ_r and μ_f independently up and down by a factor of two, whilst never allowing them to differ by a factor greater than two from each other. The combined PDF and α_s uncertainties were determined at the 68% confidence level according to the Hessian representation of the PDF4LHC21 PDF set [228]. All t -channel MC samples were normalized to their updated corresponding cross-sections.

The same $t\bar{t}$, single-top-quark s -channel production, W +jets, Z +jets, and diboson MC samples along with their respective cross-section normalizations as described in Section 6.2 were used for this analysis. The $t\bar{t}$ and all three single-top-quark MC samples were normalised to their total inclusive cross-section multiplied by the branching ratio for a top-quark decay in the ℓ +jets channel.

The same single-top-quark tW associated production samples described in Section 6.2 are used. However, these samples are normalized based on a total inclusive cross-section that was computed for a centre-of-mass energy of $\sqrt{s} = 5.02$ TeV at NLO in QCD including resummation of the NNLL terms [229], while assuming a top-quark mass of $m_t = 172.5$ GeV. The calculated inclusive cross-section with its uncertainties is $6.54 \pm^{+0.37}_{-0.36}$ pb. The quoted uncertainty includes the uncertainty due to the choice of the renormalisation scale μ_r , the factorisation scale μ_f , and the uncertainty in the parton distributions functions (PDFs). The uncertainties were determined with the same technique as the signal sample.

Table 6.1 provides a summary of basic parameters of the MC samples used in this measurement and samples unique to this analysis are highlighted in blue.

7.3 Objects and Event Selection

This analysis uses the same object definitions for electrons, muons, and E_T^{miss} , as discussed in Section 6.3. However, a slight modification is made to the jet definition and b -jet tagging working point. Due to the presence of forward jets in the final state, the jet definition is modified to include jets with $|\eta| \leq 4.0$. The p_T cuts on the leptons and jets are also modified in the selection as discussed in Section 7.3. The addition of forward jets (jets with $2.5 \leq |\eta| \leq 4.0$) also requires a slightly different in-situ JES correction which is described in Section 4.4.4. In this analysis, the DL1r b -tagging algorithm with the tighter 60% working point is used to increase the signal purity. This working point gives a rejection factor of ~ 1155 against light-quark jets and ~ 29 against jets originating from charm quarks.

The change in jet definitions is also propagated to the misidentified lepton background calculation but the same nominal and alternate parameterizations discussed in Section 6.4 are used. As shown in Appendix I, the parametrizations with the inclusion of forward jets are validated in dedicated fake-lepton-enriched control samples unique to this analysis.

Based on the expected signature of t -channel single-top-quark production, the reconstructed lepton candidate is required to have $p_T > 18$ GeV, missing transverse momentum with $E_T^{\text{miss}} > 15$ GeV to account for the neutrino, exactly two jets with $p_T > 23$ GeV, and exactly one of the jets must be b -tagged. To avoid the mis-modelling in the transition region between the central and forward electromagnetic calorimeter, electron candidates falling within $1.37 < |\eta_{\text{cl}}| < 1.52$ are excluded. Additionally, the electron candidates and the muon candidates are required to satisfy $|\eta_{\text{cl}}| < 2.47$ and $|\eta| < 2.5$, respectively.

Jets in both the central (jet $|\eta| \leq 2.5$) and forward regions ($2.5 \leq \text{jet } |\eta| \leq 4.0$) are considered. Since the spectator quark tends to be produced with higher jet $|\eta|$ in the t -channel process, the untagged jet must satisfy $1.5 < |\eta| < 4.0$. This selection enhances the signal to background ratio with respect to selecting only untagged jets in the central region. To reduce the contribution from $t\bar{t}$ background events, the separation in η between the untagged and the b -tagged jet must be larger than 1.5.

A cut of $m_T^W > 35$ GeV and $(E_T^{\text{miss}} + m_T^W) > 70$ GeV is used to reduce the misidentified lepton background as discussed in Section 6.5.

To reduce the W +jets contribution to the background, the scalar sum H_T , which is defined as the scalar sum of the p_T of the lepton, p_T of the jets, and E_T^{miss} , is required to be larger than 185 GeV. A cut on the invariant mass of the lepton and the b -tagged jet of $m_{\text{lb}} < 165$ GeV is used to exclude background events from processes not involving a top-quark.

7.3.1 Top-quark Reconstruction

To further characterize the t -channel production process, the top-quark and W boson are reconstructed using the final state particles and cuts are applied on their reconstructed masses. The 4-momentum of the W is given by $p_W^\mu = p_l^\mu + p_\nu^\mu$. The 4-momentum of the charged lepton p_l^μ is measured with good accuracy but only the x - and y -components of the neutrino 4-momentum p_ν^μ are known. Since the neutrino is assumed to be massless and does not interact with the detector material, the magnitude and ϕ direction of its transverse momentum is assumed to be exactly equal to the E_T^{miss} and ϕ^{miss} , respectively.

Since the neutrino stems from an on-shell W boson, the pole mass, $m_W = 80.399$ GeV can be used as a constraint in conjunction with a requirement that the neutrino is massless. Therefore, the z -component of the neutrino momentum (p_ν^z) can be calculated using the following quadratic equation

$$(p_l^\mu + p_\nu^\mu)^2 = m_W^2 \implies 0 = p_\nu^{z2} - 2 \cdot \frac{\alpha \cdot p_l^z}{E_l^2 - p_l^{z2}} \cdot p_\nu^z + \frac{E_l^2 \cdot p_\nu^{T2} - \alpha^2}{E_l^2 - p_l^{z2}} \quad (7.1)$$

$$\alpha = \frac{m_W^2}{2} + \cos \Delta\phi(l, E_T^{\text{miss}}) \cdot p_l^T \cdot p_\nu^T$$

Here, p_l^z and E_l are the z -component of the momentum and the energy of the charged lepton, respectively. The transverse momentum of the charged lepton and neutrino are p_l^T and p_ν^T , whereas $\Delta\phi(l, E_T^{\text{miss}})$ is the azimuthal angle difference between the charged lepton vector and missing transverse momentum vector. Since this is a quadratic equation, it can have either two real roots, one real root, or imaginary roots. A study was performed to determine the optimal method of treating these cases and is documented in Appendix J. In the case of two roots, the root which gives a reconstructed top-quark mass closest to the on-shell mass of 172.5 GeV is chosen while in the case of imaginary roots, only the real component is used for p_ν^z . Complex solutions to Equation 7.1 are observed in approximately 30% of the events and occur due to fluctuations in E_T^{miss} measurements that result in a non-physical kinematic configuration. Such cases result in a reconstructed W boson mass greater than the m_W constraint.

After calculating the z -component of the neutrino's 4-momentum, the 4-momentum of the W boson and the top quark are determined by $p_{\text{top}}^\mu = p_W^\mu + p_b^\mu$, where p_b^μ is the 4-momentum of the b -tagged jet. The invariant mass of the reconstructed W boson must satisfy $m_W < 102$ GeV and the invariant mass of the reconstructed top-quark must fall between $140 \text{ GeV} < m_{\text{top}} < 225$ GeV.

The cuts for the variables used in the event selection were determined by performing a multidimensional hyperparameter scan with the goal of maximizing the significance in a statistics-only fit (i.e. no systematic NPs are considered) to an Asimov sample.

Table 7.1 shows event cutflows for the signal, background, and data samples as they pass the various event selection cuts. Table 7.2 lists the predicted and observed event yields for the various samples after applying the selection requirements described above and splitting events into a

positive-lepton charged region (ℓ^+ +jets) and a negative-lepton charged region (ℓ^- +jets).

Comparisons between data and prediction for kinematic properties in the ℓ^+ +jets and ℓ^- +jets regions prior to the fit are documented in Appendix K.

Table 7.1: Number of events passing each selection cut for signal, background, and data samples. The signal and background samples show the weighted number of events. The ‘Other backgrounds’ category contains the Z + jets and diboson contributions.

Selection Criteria	t -channel signal	W + jets	$t\bar{t}$	single-top-quark backgrounds	Other backgrounds	Misidentified Leptons	Data
Pre-selection	924.6	148592.3	4458.9	485.1	68524.1	89459.2	960944
Single lepton passing trigger, lepton p_T and η cuts	924.0	148584.3	4025.5	448.1	29265.3	82752.6	887249
Exactly 2 jets satisfy p_T and upper $ \eta $ cut	494.8	80839.7	396.0	133.6	16370.9	41935.4	177291
Exactly 1 b -tagged jet	278.6	1422.0	203.2	65.9	338.4	4867.6	7921
Untagged jet lower η cut	191.7	570.3	49.2	16.8	142.6	2434.0	3807
Jets separation η cut	150.0	362.7	25.3	8.0	87.2	1661.9	2489
E_T^{miss} cut	141.1	332.1	24.3	7.6	62.1	1205.0	1770
m_T^W cut	122.0	307.3	20.7	6.5	38.0	361.7	731
Triangular cut	117.3	280.9	20.2	6.3	29.5	209.7	570
H_T sum cut	85.9	82.4	16.9	4.4	9.7	18.5	208
m_{lb} cut	84.2	53.1	14.1	3.6	5.7	16.1	175
Top mass cut	79.5	41.9	8.5	2.7	5.1	13.7	152
W boson mass cut	74.8	36.8	6.1	2.1	4.2	13.5	127

Table 7.2: Number of pre-fit signal, background and observed data events passing the selection in the ℓ^+ +jets and ℓ^- +jets regions. The ‘Other single top’ category contains the tW associated production and s -channel contributions. The uncertainties in the signal and background yields include the statistical uncertainties, and all systematic uncertainties described in Section 7.5.

Source	Number of events	
	ℓ^+ +jets	ℓ^- +jets
t -channel signal	51 ± 4	24 ± 2
W +jets	24 ± 7	13 ± 4
Misidentified leptons	7 ± 3	7 ± 3
$t\bar{t}$	3 ± 0.5	3 ± 0.5
Z +jets and diboson	2 ± 2	2 ± 2
Other single-top-quark production	1 ± 0.2	1 ± 0.5
Total predicted	88 ± 10	50 ± 6
Data	85	42

7.4 Signal Discrimination

A BDT trained using the `XGBoost` package [230] was used to combine several kinematic variables into one discriminant in order to separate t -channel single-top-quark signal events from the expected background.

7.4.1 BDT Training, Testing, and Validation

During the training step, the BDT is provided with the truth information, so it can learn to separate the signal events from background events via gradient boosting. All background events are trained against the signal MC events. The misidentified lepton background is included in the training because it is the second-largest background in this analysis.

The BDT is trained in the inclusive ℓ +jets region (the sum of the ℓ^+ +jets and ℓ^- +jets regions) and the input variables were chosen based on the studies done for the 13 TeV t -channel single-top-quark cross-section measurement [220, 231]. Since the BDT is trained on MC datasets without information on the MC weights, the number of trained events would not match the physical (weighted) yields expected. To correct for this, the training samples are scaled so that proportions between the number of events of each type of background used to train the BDT match their corresponding physical yield.

The nine chosen variables used for training are listed in Table 7.3 and Appendix L contains the predicted distributions and separation plots for these input variables in the ℓ +jets region. The BDT training is done with the following parameters: 100 trees where each tree has a maximum depth of 5 nodes, a learning rate of 0.01, 100 epochs, a testing sample orthogonal to the training sample that was created using 20% of the total signal and total background events. The binary cross-entropy¹ is

¹ $L = -\frac{1}{N} \sum_{i=1}^N y_i \log(p_i) + (1 - y_i) \log(1 - p_i)$. Here, the index i runs over the N training events, y_i is the truth

used as the loss function. Figure 7.2 shows different metrics used for the training and testing steps and Figure 7.3 ranks the BDT input variables according to the number of times they appear in the BDT. Such a ranking provides an indication of feature importance, and it is seen that H_T and $|\Delta p_T(W, ub)|$ are the two most important variables in the BDT.

Table 7.3: The nine variables that were used to the train the BDT ordered according to the number of times they are used by the various trees.

Variable	Definition
H_T	Scalar sum of transverse momentum of the charged lepton, the jets, and E_T^{miss}
$ \Delta p_T(W, ub) $	Absolute value of the scalar difference in transverse momentum between the reconstructed W -boson and the jet pair four-vector
$ \eta(u) $	Absolute value of the pseudo-rapidity of the light-quark (untagged) jet (u)
$ \Delta\eta(u, l) $	Absolute value of the difference in pseudo-rapidity between the charged lepton and the untagged jet
Transverse sphericity	$\frac{2\lambda_2}{\lambda_1 + \lambda_2}$ where $\lambda_1 \geq \lambda_2 \geq \lambda_3$ and $\lambda_1, \lambda_2, \lambda_3$ are eigenvalues of the matrix $S^{ab} = \frac{\sum_i p_i^a p_i^b}{\sum_i p_i^2}$; $a, b = x, y, z$; i = jet index.
m_{lb}	Invariant mass of the lepton (l) and the b -tagged jet (b)
$m(lvb)$	Invariant mass of the reconstructed top-quark
$ \eta(l) $	Absolute value of pseudo-rapidity of the charged lepton
$ \Delta\eta(b, l) $	Absolute value of the difference in pseudo-rapidity between the charged lepton and the b -tagged jet

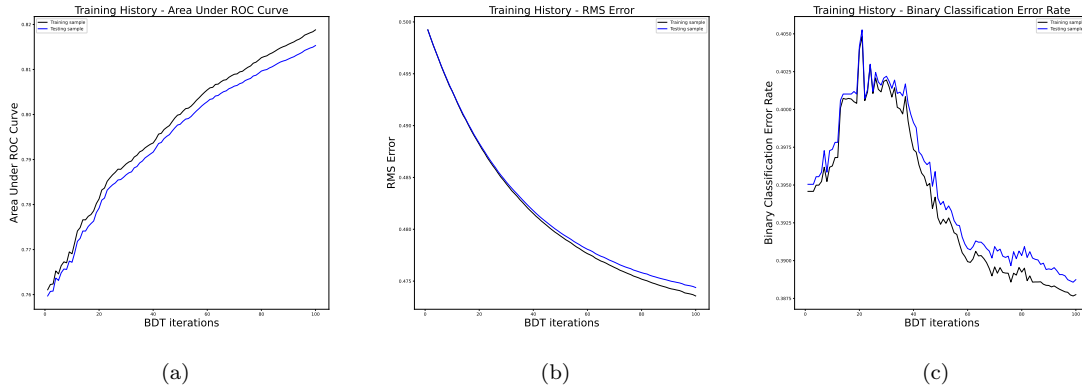


Figure 7.2: Metrics used to evaluate the BDT performance: (a) area under the background-rejection versus signal-efficiency curve (ROC curve), (b) root-mean-square error, and (c) the fraction of incorrectly categorized events. The training sample performs slightly better than the testing sample which can indicate over-training. However, this is acceptable due to the low statistics of the sample and the small absolute differences seen between the two samples in these plots.

value (0 or 1 for a binary classifier), and p_i is the prediction from the BDT.

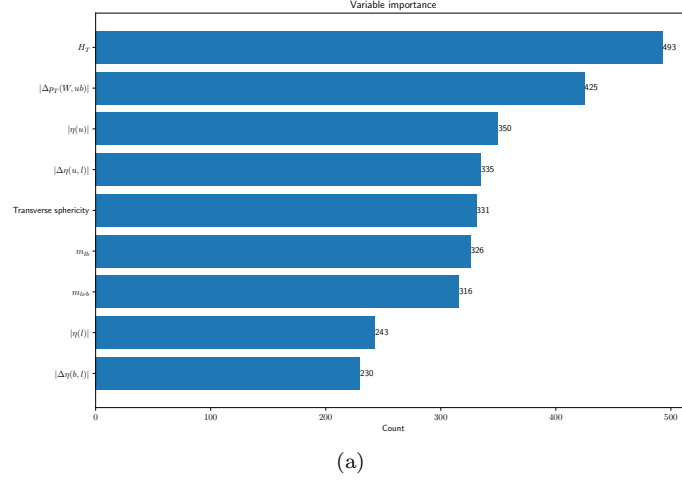


Figure 7.3: BDT input variables ranked according to their importance. The count represents how many times an input variable is used in the ensemble of decision trees.

Figure 7.4 shows the background rejection versus signal efficiency curves (ROC curves) for the training and testing samples as a whole, and the samples using k-fold cross-validation with three folds. The k-fold cross-validation study was performed on the combined training and testing dataset. The ROC curves from the cross-validation behave similarly to the ROC curves seen in the training and testing data, which indicates that over-training is not a concern.

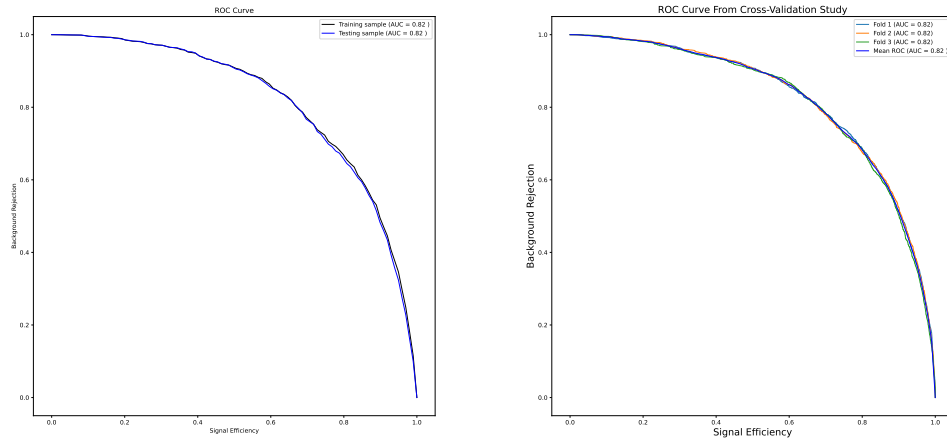


Figure 7.4: Background rejection versus signal efficiency curves for (a) events from the training and testing samples and (b) events from a BDT trained using 3 folds of the total sample. In (b), the average ROC curve of the individual folds is shown as a solid blue line.

7.4.2 BDT Application

Figure 7.5 compares, in the ℓ^+ +jets region, the observed and predicted BDT response distributions as well as the shapes of the BDT response distributions for the predicted signal and predicted background. The BDT response distribution clearly provides a better discrimination between signal and background events than any single input variable (as seen in Appendix L).

Figure 7.6 compares the expected shapes of the BDT response distributions between the signal and the total predicted background in the ℓ^+ +jets and ℓ^- +jets regions. The separation in the ℓ^- +jets is slightly worse than the separation in the ℓ^+ +jets due to the higher proportion of single-top-quark events found in the inclusive ℓ +jets region. This occurs because the individual single-top-quark and single-antitop-quark events were not normalized to have an equal effect in the training.

Figure 7.7 shows the comparison between data and prediction of the BDT response distribution in both the ℓ^+ +jets and ℓ^- +jets regions. As discussed in Section 7.7, data is fit to both BDT response distributions simultaneously in order to extract both $\sigma(tq + \bar{t}q)$ and R_t .

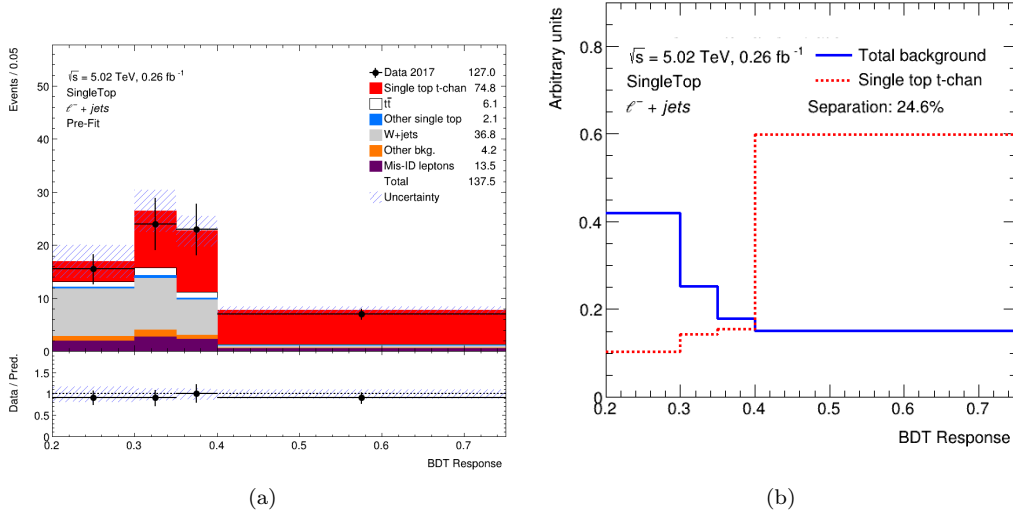


Figure 7.5: (a) shows the pre-fit BDT response distribution for data (dots) in the ℓ +jets region. The MC simulation of the signal (red histograms) and various backgrounds (represented by histograms of different colours) are also included. The error bars on the dots represent the statistical uncertainty on the data while the blue cross-hatched lines correspond to the total uncertainties on the prediction. Each bin content is scaled with respect to a bin width of 0.05. The lower panels show the ratio of the data and predicted distributions, along with the uncertainty in the ratio. (b) is a comparison between the shapes of the BDT response for the single-top-quark signal (red) and total background (blue). The distributions in (b) are normalised to unit area in order to visualize the separation in the BDT response between the signal and background.

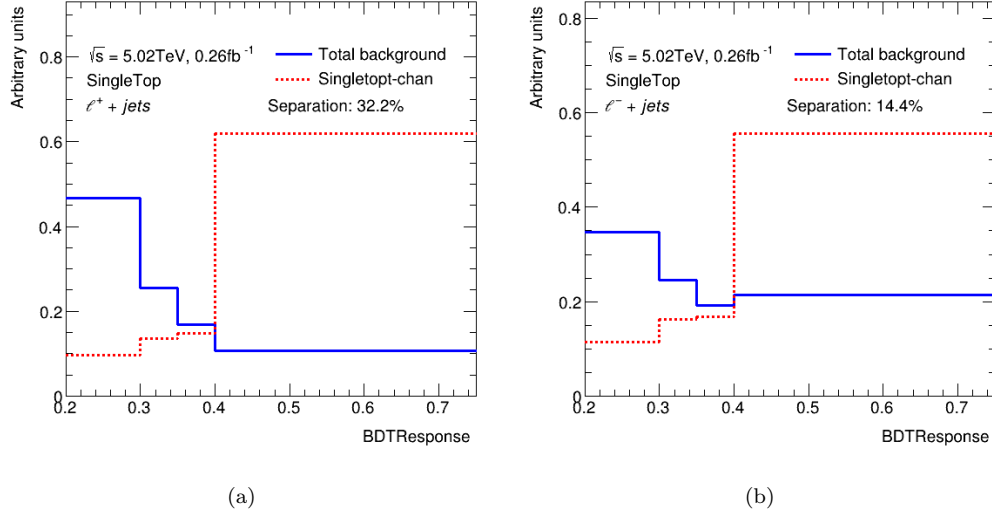


Figure 7.6: Comparison between the shapes of the BDT response for the single-top-quark signal (red) and total background (blue) in the (a) ℓ^+ +jets and (b) ℓ^- +jets regions. The distributions are normalised to unit area in order to visualize the separation in the BDT response between the signal and background.

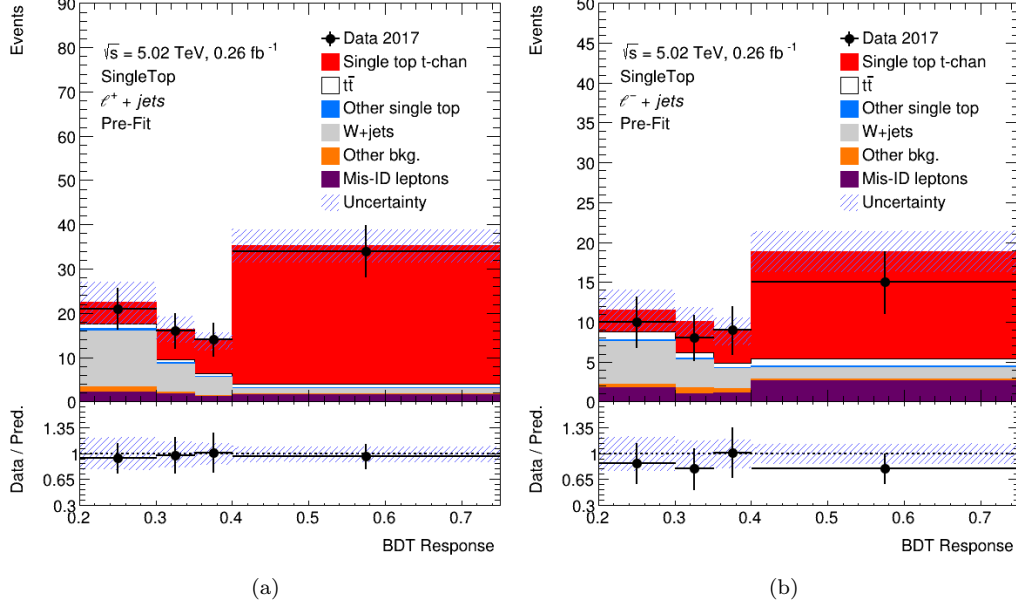


Figure 7.7: The pre-fit BDT response distribution for data (dots) in the (a) ℓ^+ +jets and (b) ℓ^- +jets regions. The MC simulation of the signal (red histograms) and various backgrounds (represented by histograms of different colours) are also included. The error bars on the dots represent the statistical uncertainty on the data while the blue cross-hatched lines correspond to the total uncertainties on the prediction. The lower panels show the ratio of the data and predicted distributions, along with the uncertainty in the ratio.

7.5 Systematic Uncertainties

Several sources of systematic uncertainties that can affect the normalization and shape of the signal and background BDT response distributions are considered. Since this analysis uses many of the same objects and MC samples as the $t\bar{t}$ measurement, it also shares a similar set of systematic uncertainties.

7.5.1 Luminosity and Pileup

The luminosity scale was measured again after the publication of the $t\bar{t}$ measurement with an uncertainty in the integrated luminosity of 1.0%. This was done by following the methodology discussed in Ref. [101], using the LUCID-2 detector [192] for the primary luminosity measurements, complemented by measurements using the inner detector and calorimeters.

Similar to the $t\bar{t}$ measurement, the pileup uncertainty is not considered for this dataset and although the LHC beam energy is known to be within 0.1%, it is unknown how the LHC beam energy affects the t -channel production cross-sections. Thus, the LHC beam energy uncertainty is not incorporated into this measurement.

7.5.2 Uncertainties on Reconstructed Objects

Uncertainties from leptons, E_T^{miss} , JER, and b -tagging are treated in exactly the same as discussed in Section 6.7.2.

The JES calibrations and uncertainties derived with the $\sqrt{s} = 13$ TeV data were applied unchanged to this dataset except for jet flavour composition uncertainties which were recalculated, exactly like the $t\bar{t}$ cross-section measurement at $\sqrt{s} = 5.02$ TeV. Due to the inclusion of forward jets in this analysis, the JES in-situ correction is slightly different from the one used for the $t\bar{t}$ measurement and two non-closure uncertainties are included in this analysis instead of one. This is done because the single uncertainty scheme used in the $t\bar{t}$ measurement was known to be a significant overestimate of the actual uncertainties, which are better represented through two NPs. To avoid double counting JES uncertainties that are covered by the in-situ measurement, only nineteen of the 29 uncorrelated components of the JES uncertainty are considered. The in-situ correction with forward jets and its corresponding uncertainties are further discussed in Section 4.4.4.

7.5.3 Uncertainties on Signal Modelling

The uncertainty due to missing higher-order QCD corrections in the ME computation, ISR, FSR, and choice of parton shower and hadronization model in the t -channel sample are determined the same way as the $t\bar{t}$ measurement (see Section 6.7.4).

The matching uncertainty in the signal is estimated by comparing the nominal sample from POWHEG BOX interfaced to PYTHIA 8 with an alternative sample generated with the pTHard parameter set to 1 instead of the nominal 0.

PDF uncertainties are evaluated for the signal the same way they were evaluated for the $t\bar{t}$ signal in the $\sigma_{t\bar{t}}$ measurement (see Section 6.7.3). The uncertainties due to the PDF choice are only estimated for the t -channel signal and $t\bar{t}$ background.

7.5.4 Uncertainties on Background Modelling

The uncertainties on the $t\bar{t}$ background from missing higher-order QCD corrections in the ME computation, ISR, FSR, choice of parton shower and hadronization mode, and matching uncertainty are the same as described in Section 6.7.3. An additional normalization uncertainty of $^{+7.5}_{-7.7}\%$ [173] arising from the uncertainty in the theoretical $t\bar{t}$ cross-section is included.

Uncertainties on the fake background estimation are considered separately for the e +jets and the μ +jets channel and a conservative 50% normalization uncertainty is used to cover the fake estimate. From Appendix I, one can see that this uncertainty overestimates the mis-modelling between data and MC in the fake lepton enriched control regions. A shape uncertainty for the fake background was studied in Appendix M, found to be negligible, and is not included in the results. However, to account for any possible shape differences in the fake lepton background, the statistical uncertainties corresponding to the fake lepton background are decorrelated from the other sources of statistical uncertainty in the prediction.

The effects of the renormalization scale, factorization scale, ISR, and FSR are evaluated for both types of single-top-quark backgrounds as fully correlated shape and normalization nuisance parameters following the prescription used for the $t\bar{t}$ background. An additional uncertainty arising from the parton shower choice is considered only in the tW production. Furthermore, the nominal tW simulated sample that uses the diagram-subtraction method [176] is compared with the nominal sample based on the diagram-removal technique [177] and the difference between the two methods is treated as an uncertainty. A normalisation uncertainty of $^{+5.6}_{-5.5}\%$ [229] and 9.5% [197] is applied to the tW , and s -channel backgrounds, respectively as independent nuisance parameters representing the theoretical uncertainty on the predicted cross-section.

The conservative Berends scaling [198] and envelope of the six point variations discussed in

Section 6.7.4 is used for the W +jets modelling uncertainties. Since there are only two jets in both regions, a 34% normalisation uncertainty on the W +jets is used for this analysis. Both the normalization and shape uncertainties are split into their W +light-quark jets, $W + \geq 1c$, and $W + \geq 1b$ contributions, for a total of six NPs representing the W +jets modelling uncertainties.

The normalisation uncertainty in the Z +jets and diboson backgrounds was conservatively taken to be 50% just like the $t\bar{t}$ measurement.

The uncertainties on the background normalisations are summarized in Table 7.4.

Table 7.4: Summary of normalisation uncertainties considered. The uncertainty on the fake background estimation is decorrelated between the e +jets and the μ +jets events.

BACKGROUND	NORMALISATION UNCERTAINTY
W +light-quark jets	$4\% \oplus 24\%$ per additional jet
$W + \geq 1c$ jets	$4\% \oplus 24\%$ per additional jet
$W + \geq 1b$ jets	$4\% \oplus 24\%$ per additional jet
$t\bar{t}$	$+7.5\%$ -7.7%
single-top-quark s -channel background	9.5%
single-top-quark tW background	$+5.6\%$ -5.5%
Diboson	50%
Z +jets	50%
Fakes	50%

7.6 Fitting Scheme

The total cross-section and ratio are measured by performing a fit to the BDT response distributions in the l^+ +jets and l^- +jets regions simultaneously. This is done by first parametrizing μ_t and $\mu_{\bar{t}}$ as functions of $\mu_{\sigma(tq + \bar{t}q)}$ and μ_{R_t} according to Equation 7.2.

$$\mu_t = \mu_{\sigma(tq + \bar{t}q)} \mu_{R_t} \frac{R_t^{\text{predicted}} + 1}{\mu_{R_t} R_t^{\text{predicted}} + 1}, \mu_{\bar{t}} = \mu_{\sigma(tq + \bar{t}q)} \frac{R_t^{\text{predicted}} + 1}{\mu_{R_t} R_t^{\text{predicted}} + 1} \quad (7.2)$$

Here, $\mu_{\sigma(tq + \bar{t}q)} = \frac{\sigma(tq + \bar{t}q)^{\text{observed}}}{\sigma(tq + \bar{t}q)^{\text{predicted}}}$, $\mu_t = \frac{\sigma_t^{\text{observed}}}{\sigma_t^{\text{predicted}}}$, $\mu_{\bar{t}} = \frac{\sigma_{\bar{t}}^{\text{observed}}}{\sigma_{\bar{t}}^{\text{predicted}}}$, $\mu_{R_t} = \frac{R_t^{\text{observed}}}{R_t^{\text{predicted}}}$. The superscripts refer to the observed and predicted cross-sections and R_t .

These equations are then used to constrain μ_t and $\mu_{\bar{t}}$ which can be measured in the l^+ +jets and l^- +jets regions, respectively, while using $\mu_{\sigma(tq + \bar{t}q)}$ and μ_{R_t} as the POIs. The statistical significance on $\sigma(tq + \bar{t}q)$ is measured according to the procedure defined in Section C.1. Note that the uncertainties on the two POIs are calculated using the MINOS minimization algorithm [232] and are thus asymmetric.

All experimental uncertainties described in Section 7.5 are taken into account and systematic uncertainties with an effect less than 0.01% are pruned in order to improve the stability of the fit.

The shape effects are smoothed when incorporated as nuisance parameters using the same algorithm as the $t\bar{t}$ pair-production cross-section measurement. All uncertainties except the first NP of the JER uncertainty and the three W +jets shape uncertainties are smoothed.

The signal **pTHard** uncertainty, uncertainties on the PS for all single-top-quark and $t\bar{t}$ samples, W +jets modelling uncertainties, uncertainties on the generator and h_{damp} variations for the $t\bar{t}$ sample, tW diagram-subtraction diagram-removal uncertainty, PDF uncertainties, JER uncertainties, MET resolution uncertainties, JES in-situ non-closure uncertainties, and lepton isolation uncertainties are symmetrized as one-sided variations. All other uncertainties are symmetrized as $\frac{\sigma_{\text{up}} - \sigma_{\text{down}}}{2}$.

7.7 Results

The fit results in

$$\sigma(tq + \bar{t}q) = 27.1^{+4.4}_{-4.1} \text{ (stat)} \text{ } ^{+4.4}_{-3.7} \text{ (syst)} \text{ pb} \quad (7.3)$$

$$R_t = 2.73^{+1.43}_{-0.82} \text{ (stat)} \text{ } ^{+1.01}_{-0.29} \text{ (syst)} \quad (7.4)$$

The observed (expected) significance for the total cross-section is measured to be 6.1σ (6.4σ) with the full fit. Figure 7.8 show the post-fit BDT response distributions for the ℓ^+ +jets and ℓ^- +jets regions and Table 7.5 shows the post-fit signal, background, and observed event yields in the ℓ^+ +jets and ℓ^- +jets regions.

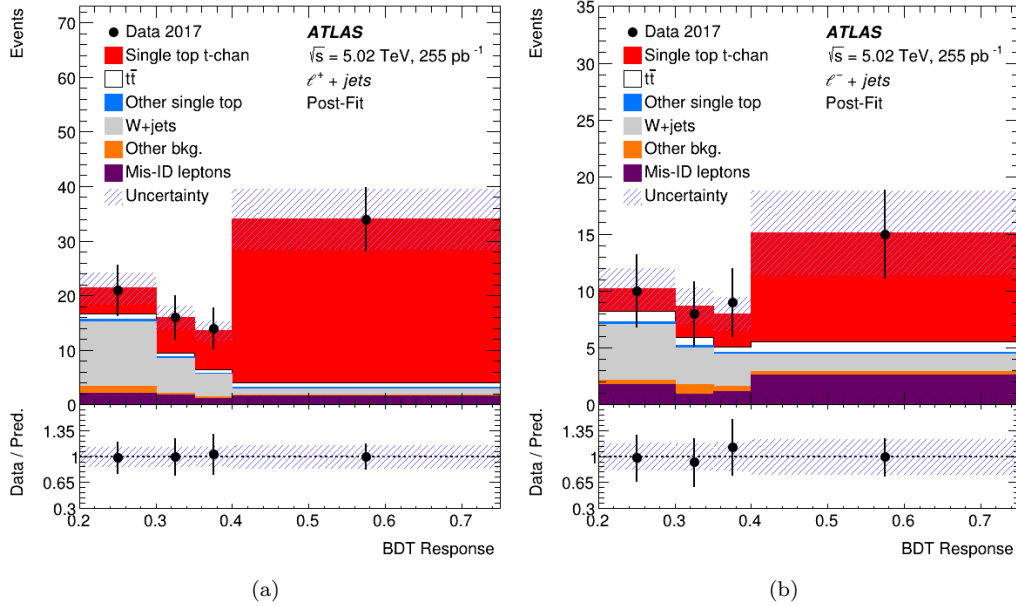


Figure 7.8: The post-fit BDT response distribution for data (dots) in the (a) ℓ^+ +jets and (b) ℓ^- +jets regions. The MC simulation of the signal (red histograms) and various backgrounds (represented by histograms of different colours) are also included. The error bars on the dots represent the statistical uncertainty on the data while the blue cross-hatched lines correspond to the total uncertainties on the prediction. The lower panels show the ratio of the data and predicted distributions, along with the uncertainty in the ratio.

Figure 7.9 shows the pulls and constraints for the fitted nuisance parameters. The pulls of all nuisance parameters are found to be within 0.2 standard deviations from their input value and all constraints are smaller than 10% of their input uncertainty.

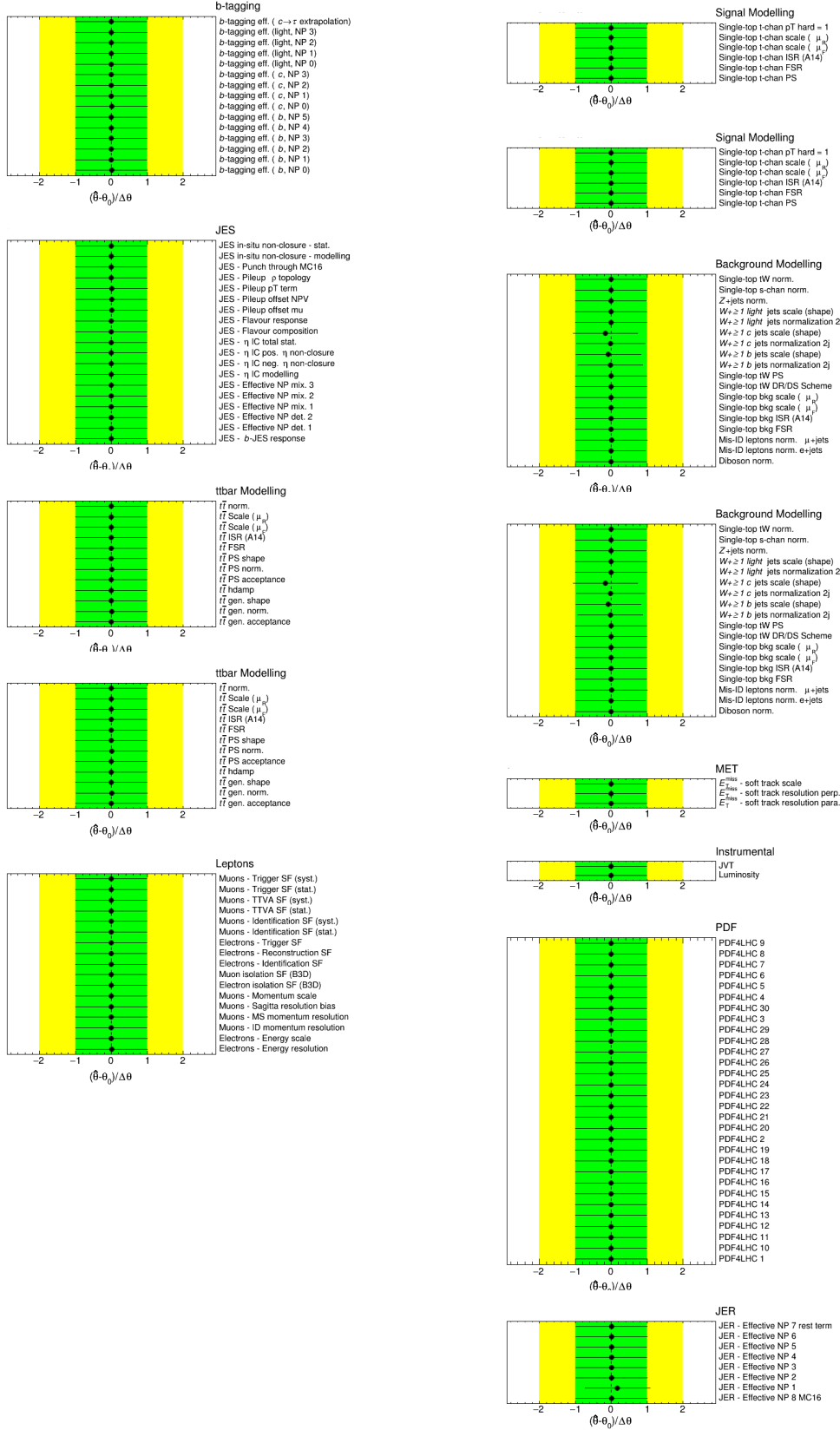


Figure 7.9: Nuisance parameter pulls after a fit to data using the BDT response distributions. NPs are arranged in different groups.

Table 7.5: Number of post-fit signal, background and observed data events in the ℓ^+ +jets and ℓ^- +jets regions. The ‘Other single top’ category contains the tW associated production and s -channel contributions. The uncertainties in the signal and background yields include the statistical uncertainties, all systematic uncertainties, and the correlations between them. The uncertainty in the total prediction includes correlations between all systematic uncertainties and thus does not equal the sum in quadrature from the individual components. In this table, the uncertainties have been symmetrised, but full asymmetric uncertainties are used to obtain the final results.

Source	Number of events	
	ℓ^+ +jets	ℓ^- +jets
t -channel signal	49 ± 9	17 ± 8
W + jets	23 ± 5	12 ± 3
Misidentified leptons	7 ± 3	7 ± 3
$t\bar{t}$	3 ± 0.5	3 ± 0.5
Z + jets and diboson	2 ± 1	2 ± 1
Other single-top-quark production	1 ± 0.2	1 ± 0.5
Total predicted	85 ± 9	42 ± 7
Data	85	42

The correlations between nuisance parameters are shown in Figure 7.10. Only NPs which have a correlation of at least 10% with a different NP are shown in the plot. The largest correlations exist between certain systematic NPs that are highly ranked and the POIs. Furthermore, there is some slight correlation between the shape and normalization NPs representing the W +jets.

JER - Effective NP 1	100.0	-2.3	4.8	0.8	3.3	0.7	12.9	2.9	9.1	6.2	16.6	-14.7
JES - Pileup offset mu	-2.3	100.0	1.1	0.1	0.4	-0.2	2.8	1.6	1.9	0.9	-5.3	13.6
Mis-ID leptons norm. e+jets	4.8	1.1	100.0	-1.8	-2.4	-0.3	-9.4	-2.1	-5.9	-1.0	23.4	-27.9
JES in-situ non-closure - stat.	0.8	0.1	-1.8	100.0	-1.7	-0.5	-4.5	2.4	-2.4	1.5	-9.1	18.1
Single-top t-chan PS	3.3	0.4	-2.4	-1.7	100.0	-0.3	-6.0	1.1	-3.4	0.5	-3.8	37.8
Single-top t-chan pT hard = 1	0.7	-0.2	-0.3	-0.5	-0.3	100.0	-0.2	-0.0	-0.0	-0.5	0.5	-13.1
$W_{\geq 1} b$ jets normalization 2j	12.9	2.8	-9.4	-4.5	-6.0	-0.2	100.0	-2.2	-14.0	-2.0	5.3	-17.4
$W_{\geq 1} b$ jets scale (shape)	2.9	1.6	-2.1	2.4	1.1	-0.0	-2.2	100.0	-2.2	-16.6	-8.5	5.6
$W_{\geq 1} c$ jets normalization 2j	9.1	1.9	-5.9	-2.4	-3.4	-0.0	-14.0	-2.2	100.0	-1.2	7.5	-11.8
$W_{\geq 1} c$ jets scale (shape)	6.2	0.9	-1.0	1.5	0.5	-0.5	-2.0	-16.6	-1.2	100.0	-0.2	3.5
$\mu(R_t)$	16.6	-5.3	23.4	-9.1	-3.8	0.5	5.3	-8.5	7.5	-0.2	100.0	-29.9
$\mu(\text{tot. } t\text{-chan})$	-14.7	13.6	-27.9	18.1	37.8	-13.1	-17.4	5.6	-11.8	3.5	-29.9	100.0

Figure 7.10: Correlations of nuisance parameters in a fit to data using the BDT response distributions.

To check the fit stability and map the likelihood function, a likelihood scan was calculated by scanning over various values of the two POIs and determining the difference in the negative log-likelihood between the scanned value and the best fit value. The resulting plot is shown in Figure 7.11. The same plot is also shown in Figure 7.12, but the scan was performed over a smaller range. From these plots, it is clear that the likelihood has a minimum near its best-fit value. It is interesting to note that there is a significant asymmetry in the likelihood and smaller values of both R_t and the total cross-section lead to large differences in the negative log-likelihood, with respect to the minimum. This is to be expected since there is a clear asymmetry in the single-top-quark and single-antitop-quark yields as well as the total yields. The uncertainties on the two variables can be extracted by determining the point where the negative log-likelihood difference is equal to 0.5.

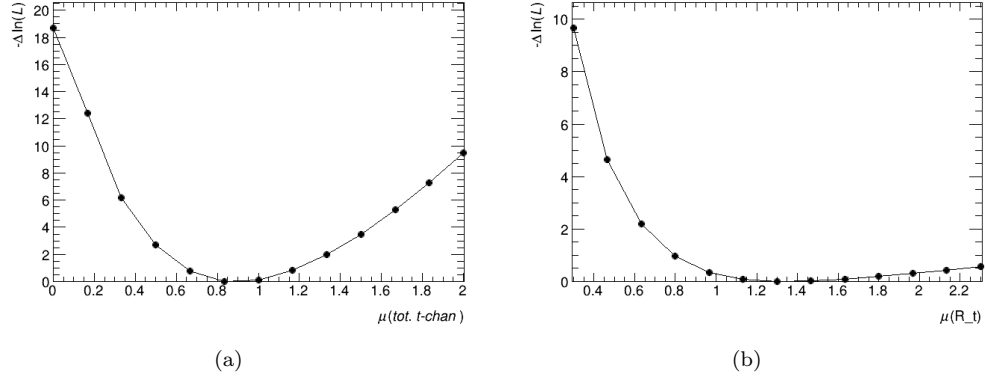


Figure 7.11: Likelihood scan for (a) $\mu_{\sigma(tq + \bar{t}q)}$ and (b) μ_{R_t} in a fit to data using the BDT response. The x-axis is the value of the scanned variable and the y-axis shows the difference in the negative log-likelihood between the scanned value and the best fit value.

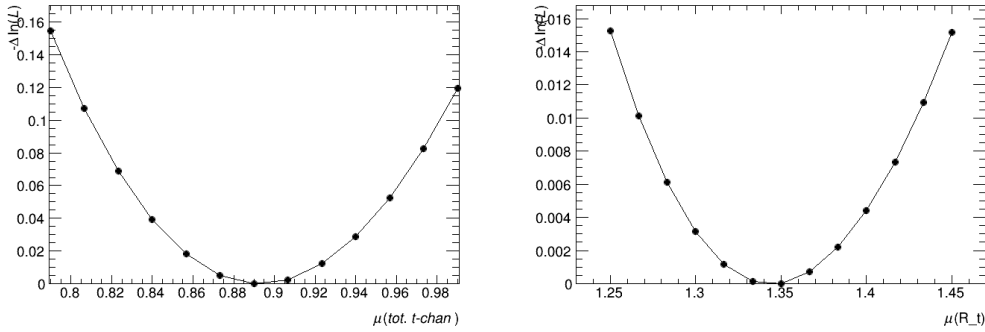


Figure 7.12: Likelihood scan for (a) $\mu_{\sigma(tq + \bar{t}q)}$ and (b) μ_{R_t} in a fit to data using the BDT response. The x-axis is the value of the scanned variable and the y-axis shows the difference in the log-likelihood between the scanned value and the best fit value.

The ranking plots for both $\mu_{\sigma(tq + \bar{t}q)}$ and μ_{R_t} after a fit to data are shown in Figure 7.13.

For the $\mu_{\sigma(tq + \bar{t}q)}$ parameter, the signal PS uncertainty is the systematic uncertainty with the largest effect and one would expect it to be a leading uncertainty due to the explicit requirement of two jets in the selection - which is highly correlated with the choice of PS. The PS uncertainty is followed by the over-estimated normalization uncertainty in the fake lepton background, which is similar in magnitude to the dominant signal-modelling uncertainty. Note that the fake lepton background is $\sim 90\%$ dominated by fake electron events and so only the e +jets fake lepton normalization uncertainty appears in the ranking plot. This is followed by a W +jets normalization uncertainty which is also an overestimate since it is based on Berends scaling. This uncertainty is followed by the statistical component of the JES in-situ uncertainty due to the low statistics for the forward jets, as seen in Section 4.4.4. Finally, there are some JES uncertainties which show up in the ranking plot due to the multiple p_T cuts in the selection.

For μ_{R_t} , the normalization uncertainty in the fake lepton background is the largest uncertainty contribution and is followed by uncertainties from the JER, the statistical uncertainties in the prediction, uncertainties from the JES, and the W +jets background. In the ratio, uncertainties sensitive to the lepton charge appear high in the ranking since most other uncertainties must cancel out.

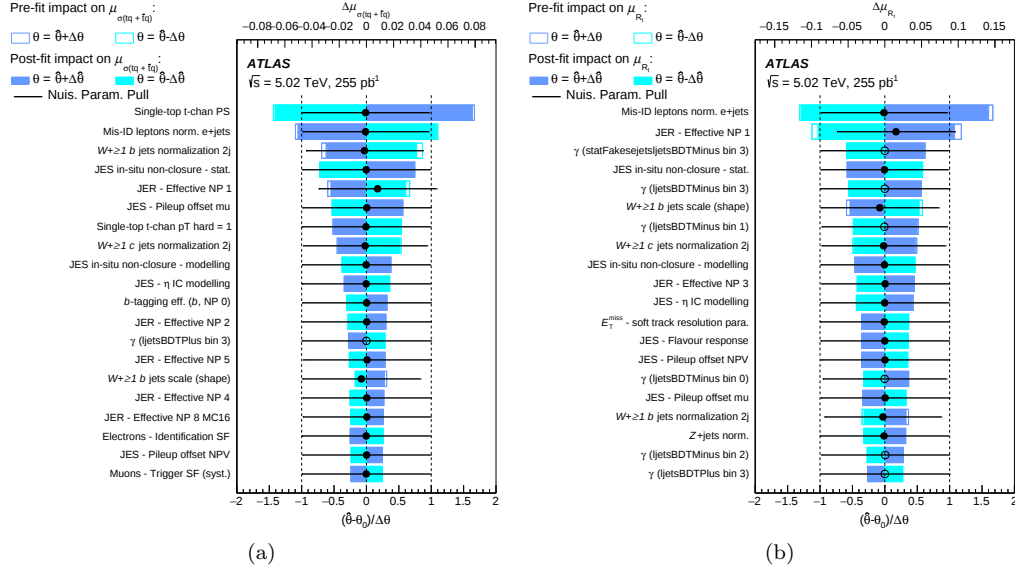


Figure 7.13: Ranking plots showing the effect of the top 20 sources of uncertainties on the signal strength in a fit to data with the BDT response distributions for (a) $\mu_{\sigma(tq + \bar{t}q)}$ and (b) μ_{R_t} . The black point shows the pulls of various NPs (along the bottom x-axis) whereas the shaded coloured bands show the difference in the POI (along the top x-axis) when varying a NP by $+1\sigma$ (dark blue) and -1σ (light blue). The shaded bands represent the post-fit uncertainties whereas the band with an outline is based on the pre-fit uncertainties.

Table 7.6 shows a breakdown of the contributions from different categories of systematic uncertainties for $\sigma(tq + \bar{t}q)$ and R_t in a fit to data. The squared uncertainties are calculated by fixing the

Table 7.6: Sources of uncertainty for measurements of $\sigma(tq + \bar{t}q)$ and R_t at $\sqrt{s} = 5.02$ TeV. The systematic uncertainties for both the values do not add up in quadrature to the total systematic uncertainty because of correlations in the fit parameters. In this table, the uncertainties have been symmetrized, but full asymmetric uncertainties are used to obtain the final results.

Category	$\delta\sigma(tq + \bar{t}q)/\sigma(tq + \bar{t}q)[\%]$	$\delta R_t/R_t[\%]$
Single-top-quark signal modelling	8.6	4.1
Parton distribution functions	0.5	0.8
Misidentified lepton background	6.3	11.1
$W + \geq 1b$ jets modelling	3.9	4.4
$W + \geq 1c$ jets modelling	2.7	3.4
Z +jets normalisation	1.1	2.1
$t\bar{t}$ modelling	0.8	1.2
Single-top-quark background modelling	0.6	2.1
$W + \geq 1$ light jets modelling	0.3	0.4
Diboson normalisation	0.1	0.3
Jet energy resolution	4.6	7.8
$\sqrt{s} = 5.02$ TeV JES correction	4.4	5.1
Jet energy scale	4.0	5.3
Flavour tagging	2.0	1.3
Electron reconstruction	1.4	0.5
Muon reconstruction	1.3	0.7
Integrated luminosity	1.3	0.4
E_T^{miss}	0.6	2.4
Jet-vertex tagging	0.07	0.05
Simulation's statistical uncertainty	2.3	6.5
Data's statistical uncertainty	16	38
Total systematic uncertainty	15	18
Total uncertainty	21	42

set of nuisance parameters corresponding to a category, repeating the fit, and taking a difference between the squares of the resulting uncertainty and the total uncertainty of the nominal fit. The total uncertainty quoted is the sum in quadrature of the total systematic uncertainty and the data's statistical uncertainty. The total uncertainty on $\sigma(tq + \bar{t}q)$ is dominated by the statistical uncertainty followed by uncertainties in the signal modelling, misidentified lepton modelling, JER, the in-situ correction, JES, and the modelling of $W + \geq 1b$ jets. The total uncertainty on R_t is dominated by the statistical uncertainty, followed by uncertainties in the misidentified lepton modelling, JER, the statistical uncertainty in the prediction, the JES in-situ correction, and other JES uncertainties.

7.7.1 Calculation of $\sigma(tq)$, $\sigma(\bar{t}q)$, and $f_{LV} \cdot |V_{tb}|$

The individual cross-sections are calculated to be

$$\sigma(tq) = 19.8_{-3.1}^{+3.9} \text{ (stat)} \text{ }_{-2.2}^{+2.9} \text{ (syst)} \text{ pb} \quad (7.5)$$

$$\sigma(\bar{t}q) = 7.3_{-2.1}^{+3.2} \text{ (stat)} \text{ }_{-1.5}^{+2.8} \text{ (syst)} \text{ pb} \quad (7.6)$$

The uncertainties are calculated using linear error propagation techniques that account for the -30% correlation between μ_{R_t} and $\mu_{\sigma(tq + \bar{t}q)}$.

The t -channel single-top-quark production cross-section depends on $f_{LV}^2 \cdot |V_{tb}|^2$, where f_{LV} is a left-handed form factor that is unity in the SM and V_{tb} is a component of the CKM matrix [233]. By assuming that the CKM matrix elements $|V_{td}|$ and $|V_{ts}|$ are much smaller than $|V_{tb}|$ ² and that the Wtb vertex is left-handed, the measured cross-section gives

$$f_{LV} \cdot |V_{tb}| = 0.94^{+0.08}_{-0.07} \text{ (stat)} \quad {}^{+0.08}_{-0.06} \text{ (syst)} \quad (7.7)$$

The experimental uncertainties in the measured $\sigma(tq + \bar{t}q)$ and the uncertainties in the predicted $\sigma(tq + \bar{t}q)$ arising from scale variations, choice of PDF, α_s , and m_t dependence are all summed in quadrature.

7.7.2 Summary Plots

Figure 7.14 compares the measured $\sigma(tq + \bar{t}q)$ and R_t with various PDF predictions at $\sqrt{s} = 5.02$ TeV. Similarly, Figure 7.15 compares the measured $\sigma(tq)$ and $\sigma(\bar{t}q)$ with predictions obtained using various PDF sets. From these plots, a slight 1σ “tension” can be seen between the observed cross-sections and the ATLASpdf21 predictions. Figure 7.16 shows the various inclusive single-top-quark production cross-sections and R_t , as measured by the ATLAS and CMS Collaborations, as a function of the centre-of-mass energy. Finally, Figure 7.17 shows the various ATLAS and CMS measurements of $f_{LV} \cdot |V_{tb}|$.

²Consistent with estimates of their values when assuming unitarity of the CKM matrix [50]

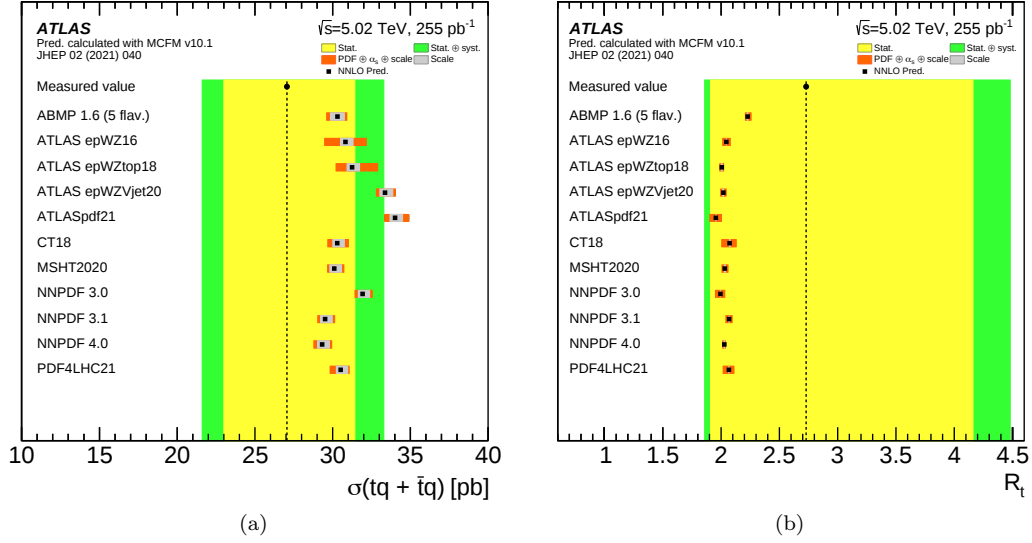


Figure 7.14: Comparison of (a) $\sigma(tq + \bar{t}q)$ and (b) R_t measured at $\sqrt{s} = 5.02$ TeV to various predictions from NLO and NNLO PDF sets. The dashed line shows the experimental measurement with the statistical (inner yellow band) and total (outer green band) uncertainties overlaid. Uncertainties from the scale variations (inner grey band) and the sum in quadrature of the scale variations, PDF variations, and α_s variations (outer orange band) are shown for the various PDF predictions.

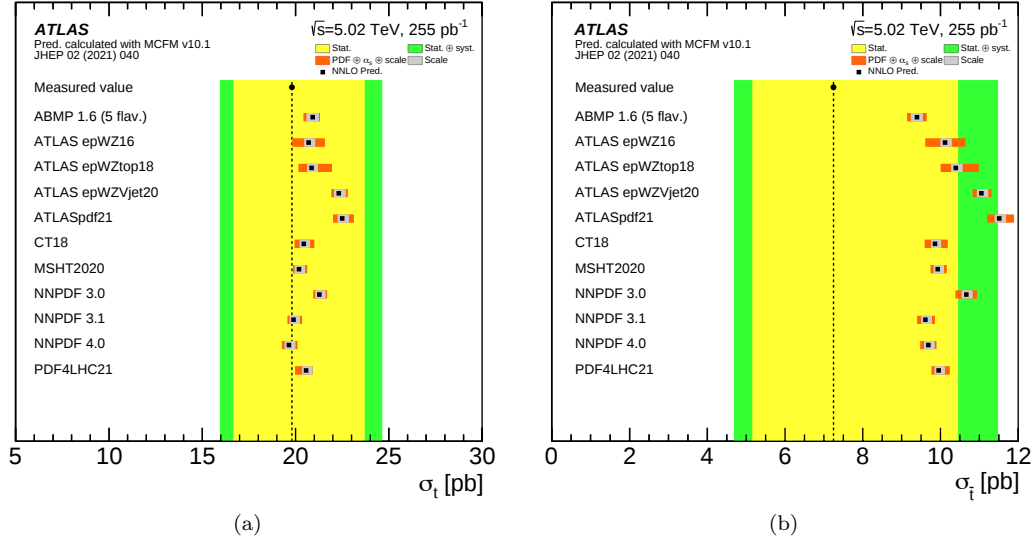


Figure 7.15: Comparison of (a) $\sigma(tq)$ and (b) $\sigma(\bar{t}q)$ measured at $\sqrt{s} = 5.02$ TeV to various predictions from NLO and NNLO PDF sets. The dashed line shows the experimental measurement with the statistical (inner yellow band) and total (outer green band) uncertainties overlaid. Uncertainties from the scale variations (inner grey band) and the sum in quadrature of the scale variations, PDF variations, and α_s variation (outer orange band) are shown for the various PDF predictions.

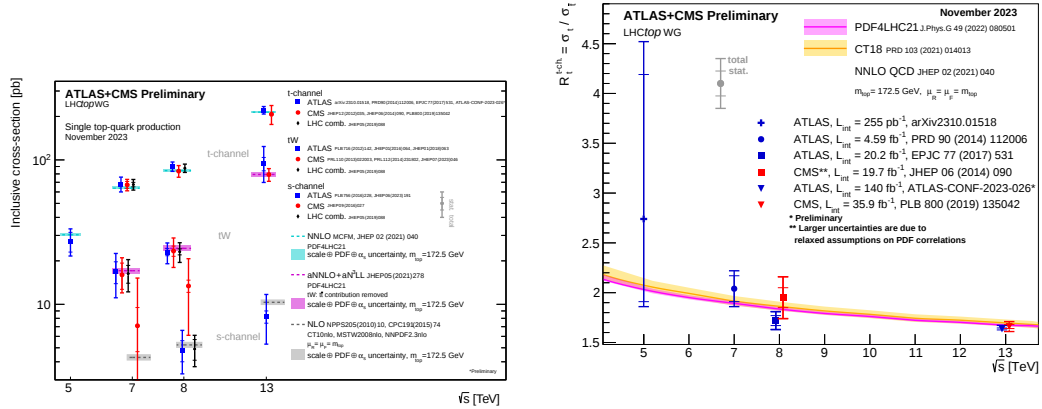


Figure 7.16: Summary of ATLAS and CMS measurements of (a) the single-top-quark production cross-sections in various channels and (b) the t -channel single-top-quark production cross-section to the t -channel single-antitop-quark production cross-section (R_t), as a function of the centre-of-mass energy. The measurements in (a) are compared to theoretical calculations that are approximately NNLO in QCD with an approximate NNNLL resummation for the tW -associated production, NNLO in QCD for the t -channel production, and only NLO in QCD for the s -channel production. The measurements in (b) are compared to predictions that are NNLO in QCD.

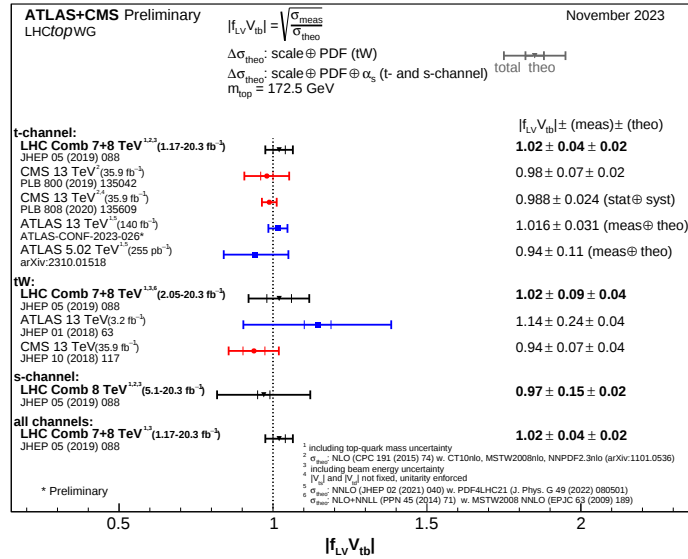


Figure 7.17: Summary of the ATLAS and CMS extractions of the CKM matrix $f_{LV} \cdot |V_{tb}|$ term from single top-quark measurements. The total uncertainty is composed of the uncertainty on the theoretical prediction for the single-top-quark production cross-section along with the uncertainty originating from the experimental measurement of the cross-section.

Chapter 8

Conclusion

Although no new physics beyond the SM have been directly observed in the data collected by the LHC, it is still possible to probe the SM by performing precision measurements. Given enough precision, measurements can be compared with SM predictions to allow for a model-independent approach to searching for physics beyond the SM. With no new particles discovered at the LHC, precision measurements are becoming an important contribution to understanding and testing the SM.

With the near future of high energy particle physics being dominated by hadron colliders, the understanding of the proton PDFs is a necessity. A better understanding of PDFs would lead to improved theoretical and experimental results in particle physics such as Higgs boson precision measurements. Another such experimental result that would benefit from improved PDFs is the controversial W boson mass measurement by CDF [41], which is higher than the theoretical prediction (extracted from fits of electroweak parameters) by $\sim 7\sigma$. Due to the sensitivity of the measured W boson mass measurements to the PDFs, improvements to PDFs would help confirm or deny the CDF results.

Certain cross-section measurements of processes at a lower centre-of-mass energies can provide unique information that can help constrain select PDFs in certain phase spaces. Thus, the measurements of the $t\bar{t}$ pair-production and single-top-quark t -channel production cross-sections at $\sqrt{s} = 5.02$ TeV presented in this thesis can be used to improve our knowledge of PDFs since PDFs are sensitive to cross-section measurements at various centre-of-mass energies. At different centre-of-mass energies, the production mechanism can change (i.e. top-quark pair production) and thus be sensitive to alternate PDFs. Furthermore, measurements of cross-sections at various centre-of-mass energies can provide constraints when determining PDFs due to the DGLAP evolution of PDFs. Since these measurements are made at $\sqrt{s} = 5.02$ TeV, they can also provide a unique test of the SM at a different centre-of-mass energy.

Both cross-section measurements were performed using $\sim 255 \text{ pb}^{-1}$ of pp collision data collected by the ATLAS detector in 2017. The $t\bar{t}$ cross-section measurement was performed in both the dilepton and lepton+jets channels, and then statistically combined. The dilepton channel measurement was performed by applying kinematic cuts and extracting the fitted cross-section. The lepton+jets channel measurement on the other hand trained two BDTs to separate signal from background in six regions. The regions were defined by kinematic cuts and the number of total jets and jets associated with a b -hadron decay. A profile likelihood fit to the BDT distribution was then used to extract the cross-section. The cross-section from the dilepton channel at $\sqrt{s} = 5.02 \text{ TeV}$ is measured to be

$$\sigma_{t\bar{t}} = 65.7 \pm 4.5 (\text{stat.}) \pm 1.6 (\text{syst.}) \pm 1.2 (\text{lumi.}) \pm 0.2 (\text{beam}) \text{ pb} \quad (8.1)$$

whereas the cross-section in the lepton+jets channel was measured to be

$$\sigma_{t\bar{t}} = 68.2 \pm 0.9 (\text{stat.}) \pm 2.9 (\text{syst.}) \pm 1.1 (\text{lumi.}) \pm 0.2 (\text{beam}) \text{ pb} \quad (8.2)$$

The four uncertainties correspond to the statistical uncertainty in the data, systematic uncertainties in the detector, signal modelling, and background modelling, uncertainty in the integrated luminosity, and the LHC beam energy uncertainty. These values are in good agreement with the NNLO+NNLL SM prediction of $\sigma_{t\bar{t}} = 68.2^{+5.2}_{-5.3} \text{ pb}$. The uncertainty in both channels is dominated by low statistics, the uncertainty in the integrated luminosity, and uncertainties associated with jets and signal modelling. With a relative uncertainty of 4.5%, the lepton+jets $t\bar{t}$ cross-section measurement at $\sqrt{s} = 5.02 \text{ TeV}$ is the most precise measurement performed by ATLAS in this channel! This is possible due to the optimizations of the BDT and analysis regions and lower signal-modelling uncertainties than ones seen at $\sqrt{s} = 13 \text{ TeV}$. The lower signal-modelling uncertainties occur because the MC is tuned using data collected at $\sqrt{s} = 7 \text{ TeV}$ and $\sqrt{s} = 8 \text{ TeV}$, which models $\sqrt{s} = 5.02 \text{ TeV}$ data better than data at $\sqrt{s} = 13 \text{ TeV}$.

The combined cross-section is determined to be

$$\sigma_{t\bar{t}} = 67.5 \pm 0.9 (\text{stat.}) \pm 2.3 (\text{syst.}) \pm 1.1 (\text{lumi.}) \pm 0.2 (\text{beam energy}) \quad (8.3)$$

This is also in good agreement with the SM prediction and has a lower relative uncertainty of 3.9% due to the combination. The combined measurement was compared with predictions from various PDF sets in Figure 6.16. The measured value is compatible with the predictions from all the PDF sets considered, except for ABMP16, which has a softer gluon distribution and predicts a $\sigma_{t\bar{t}}$ value 2.2 standard deviations lower than measured. The effect of the measurement on the ATLASpdf21 set [60] is determined for $Q^2 = 10^4 \text{ GeV}^2$. At $Q^2 = 10^4 \text{ GeV}^2$, the addition of the new data reduces the gluon PDF uncertainty in the region of Bjorken- x above $x \approx 0.05$. The uncertainties in the valence and sea quark PDFs are unaffected. The inclusion of $\sqrt{s} = 5.02 \text{ TeV}$ data also seems to prefer a harder gluon for $x > 0.1$, as the gluon PDF increases by $\mathcal{O}(1\%)$. In this range, this is approximately equivalent to the effect of including 8 TeV and 13 TeV differential $t\bar{t}$ cross-section data used for the ATLASpdf21 fit. Thus, it can be seen that the gluon PDF is highly sensitive to $t\bar{t}$ measurements at $\sqrt{s} = 5.02 \text{ TeV}$ and differential measurements at $\sqrt{s} = 5.02 \text{ TeV}$ could lead to further reductions in uncertainties and increased understanding of the proton structure.

The t -channel cross-section measurement is the first one made at $\sqrt{s} = 5.02$ TeV and was made after the success of the $t\bar{t}$ cross-section measurement. The measurement was performed by applying selection cuts and training a BDT to separate t -channel single-top-quark events from background, with a leptonic decay of the W boson associated with the top quark. Major sources of background include the W +jets, misidentified lepton, and $t\bar{t}$ processes. The events are categorized as arising from the top quark (positively charged lepton) or the antitop quark (negatively charged lepton). A profile likelihood fit is then used to extract the t -channel cross-section and the ratio of top-to-antitop quark production. From these two quantities, it is possible to calculate the measured value of the individual top-quark and antitop-quark production cross-sections and the $f_{LV} \cdot |V_{tb}|$ term of the CKM matrix. The total cross-section and ratio are measured to be

$$\sigma(tq + \bar{t}q) = 27.1_{-4.1}^{+4.4} \text{ (stat)} \text{ }_{-3.7}^{+4.4} \text{ (syst)} \text{ pb} \quad (8.4)$$

$$R_t = 2.73_{-0.82}^{+1.43} \text{ (stat)} \text{ }_{-0.29}^{+1.01} \text{ (syst)} \quad (8.5)$$

The observed (expected) significance for the total cross-section is measured to be 6.1σ (6.4σ) and allows one to claim an observation of single-top-quark production at $\sqrt{s} = 5.02$ TeV. The dominant sources of uncertainties in this measurement are the data statistics, background modelling, and signal modelling. The individual cross-sections are measured to be

$$\sigma(tq) = 19.8_{-3.1}^{+3.9} \text{ (stat)} \text{ }_{-2.2}^{+2.9} \text{ (syst)} \text{ pb} \quad (8.6)$$

$$\sigma(\bar{t}q) = 7.3_{-2.1}^{+3.2} \text{ (stat)} \text{ }_{-1.5}^{+2.8} \text{ (syst)} \text{ pb} \quad (8.7)$$

All of these are in good agreement with the NNLO+NNLL SM prediction of $\sigma(tq) = 20.3_{-0.4}^{+0.5}$ pb, $\sigma(\bar{t}q) = 10.0_{-0.3}^{+0.2}$ pb, $\sigma(tq + \bar{t}q) = 30.3_{-0.5}^{+0.7}$ pb. The ratio R_t is predicted to be $R_t = 2.03_{-0.07}^{+0.06}$. Finally, the $f_{LV} \cdot |V_{tb}|$ term is measured to be

$$f_{LV} \cdot |V_{tb}| = 0.94_{-0.07}^{+0.08} \text{ (stat)} \text{ }_{-0.06}^{+0.08} \text{ (syst)} \quad (8.8)$$

which is found to be in good agreement with the PDG value of 1.014 ± 0.029 [50].

The measured values of all t -channel cross-sections are compared to predictions from various PDF sets but due to the large statistical uncertainty in the measured value, no PDF sets can be excluded. However, all PDF sets seem to systematically prefer a larger value of the antitop-quark production cross-section and the total cross-section, and consequently a lower value of R_t than what is observed. This could indicate a systematic effect in the PDFs that this measurement could affect.

Both cross-section measurements at $\sqrt{s} = 5.02$ TeV are in good agreement with their SM prediction and as seen by the study on the ATLASpdf21 set, such measurements can provide additional information in PDF fits. Although the quantitative effect of the t -channel measurement on PDFs was not studied, there is some indication that it could also provide new information to PDF fits. With these two measurements and a renewed interest in PDFs, unique datasets such as the 5.02 TeV dataset can be used to address phenomena that goes above their original scope. With more pp data at lower centre-of-mass energies ($\sqrt{s} = 5.36$ TeV) expected in Run 3, there are unique opportunities to increase the precision of these two measurements and also perform differential

cross-section measurements. Differential cross-section measurements may be even more sensitive to variations in PDFs. Additionally, there might be a possibility to observe and measure other top-quark production processes such as tW associated single-top-quark production, at $\sqrt{s} = 5.02$ TeV.

In summary, the precision measurements presented in this thesis not only reaffirm the robustness of the SM but also show the utility of analyzing lower-energy datasets in conjunction with those coming from the highest pp collisions, while also paving the way for further advancements in the understanding of particle physics, at the intersection of precision measurements and PDF studies. These hold promise for increasing our understanding of proton structure and improving precision SM measurements that rely on this knowledge.

Appendices

Appendix A

Contributions to the ATLAS Collaboration

Over the course of my PhD I had the pleasure of working on many different projects, which are summarized in this appendix. Beyond the two analyses presented in this thesis, I was involved in a search for a hypothetical fourth generation “vector-like quark” (VLQ) that decayed into an energetic top quark and Higgs boson, in an all-hadronic final state [234]. This was the first measurement that searched for a VLQ with the full Run 2 dataset. In this analysis, I was responsible for developing the analysis framework, implementing the data-driven multijet estimate, the fitting framework, editing the internal note and paper draft, and acting as the liaison with the VLQ combination analysis. Through the effort of the analysis team, we were the first analysis using the full LHC Run 2 data and were able to place the most stringent limits on single VLQ production at the time. In conjunction with this analysis, I started working on the $\sqrt{s} = 5.02$ TeV $t\bar{t}$ cross-section measurement in the single-lepton channel. For this measurement, I was the internal note editor, participated in paper writing and editing, contributed to general framework development, was responsible for the fitting and plotting framework, and the combination effort.

Since Spring 2020, I have been participating in the operation of the ATLAS LAr calorimeter and commissioning of its Phase-1 upgrade. I was one of the Run Coordinators, responsible for the efficient operation of the LAr detector during the shutdown and Run 3. I have made significant contributions to the development and maintenance of online software, specifically for the tools used to run and validate calibration during commissioning and the low-level software that controls the calorimeter. Due to my contributions, I have been appointed as the Co-coordinator in charge of the LAr online software team since September 2022. As the online software coordinator, I continued my responsibilities for the development, maintenance, and integration of the online software used by the LAr calorimeter. Beyond my personal contributions, I coordinated a team of 20 engineers and researchers to tackle various operations issues and was one of the many experts that helped optimize and ensure steady LAr operations. Major projects undertaken during my tenure as online

software coordinator include the development of the LAr Super Cell Killer (LArSkill) and an imagery framework for supercell rates (LArSoup). The tools were used to mask noisy LAr supercells and visualize the rate of events passing an energy threshold, respectively. I also submitted a proposal for a CERN summer student project that was accepted for the summer off 2023. My student and I investigated the energy spectrum seen by the LAr calorimeter and developed a visualization tool to plot energy spectrums of a calorimeter supercell. This study eventually led us to discover a bug in the firmware of the LAr hardware that was successfully fixed by the end of the summer. I am one of the internal authors of the paper summarizing the Phase-1 upgrade and its performance [235].

In the summer of 2022, I initiated and lead the measurement of the t -channel single-top-quark production cross-section at $\sqrt{s} = 5.02$ TeV. I was responsible for all aspects of the analysis, including the framework development, JES studies, BDT implementation, fitting, and internal note and paper writing.

Beyond the official analyses, I am working on studies of the measurement of the SM tH production and the constraints offered by a differential top-quark pair cross-section measurement at $\sqrt{s} = 5.02$ TeV on the proton PDFs.

Appendix B

Details on the Reconstruction Algorithms in ATLAS

B.1 Electron Reconstruction, Identification, and Isolation

Figure B.1 shows the effect of applying the GSF algorithm on the $q \cdot \frac{d_0}{\sigma(d_0)}$ distribution for tracks matched to truth level electrons in MC, and the relative difference between the truth and reconstructed q/p for a candidate electron. Both figures show an improved response on track parameters associated with electrons, after applying the GSF algorithm [113].

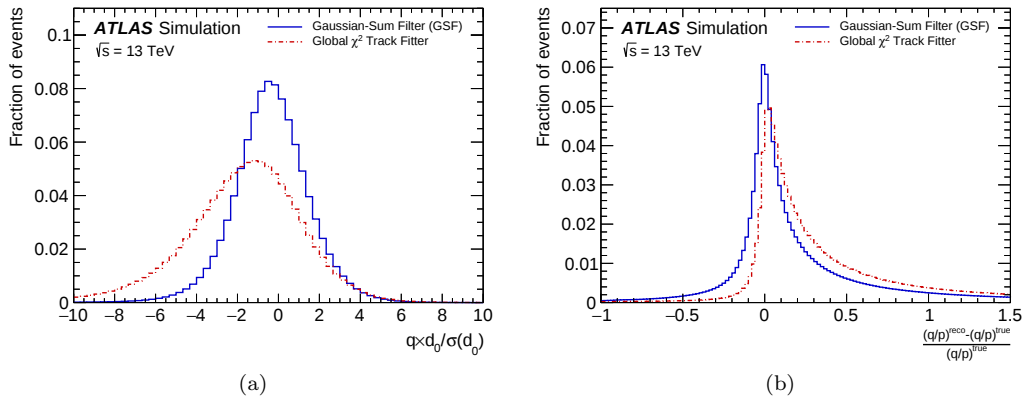
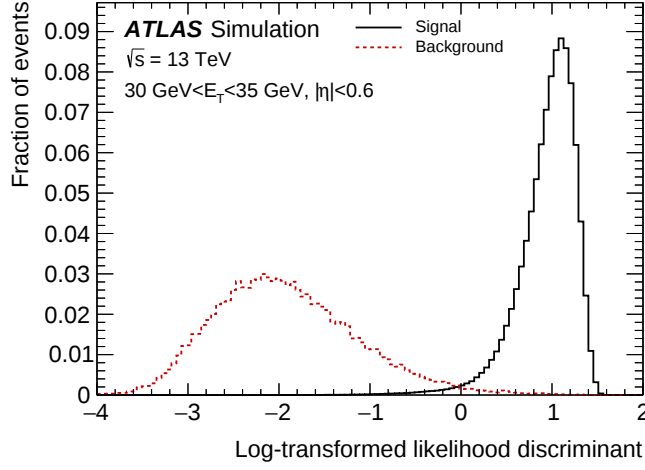


Figure B.1: Distributions of (a) the reconstructed electron charge divided by the relative uncertainty on the transverse impact parameter d_0 of the electron track and (b) the relative difference between the reconstructed and generator level electron candidate's, charge-to-momentum ratio q/p . The distributions are shown for tracks fitted with only the Global χ^2 track fitter (dashed red lines) and for tracks fitted with the additional GSF (solid blue line). All distributions were simulated using single-electron samples and both distributions are normalized to unity.

Figure B.2 shows an example of the d_L ¹ distribution for $Z \rightarrow ee$ MC and the set of various simulated backgrounds discussed in Ref. [113]. Note the distinct shape difference between the signal and background distributions.



(a)

Figure B.2: The d_L discriminant distributions scaled by $\frac{1}{15}$, for reconstructed electron candidates with $|\eta| < 0.6$ and E_T between 30 and 35 GeV, from $Z \rightarrow ee$ signal events (solid black line) and background events simulating fake electrons (dashed red line). Both distributions are normalized to unity.

Figure B.3 shows the average $E_{T, \text{cone}}^{\text{isol}}$ as a function of the simulated single electron E_T after subtracting the three terms [113]. The leakage correction increases with E_T whereas the pileup correction is constant over the E_T range.

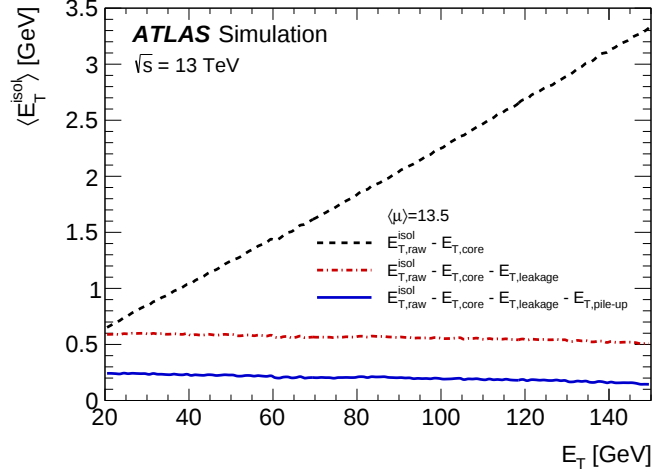
B.2 Electron Efficiencies and Scale Factors

This section discusses the efficiency and scale factor measurements measured by the ATLAS detector between 2015 and 2017. Details on the data and simulation samples, selection requirements, and background treatments used in the efficiency measurements can be found in Ref. [108]. Systematic uncertainties on the efficiencies and their relevant scale factors are determined by varying selection requirements, tag-electron requirements, background estimate variations, and signal estimate fits where appropriate [108].

Figure B.4 shows $\epsilon_{\text{Cluster}}^{\text{MC}}$ and $\epsilon_{\text{Reco}}^{\text{MC}}$ as a function of electron candidate E_T . Both the clustering and reconstruction efficiencies are measured to be $\sim 100\%$ in simulation, for $E_T > 20$ GeV.

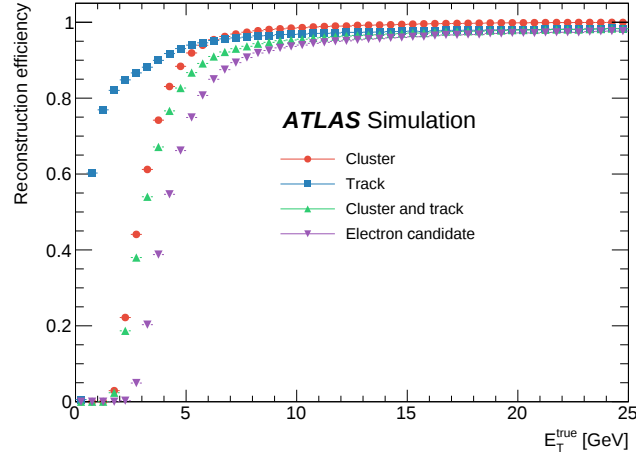
Figure B.5 shows the measured electron identification efficiencies and the electron identification scale factors for the various working points, as functions of the reconstructed electron E_T and $\langle\mu\rangle$.

¹The distribution is scaled down slightly for visibility and is defined as: $\frac{1}{15} \ln \left(\frac{L_S}{L_B} \right)$.



(a)

Figure B.3: The average isolation cone energy $E_{T,\text{cone}}^{\text{isol}}$ as a function of the simulated single electron E_T built using a cone of $\Delta R = 0.2$. The dashed black line represents the isolation energy without any additional corrections whereas the dashed red and solid blue lines represent the isolation energy after correcting for leakage and pileup effects, respectively. The energies are calculated using simulated single electron samples that include pileup effects corresponding to a $\langle \mu \rangle = 13.5$ and satisfy the **Tight** electron identification requirements.



(a)

Figure B.4: The reconstruction efficiency observed in MC simulation as a function of the generator level electron E_T , for the various steps in the electron reconstruction chain. The red circle is the EM calorimeter clustering efficiency $\epsilon_{\text{Cluster}}$ whereas the blue square and green triangles are the efficiency to reconstruct an electron track and match it to a calorimeter cluster, respectively. Finally, the inverted purple triangle is the efficiency to fully reconstruct and electron candidate (ϵ_{Reco}).

The **Medium** working point is $\sim 80\%$ efficient at $E_T = 20$ GeV and increases to an efficiency of $\sim 93\%$ for $E_T = 100$ GeV. The identification scale factors have a distinct shape when considering electrons with E_T below 20 GeV. However, they follow a slight linear relation at higher E_T and are a few percent off from unity. Similarly, the **Medium** working point efficiency varies linearly from $\sim 88\%$ to $\sim 84\%$ for $\langle\mu\rangle$ between 15 and 60. The linear dependence of the identification efficiency as a function of $\langle\mu\rangle$ arises due to a deliberate choice made in the construction of the working points. A constant efficiency across $\langle\mu\rangle$ would lead to a significant loss of background rejection, thus a slight linear dependence is chosen when constructing the working points [108, 113].

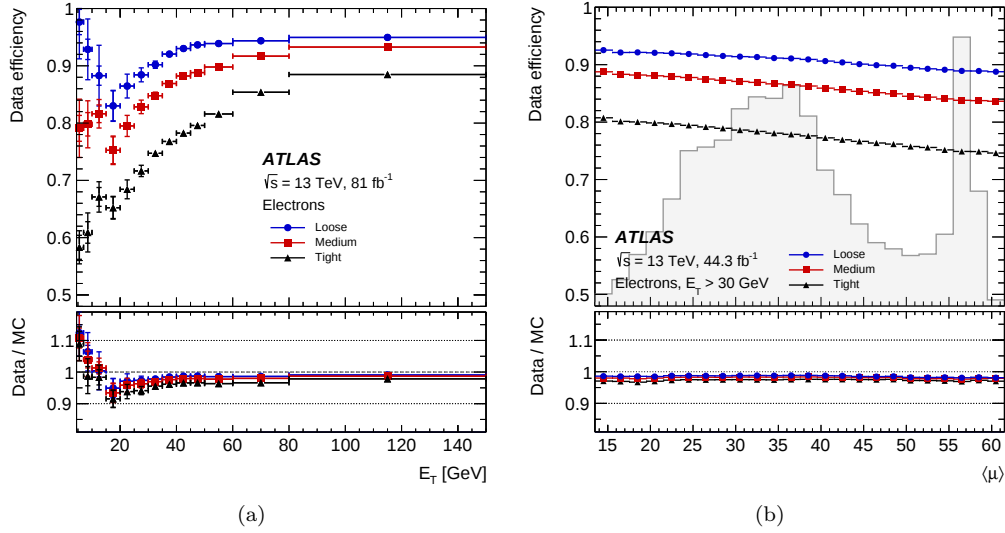


Figure B.5: The electron identification efficiencies ϵ_{ID} measured in data, for the **Loose** (blue dot), **Medium** (red square), and **Tight** (black triangle) working points. The efficiencies are plotted as functions of (a) E_T and (b) $\langle\mu\rangle$ with a requirement that $E_T > 30$ GeV. The efficiencies shown in (a) were measured using $Z \rightarrow ee$ and $J/\psi \rightarrow e^+e^-$ decays whereas the efficiencies in (b) were measured with only $Z \rightarrow ee$ events. The shape of the $\langle\mu\rangle$ distribution is shown as a shaded histogram in (b). The inner (outer) error bars represent the statistical (total) uncertainty. The lower panels show the ratio of the data and the MC simulation (scale factors), along with the uncertainty in the ratio.

Figure B.6 presents the measured isolation efficiencies for the various working points described in Ref. [108], as a function of the electron E_T and η . The isolation efficiency for the **FixedCutTight** working point is $\sim 76\%$ at $E_T = 20$ GeV and increases as a function of E_T . Across η , the **FixedCutTight** working point is between 86% and 92% efficient. The scale factors show a $\sim 2\%$ higher efficiency in data when compared to MC. This deviation is typically associated with low energy electrons that are produced within $|\eta| < 0.5$.

Figure B.7 shows the trigger efficiency for the **HLT_e15_lhloose_nod0_L1EM12** trigger², as a function of electron η and E_T . This was the trigger used during the low-pileup runs taken at $\sqrt{s} = 13$ TeV and $\sqrt{s} = 5.02$ TeV in 2017. In low-pileup 13 TeV data, the trigger is found to be

²Trigger names in ATLAS have either the L1 or HLT prefix, followed by a designation representing the type and energy of the particle the trigger selects for (i.e. **mu14** for muons with p_T greater than 14 GeV). This is occasionally followed by special reconstruction, identification, and isolation criteria [103, 104].

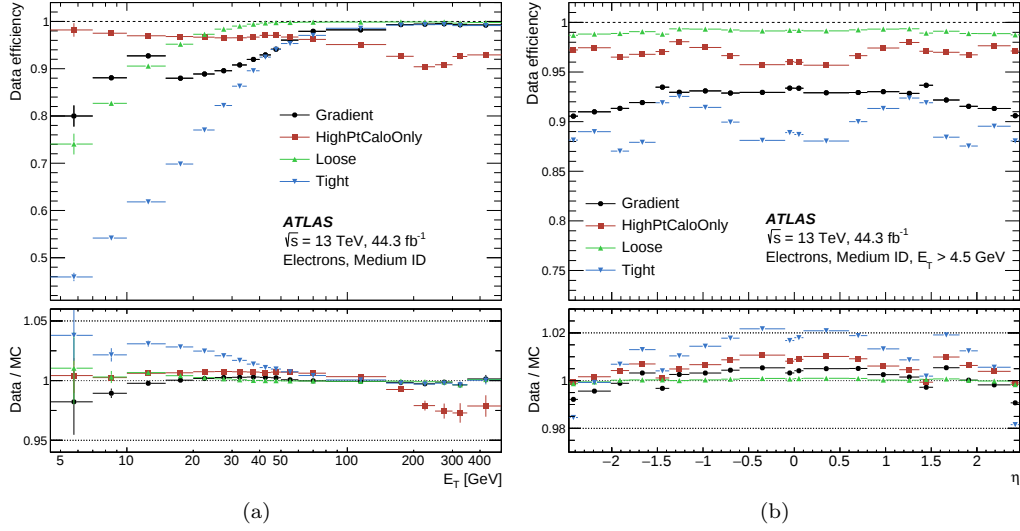


Figure B.6: The electron isolation efficiencies ϵ_{Isol} measured in $Z \rightarrow ee$ data events, as a function of the electron (a) E_T and (b) η . Efficiencies for various working points discussed in [108] are shown, including the **FixedCutLoose** (green triangle) and **FixedCutTight** (inverted blue triangle) working points that are relevant to this thesis. In (b), an additional cut of $E_T > 4.5$ GeV is applied. The inner (outer) error bars represent the statistical (total) uncertainty. The lower panels show the ratio of the data and the MC simulation (scale factors), along with the uncertainty in the ratio.

$\sim 95\%$ efficient outside the crack region and the scale factors are a few percent around unity. The $\sqrt{s} = 5.02$ TeV trigger efficiency was found to match the $\sqrt{s} = 13$ TeV trigger efficiency in MC to the per-mille level. Thus, the low-pileup $\sqrt{s} = 13$ TeV trigger efficiencies were used for the $\sqrt{s} = 5.02$ TeV analyses [118].

B.3 Muon Reconstruction, Identification, and Isolation Efficiencies

Figure B.8 shows the reconstruction and identification efficiencies measured in data as a function of p_T , and the scale factor map for the **Medium** working point, in the $\eta - \phi$ plane since scale factors are applied in bins of η and ϕ . The scale factors are approximately unity for muons with p_T greater than 20 GeV. The largest deviation from unity in the scale factors is seen in the MS crack region, although Local deviations in the $|\eta| < 1$ regions also arise due to MS support structures.

Similarly, Figure B.9 shows the muon vertex association efficiency measured in data and its scale factor in the $\eta - p_T$ plane. The vertex association efficiency is measured to be $\sim 99\%$ for muons with a $p_T > 20$ GeV, and the scale factor is measured to be approximately one.

Finally, Figure B.10 shows the isolation efficiency measured in data and MC, as a function of p_T

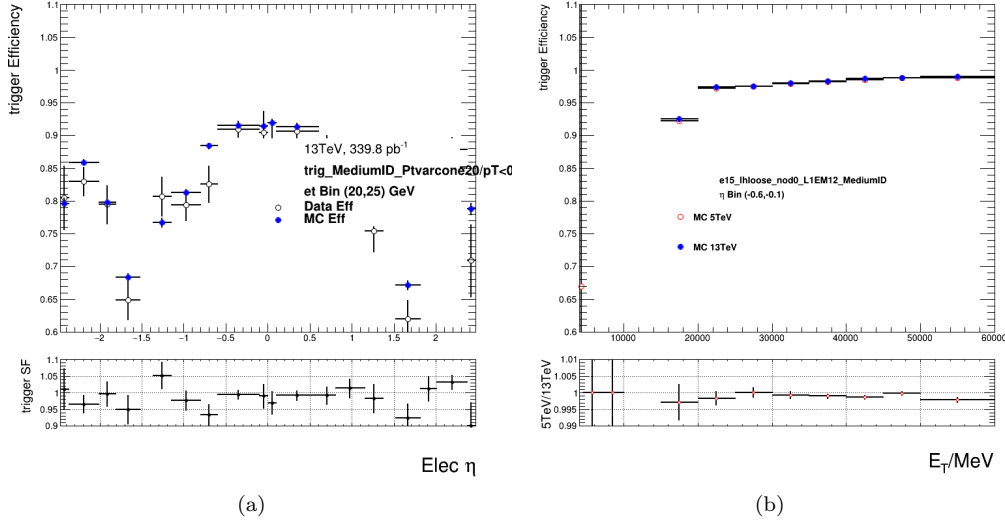


Figure B.7: (a) shows the `HLT_e15_lhloose_nod0_L1EM12` trigger efficiency measured in low-pileup $\sqrt{s} = 13$ TeV data collected in 2017 (white circle) and MC (blue circle), as a function of electron η . The electron E_T is required to be between 25 GeV and 30 GeV. The inner (outer) error bars represent the statistical (total) uncertainty. The lower panels show the ratio of the data and the MC simulation (scale factors), along with the uncertainty in the ratio. (b) compares the trigger efficiencies measured in MC from $\sqrt{s} = 5.02$ TeV (white circle) and $\sqrt{s} = 13$ TeV conditions (blue circle), as a function of E_T . The electron η must be between -0.1 and -0.6. The error bars represent the total uncertainty and the lower panel shows the ratio between the 5.02 TeV and 13 TeV efficiencies, along with the total uncertainty in the ratio.

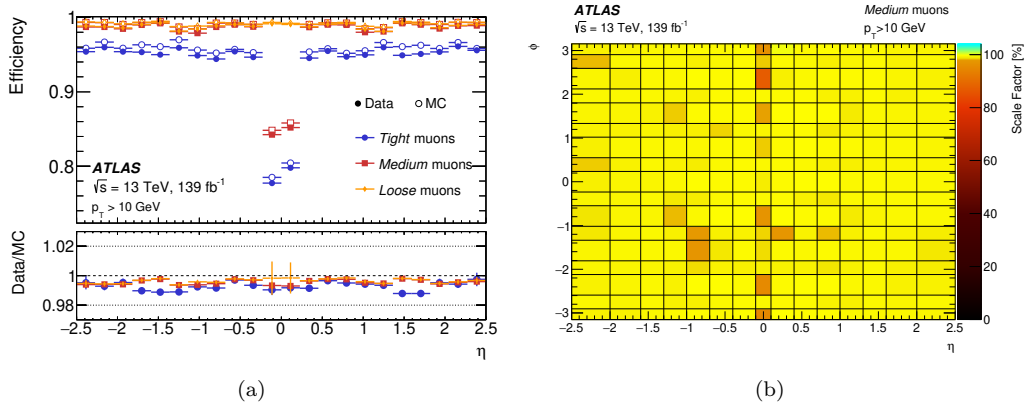


Figure B.8: (a) shows the muon reconstruction and identification efficiencies for the `Medium` working point, as a function of the muon p_T . The efficiencies are measured in data (filled triangles) and simulation (open triangles) using $Z \rightarrow ee$ (inverted triangles) and $J/\psi \rightarrow e^+e^-$ (upright triangles) events with muons of $0.1 < |\eta| < 2.5$. The error bars in the top panel show only the statistical uncertainty on the measurement. The lower panel shows the ratio of the data and the MC simulation (scale factors), along with the total uncertainty in the ratio. (b) shows the scale factors measured for the `Medium` working point using $Z \rightarrow \mu\mu$ events with a muon $p_T > 10$ GeV, in the $\eta - \phi$ plane.

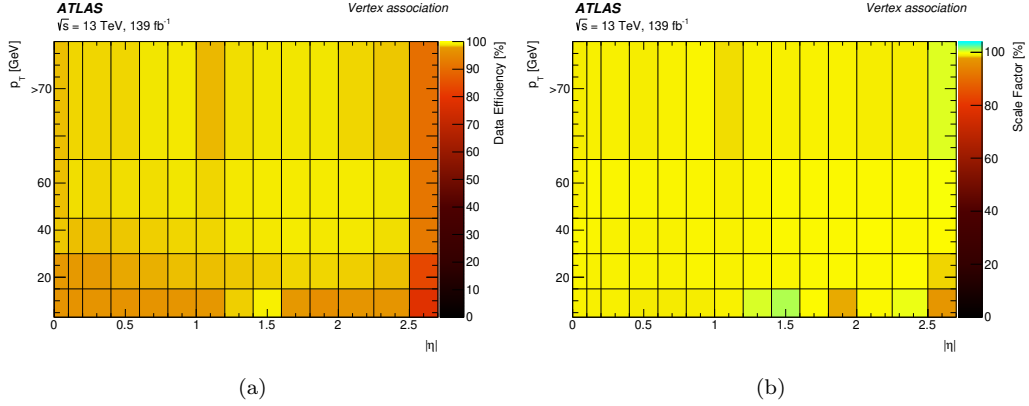


Figure B.9: The (a) track to vertex association efficiency measured in data and (b) the relevant scale factor determined using $Z \rightarrow \mu\mu$ events with a muon $p_T > 3$ GeV, as a function of muon $|\eta|$ and p_T .

and ΔR between a reconstructed jet and muon. The isolation efficiency is measured to be $\sim 70\%$ for a muon with $p_T = 20$ GeV and found to increase with p_T . In the same p_T range, the scale factor is observed to be equal to one.

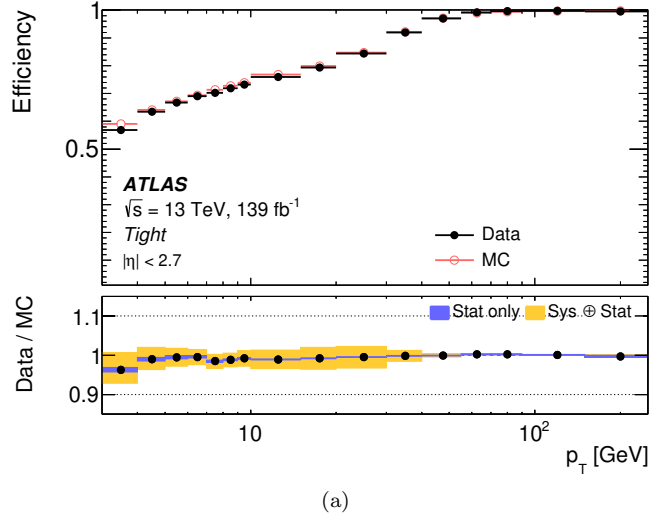


Figure B.10: The FCTight.FixedRad isolation efficiency measured in data (filled black dots) and simulation (open red dots) using $Z \rightarrow \mu\mu$ events, as a function of p_T . The lower panel shows the ratio of the data and the MC simulation (scale factors), along with the statistical (blue band) and total (yellow band) uncertainties on the ratio.

Figure B.11 shows the HLT.MU14 trigger efficiency measured using $\sqrt{s} = 5.02$ TeV data and MC, as a function of p_T . The scale factor for the trigger is also shown as a function of p_T and η . The isolation requirement used to define the denominator, MC datasets, and systematic uncertainties considered are all described in Ref. [127]. The trigger is observed to have a constant efficiency of $\sim 82\%$ for p_T greater than 20 GeV, which is slightly lower than the MC prediction. The scale factor is also observed to be constant over p_T but it varies between 80% and 95% as a function of η . The

larger discrepancies between data and MC are observed in the barrel and around $|\eta| \sim 1.0$.

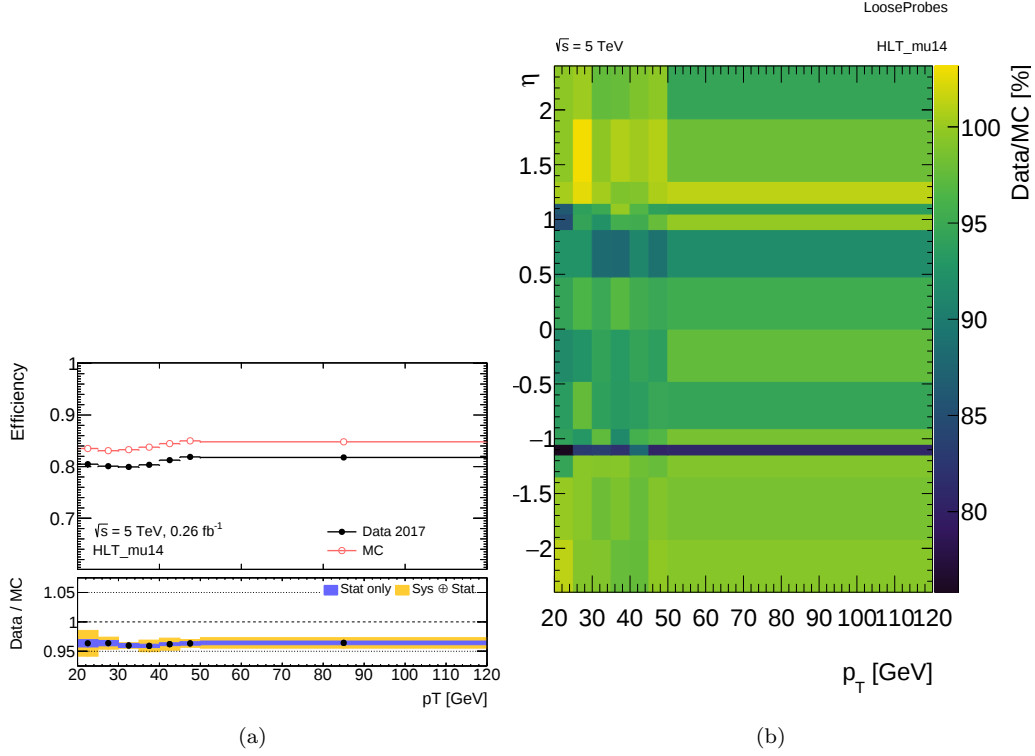


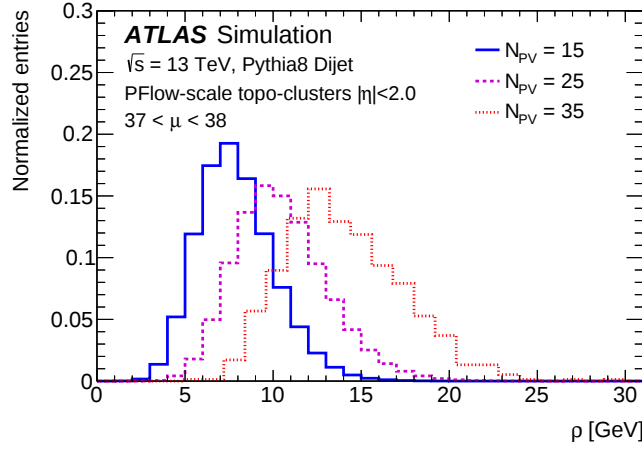
Figure B.11: The HLT_mu14 trigger efficiency as measured in 5.02 TeV data (filled black dots) and simulation (open red dots) using $Z \rightarrow \mu\mu$ events, as a function of muon p_T . The lower panel shows the ratio of the data and the MC simulation (scale factors), along with the statistical (blue band) and total (yellow band) uncertainties on the ratio. (b) shows the scale factor as a function of muon p_T and η .

B.4 JES MC Based Corrections

B.4.1 Pileup Correction

The median p_T surface density ($\text{median}(p_T)/\text{area}$) of jets in the $\eta - \phi$ plane (ρ), is the metric used to determine the sensitivity of the jet's energy to pileup. The area of a jet is measured by determining the fractional area in the $\eta - \phi$ plane of ghost matched particles to a clustered jet. The ρ is calculated using $R = 0.4 k_t$ jets [236] instead of anti- k_t jets since the former algorithm is less biased towards jets arising from the hard scatter, and tends to reconstruct softer jets such as the ones arising from ghost particles [133]. Furthermore, only calorimeter clusters in the $|\eta| < 2.0$ region are considered since ρ drops to zero above that $|\eta|$ range. Figure B.12 shows the normalized distributions of ρ for various number of reconstructed primary vertices, as seen in MC. The location of the peak of the

ρ distribution increases approximately linearly with the number of reconstructed primary vertices N_{PV} [134].



(a)

Figure B.12: The median energy surface density distribution for particle flow jets, as seen in PYTHIA 8 dijet events at $\sqrt{s} = 13$ TeV and a $\langle\mu\rangle$ between 37 and 38. The three distributions are all normalized to unity and represent cases where the number of primary vertices is 15 (solid blue), 25 (dashed pink), and 35 (dashed red).

The jet energy contribution from pileup is corrected for, by subtracting $\rho \times A_{\text{reco}}$ from the reconstructed jet p_T . This density-based correction still leads to residual differences between the truth and reconstructed jet p_T since it does not describe the pileup sensitivity in high- p_T tails of jets or from jets produced in the forward regions. These residual effects can be parametrized in terms of two constants, α and β which are proportional to the number of pileup vertices ($N_{PV} - 1$) and the average number of collisions $\langle\mu\rangle$, respectively. The residual δ_{PU} can then be expressed as: $\delta_{PU} = \alpha \cdot (N_{PV} - 1) + \beta \cdot \langle\mu\rangle$. The two constants are determined by geometrically matching reconstructed jets to truth jets ($\Delta R < 0.3$) in MC, and then fitting for the residuals in bins of truth jet p_T and η_{det} ³. Details on the fitting procedure are discussed in Ref. [134]. Figure B.13 shows the proportionality constants α and β as functions of $|\eta_{\text{det}}|$, and the various corrections considered. After correcting for the residual effects, the jet p_T is observed to be constant over N_{PV} and $\langle\mu\rangle$.

B.4.2 Absolute JES Calibration

For the absolute JES correction, reconstructed jets are geometrically matched to truth jets similar to the procedure used for the residual pileup correction, and additional isolation requirements on the truth and reconstructed jets are applied. Truth (reconstructed) jets must not have another truth (reconstructed) jet within a ΔR of 1.0 (0.6).

³ η_{det} is measured from the centre of the detector and does not include the origin correction which defines η with respect to the primary vertex.

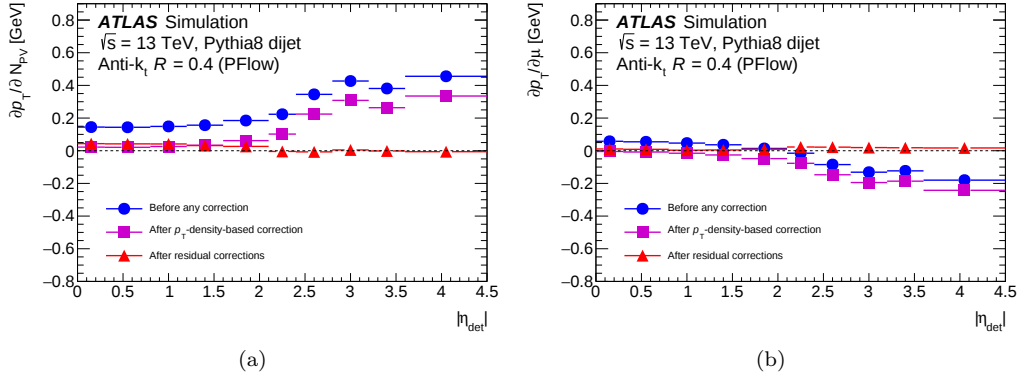


Figure B.13: The distribution of (a) α and (b) β as functions of η_{det} for particle flow $R = 0.4$ jets, as seen in PYTHIA 8 dijet events at $\sqrt{s} = 13$ TeV. The distributions are shown before any correction (blue circles), after the ρ correction (purple squares), and the residual correction (red triangle).

The ratio of the reconstructed jet energy (E^{reco}) to the truth level jet energy (E^{true}) is then fit to Gaussian distributions in bins of E^{true} and η_{det} . The mean of these Gaussian fits is called the “average jet energy response” and is parametrized as a function of E^{reco} using a fit [237]. The inverse of the average energy response is then taken as the correction factor that must be applied to reconstructed jets, also in bins of η_{det} and E^{reco} . Figure B.14 shows the average jet energy response for $R = 0.4$ particle flow jets, as a function of E^{reco} and η_{det} . Jets produced outside the forward and transition regions have a higher response than ones produced in those regions. The response is recalculated after applying the calibration, and is observed to diverge by a maximum of 5% for jets with $p_T = 20$ GeV. This deviation decreases to 1% for jets with $p_T = 50$ GeV [134]. A similar correction on reconstructed jet η is performed in order to correct for biases from the detector geometry [134].

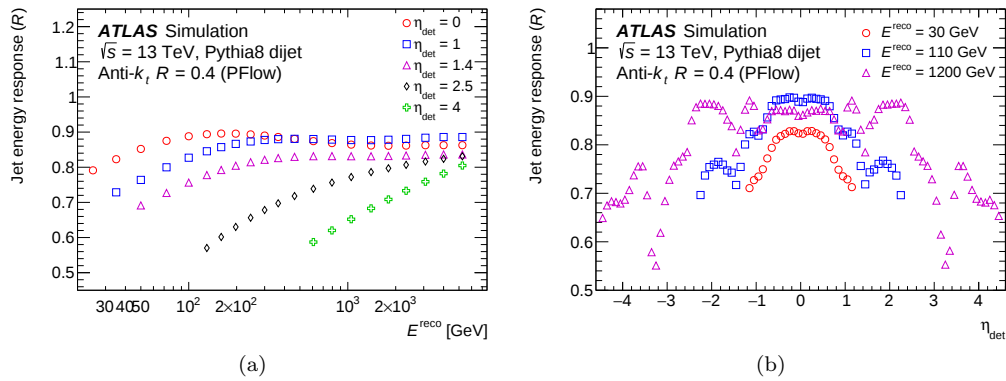


Figure B.14: The distribution of the average jet energy response in particle flow $R = 0.4$ jets seen in PYTHIA 8 dijet events at $\sqrt{s} = 13$ TeV, as a function of (a) E^{reco} and (b) η_{det} .

B.4.3 Global Sequential Calibration

The GSC is an extension of the absolute JES calibration that applies the correction as a function of a third variable x . Similar to the absolute JES correction, GSC corrections are derived in bins of p_T^{true} and η_{det} , but they use the jet p_T response ($\mathcal{R}_{p_T}^{ijk}$) instead of the jet energy response. $\mathcal{R}_{p_T}^{ijk}$ is defined as the mean given by a Gaussian fit to the ratio of reconstructed jet p_T to the truth jet p_T , in bin i of p_T^{true} , bin j of η_{det} , and bin k of the variable x . The correction factors are then determined in three dimensions using the same algorithm as the absolute JES calibration. Note that corrections from multiple variables can be applied sequentially.

Six variables are used for the ATLAS GSC calibration:

- f_{charged} : The fraction of the jet p_T measured from ghost associated tracks with p_T greater than 500 GeV;
- f_{Tile0} : The fraction of energy measured in the first layer of the tile calorimeter;
- f_{LAr3} : The fraction of energy measured in the third layer of the LAr calorimeter;
- n_{trk} : Number of tracks with p_T greater than 1 GeV that are ghost associated with the jet;
- w_{trk} : p_T weighted distance in the $\eta - \phi$ plane for all tracks with $p_T > 1$ GeV, that are also ghost associated with a jet;
- n_{segments} : The number of MS tracks ghost associated with a jet;

The variables and their applicable η , p_T^{true} bins are further discussed in Ref. [134]. The effect of the GSC is visible in the relative jet p_T resolution $\frac{\sigma(\mathcal{R}_{p_T}^{ij})}{\mathcal{R}_{p_T}^{ij}}$. $\sigma(\mathcal{R}_{p_T}^{ij})$ is the standard deviation from the Gaussian fit discussed above, that is integrated over index k . Figure B.15 shows the effect of the GSC on the relative resolution, as a function of p_T^{true} , and using dijet MC particle flow jets with $0.2 < |\eta_{\text{det}}| < 0.3$. The track variables have a larger effect than the calorimeter variables at lower p_T whereas this is the opposite at higher p_T , exactly as one would expect from the particle flow algorithm.

B.5 JER

Figure B.16 shows such dijet asymmetry distributions for particle flow jets in simulation and data, for various bins of p_T^{avg} and $\eta_{\text{det}}^{\text{probe}}$. The truth level resolution in simulation is found to be smaller than the detector level resolution measured in data since the former does not account for the detector level resolution.

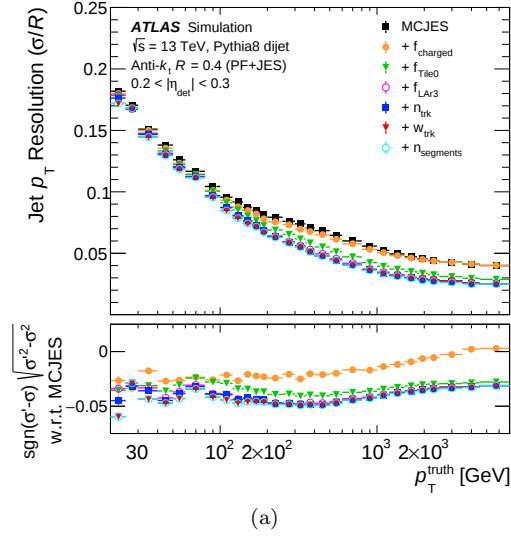


Figure B.15: The relative jet p_T resolution before the GSC (filled black dots) and after the various steps of the GSC, as a function of p_T^{truth} . The distribution is shown for particle flow $R = 0.4$ jets with $|0.2 < \eta_{\text{det}} < 0.3|$, as seen in PYTHIA 8 dijet events at $\sqrt{s} = 13$ TeV. The lower panel shows the difference in quadrature between the resolution before any GSC correction is applied (σ) and after the corresponding GSC step is applied (σ').

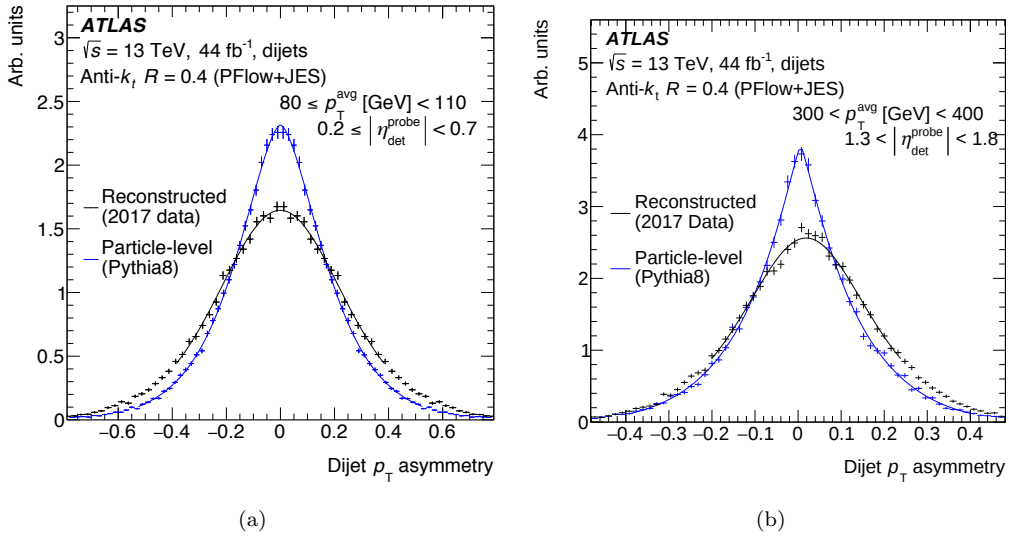


Figure B.16: Asymmetry distributions measured in data (black dots) and particle level simulation (blue dots) using PYTHIA 8, for particle flow jets. (a) shows the distributions for events with p_T^{avg} between 80 GeV and 110 GeV, and $0.2 < \eta_{\text{det}} < 0.7$ whereas (b) shows the distributions for events with p_T^{avg} between 300 GeV and 400 GeV, and $1.3 < \eta_{\text{det}} < 1.8$. Error bars in both plots represent the statistical uncertainty. The curves represent the fitted distributions.

Appendix C

Statistical analysis

C.1 Profile Likelihood Fits

The statistical interpretation of all analyses discussed in this thesis is based on the use of the binned likelihood function $\mathcal{L}(\mu, \gamma, \theta)$ that is constructed as a product of Poisson probability terms over all bins considered in the measurement. The likelihood function further depends on the ratio of the observed cross-section to the predicted cross-section, μ , and is denoted as the parameter of interest (POI), a set of Poisson NPs (γ_j) corresponding to the statistical uncertainty in the prediction of a bin, and a set of nuisance parameters (NPs) that have PDFs defined by normal Gaussian distributions that encode the effect of systematic uncertainties on the signal and background (θ). The effect of the NPs is parametrized by interpolating between templates of histograms. Typically, for each NP, three histograms are used, a nominal histogram representing no systematic variation along with the “up” and “down” variations on the nominal histogram that correspond to a $\pm 1\sigma$ uncertainty for a given NP. These templates will typically have shape effects which change the shape of a distribution with a change in the NP and normalization effects that change the number of entries seen across the entire histogram.

Thus, their fitted values correspond to the deviations from the nominal expectations that provide the best fit to the data and can be used to reduce the effect of systematic uncertainties on the measurement via profiling. A summary of the binned likelihood function is given in Equation C.1.

$$\mathcal{L}(\mu_X, \hat{\theta}; S, B, n, h) = \prod_{i=1}^{N_b} \text{Pois}(n_i; S_i(\mu_X) + B_i) \cdot \text{Pois}(h_i; \gamma_i) \prod_{j=1}^{N_p} \text{Gauss}(\theta_j, \sigma_j) \quad (\text{C.1})$$

The variables involved in Equation C.1 are defined as:

- N_b : Number of bins
- n_i : Number of data events in the i -th bin
- μ_X : The POI, a special NP defined as the ratio of the observed quantity to the expected quantity, $\mu_X = \frac{X_{\text{observed}}}{X_{\text{expected}}}$. The quantity X is typically the cross-section of the signal process
- $S_i(B_i)$: Number of predicted signal (background) events
- h_i : Total number of predicted events (signal + background)
- γ_i : Uncertainty on the predicted events for the i -th bin
- N_p : Number of Gaussian NPs considered (systematic uncertainties)
- θ_j : The set of nuisance parameters corresponding to systematic uncertainties
- σ_j : The uncertainty in the nuisance parameters corresponding to systematic uncertainties

With such a function, the optimal value for the POI can be found by performing an N-dimensional maximization on the likelihood function (where N is the number of NPs), or equivalently by minimizing the negative-log likelihood $q(\mu)$ ($q(\mu) = -2 \log \mathcal{L}$). The optimal values of μ , the sets of γ_i , θ_j , and σ_j are found by minimizing $q(\mu)$ using MINUIT2 [238] or MINOS [232] minimization algorithms. The Hessian of the negative-log likelihood can then be inverted to calculate the covariance and correlation matrices for the various NPs and propagate this information into the post-fit uncertainties. This is implemented through profiling wherein the negative-log likelihood is minimized for a given value of the POI, and an optimal set of values for the NPs is found. By going through the phase space and profiling, one can obtain the dependence of the NPs on the POI. The uncertainties on the variables can be extracted by determining the point where the negative log-likelihood difference is equal to 0.5. This is typically done by scanning over various values of the two POIs and determining the difference in the negative log-likelihood between the scanned value and the best fit value.

Values or plots based on the fitted NP values (after minimization) are denoted as “post-fit” whereas values and plots using the standard Gaussian PDFs are denoted as “pre-fit”.

C.2 Significance of a Measurement

The p-value is defined as the probability, while assuming the “null hypothesis” (i.e. no signal), of observing data of equal or greater incompatibility with the predictions of null-hypothesis (i.e.: background only hypothesis). From this, one can define the significance through a transformation on the p-value. One can define two testing hypotheses: H_1 with a presence of signal ($\mu > 0$), and the null hypothesis H_0 with no signal ($\mu = 0$). From these two hypotheses, one can define $\mathcal{L}(\mu, \hat{\theta}_\mu)$ as the maximized likelihood function for a given μ that corresponds to the hypothesis H_0 being true. Similarly, one defines $\mathcal{L}(\hat{\mu}, \hat{\theta})$ as the maximized likelihood function that corresponds to the hypothesis

H_1 being true where $\hat{\mu}$ is the POI preferred by the data and $\hat{\hat{\theta}}_\mu$ is the set of NP values assuming a background only hypothesis.

To test a hypothesized value of μ , the profile likelihood ratio defined in Equation C.2 is considered to be the best discriminant.

$$\lambda(\mu) = \frac{\mathcal{L}(\mu, \hat{\hat{\theta}}_\mu)}{\mathcal{L}(\hat{\mu}, \hat{\theta})} \quad (\text{C.2})$$

And the test statistic is defined as

$$q_0 = \begin{cases} -2 \log \lambda(0) & \hat{\mu} \geq 0 \\ 0 & \hat{\mu} < 0 \end{cases} \quad (\text{C.3})$$

The p -value defined in Equation C.4 can then be used to quantify the level of disagreement.

$$p_0 = \int_{q_{0,\text{obs}}}^{\infty} f(q_0|0) dq_0 \quad (\text{C.4})$$

Here, $q_{0,\text{obs}}$ is the value of q_0 observed from data, and $f(q_0|0)$ denotes the probability density function of q_0 under the assumption of signal strength $\mu = 0$. Finally, the significance Z_0 can be computed by

$$Z_0 = \Phi^{-1}(1 - p_0) \quad (\text{C.5})$$

where Φ^{-1} is the quantile (inverse of the cumulative distribution) of the standard Gaussian probability distribution.

Although p_0 can be evaluated using toy models, this is a resource and time intensive process. The **TRExFitter** package instead calculates the p_0 using the asymptotic Gaussian approximation [239] which states

$$Z_0 \approx \sqrt{q_0} \quad (\text{C.6})$$

Note that q_0 can be written as $2 \cdot \left(\mathcal{L}(\hat{\mu}, \hat{\theta}) - \mathcal{L}(0, \hat{\hat{\theta}}_\mu) \right)$ and computed through a scan of the likelihood function.

Appendix D

Misidentified Lepton Background Validation - $\sigma_{t\bar{t}}$ Measurement

In order to validate the nominal estimate of misidentified lepton background using the matrix method technique, two validation regions enriched in fake lepton events are constructed. These regions are similar to the analysis regions and are constructed separately for the μ +jets and e +jets channels. This is done by keeping the nominal selection but reversing the E_T^{miss} and m_T^{W} cuts. Note that such a selection is orthogonal to the nominal analysis selection.

For the μ +jets channel, the $E_T^{\text{miss}} + m_T^{\text{W}}$ cut is reversed and events must have $E_T^{\text{miss}} + m_T^{\text{W}} < 60 \text{ GeV}$. The observed and predicted distributions for the H_T^{had} , muon η , and minimum azimuthal angle between the muon and jets are shown for the $\mu+2j \geq 1b$, $\mu+3j \text{ 1b}$, and $\mu+\geq 4j \text{ 1b}$ fake lepton enriched control regions in Figures [D.1](#), [D.2](#), and [D.3](#), respectively.

In the e +jets channel, events are required to have $E_T^{\text{miss}} < 30 \text{ GeV}$ and $m_T^{\text{W}} > 30 \text{ GeV}$. The observed and predicted distributions for the H_T^{had} , electron η , and minimum azimuthal angle between the electron and jets are shown for the $e+2j \geq 1b$, $e+3j \text{ 1b}$, and $e+\geq 4j \text{ 1b}$ fake lepton enriched control regions in Figures [D.4](#), [D.5](#), and [D.6](#), respectively.

The uncertainty bands in these plots represent only the statistical uncertainty on the prediction and the 50% normalization uncertainty on the misidentified lepton background. Good agreement between data and the predicted distributions is seen in all control regions and the 50% normalization uncertainty accounts for any mis-modelling that might be present.

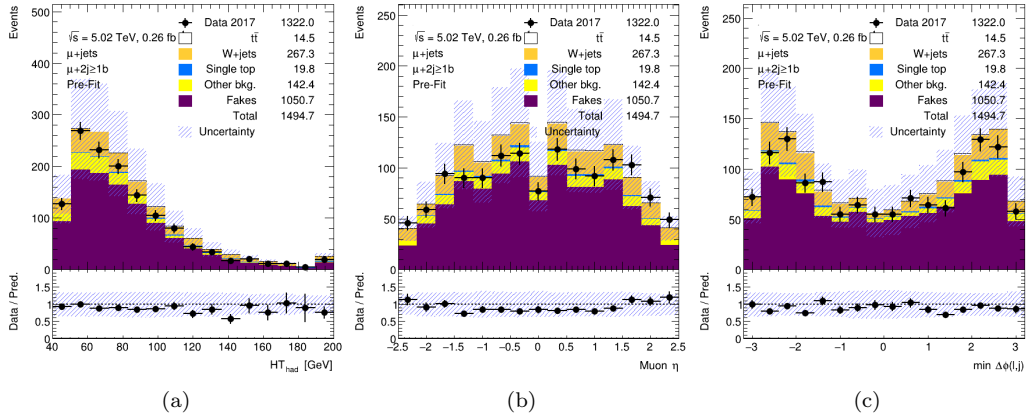


Figure D.1: The (a) H_T^{had} , (b) muon η , and (c) minimum $\Delta\phi(\mu, j)$ distributions for data (dots) in the $\mu+2j\geq 1b$ misidentified lepton enriched control region. The misidentified lepton background was estimated using fake efficiencies parametrized in lepton $|\phi|$ in the $\geq 1j, \geq 1b$ region. The MC simulation of the signal (white histograms) and various backgrounds (represented by histograms of different colours) including the misidentified lepton background (purple histograms) are also included. The error bars on the dots represent the statistical uncertainty on the data while the blue cross-hatched lines correspond to the sum in quadrature between the statistical uncertainties on the prediction and the 50% normalization uncertainty on the misidentified lepton background. The lower panels show the ratio of the data and predicted distributions, along with the uncertainty in the ratio. The first and last bins contain any underflow and overflow events, respectively.

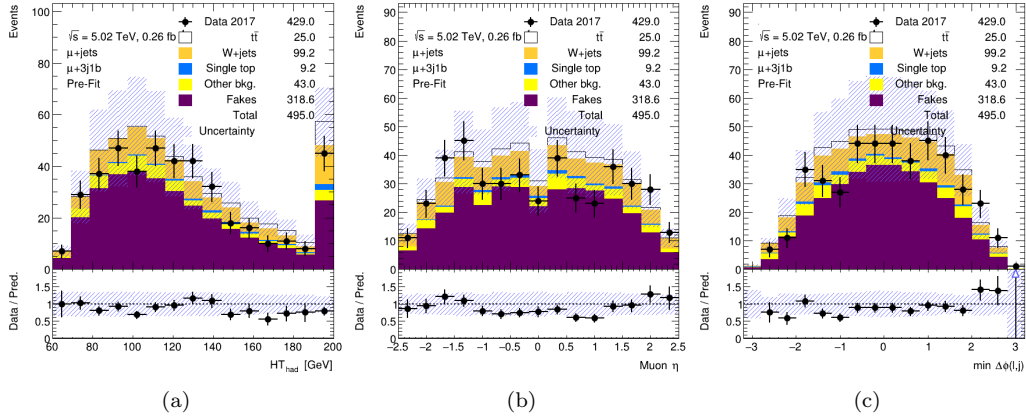


Figure D.2: The (a) H_T^{had} , (b) muon η , and (c) minimum $\Delta\phi(\mu, j)$ distributions for data (dots) in the $\mu+3j\ 1b$ misidentified lepton enriched control region. The misidentified lepton background was estimated using fake efficiencies parametrized in lepton $|\phi|$ in the $\geq 1j, \geq 1b$ region. The MC simulation of the signal (white histograms) and various backgrounds (represented by histograms of different colours) including the misidentified lepton background (purple histograms) are also included. The error bars on the dots represent the statistical uncertainty on the data while the blue cross-hatched lines correspond to the sum in quadrature between the statistical uncertainties on the prediction and the 50% normalization uncertainty on the misidentified lepton background. The lower panels show the ratio of the data and predicted distributions, along with the uncertainty in the ratio. The first and last bins contain any underflow and overflow events, respectively.

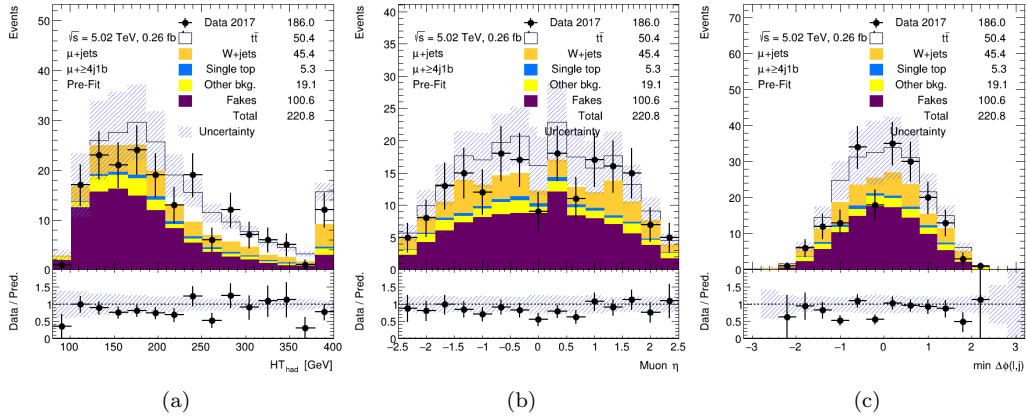


Figure D.3: The (a) H_T^{had} , (b) muon η , and (c) minimum $\Delta\phi(\mu, j)$ distributions for data (dots) in the $\mu + \geq 4j$ 1b misidentified lepton enriched control region. The misidentified lepton background was estimated using fake efficiencies parametrized in lepton $|\phi|$ in the $\geq 1j, \geq 1b$ region. The MC simulation of the signal (white histograms) and various backgrounds (represented by histograms of different colours) including the misidentified lepton background (purple histograms) are also included. The error bars on the dots represent the statistical uncertainty on the data while the blue cross-hatched lines correspond to the sum in quadrature between the statistical uncertainties on the prediction and the 50% normalization uncertainty on the misidentified lepton background. The lower panels show the ratio of the data and predicted distributions, along with the uncertainty in the ratio. The first and last bins contain any underflow and overflow events, respectively.

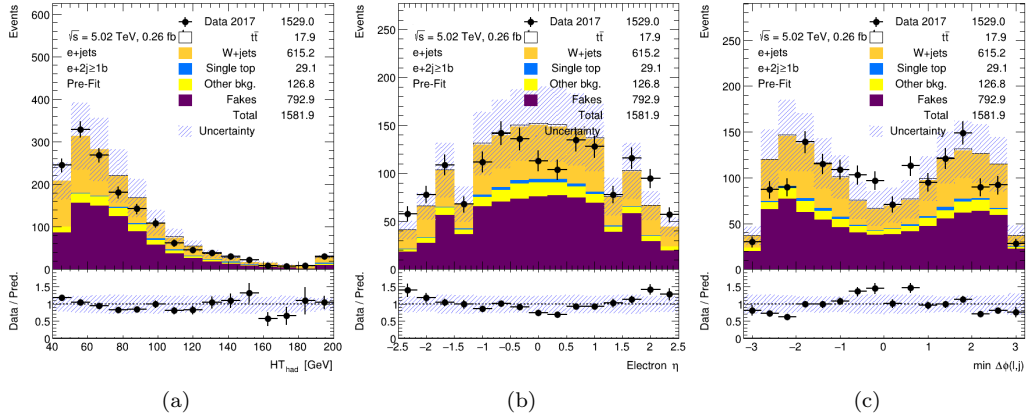


Figure D.4: The (a) H_T^{had} , (b) electron η , and (c) minimum $\Delta\phi(e, j)$ distributions for data (dots) in the $e + 2j \geq 1b$ misidentified lepton enriched control region. The misidentified lepton background was estimated using fake efficiencies parametrized in lepton $|\phi|$ in the $\geq 1j, \geq 1b$ region. The MC simulation of the signal (white histograms) and various backgrounds (represented by histograms of different colours) including the misidentified lepton background (purple histograms) are also included. The error bars on the dots represent the statistical uncertainty on the data while the blue cross-hatched lines correspond to the sum in quadrature between the statistical uncertainties on the prediction and the 50% normalization uncertainty on the misidentified lepton background. The lower panels show the ratio of the data and predicted distributions, along with the uncertainty in the ratio. The first and last bins contain any underflow and overflow events, respectively.

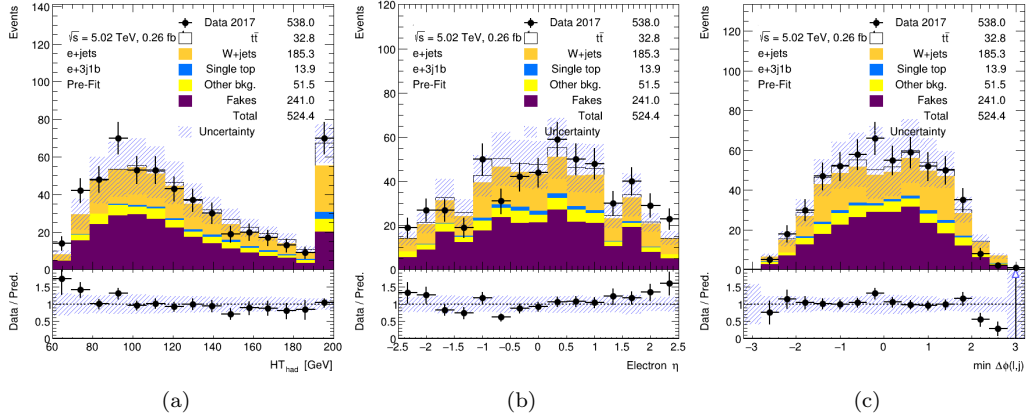


Figure D.5: The (a) H_T^{had} , (b) electron η , and (c) minimum $\Delta\phi(e, j)$ distributions for data (dots) in the $e+3j$ 1b misidentified lepton enriched control region. The misidentified lepton background was estimated using fake efficiencies parametrized in lepton $|\phi|$ in the $\geq 1j, \geq 1b$ region. The MC simulation of the signal (white histograms) and various backgrounds (represented by histograms of different colours) including the misidentified lepton background (purple histograms) are also included. The error bars on the dots represent the statistical uncertainty on the data while the blue cross-hatched lines correspond to the sum in quadrature between the statistical uncertainties on the prediction and the 50% normalization uncertainty on the misidentified lepton background. The lower panels show the ratio of the data and predicted distributions, along with the uncertainty in the ratio. The first and last bins contain any underflow and overflow events, respectively.

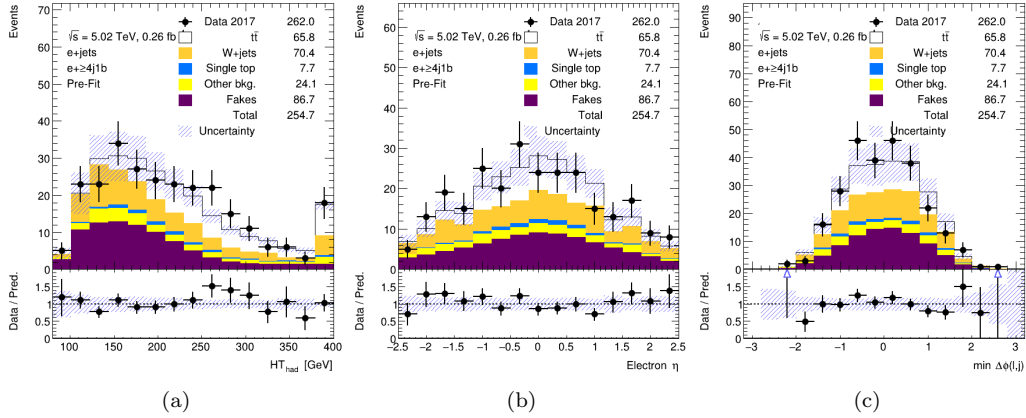


Figure D.6: The (a) H_T^{had} , (b) electron η , and (c) minimum $\Delta\phi(e, j)$ distributions for data (dots) in the $e+\geq 4j$ 1b misidentified lepton enriched control region. The misidentified lepton background was estimated using fake efficiencies parametrized in lepton $|\phi|$ in the $\geq 1j, \geq 1b$ region. The MC simulation of the signal (white histograms) and various backgrounds (represented by histograms of different colours) including the misidentified lepton background (purple histograms) are also included. The error bars on the dots represent the statistical uncertainty on the data while the blue cross-hatched lines correspond to the sum in quadrature between the statistical uncertainties on the prediction and the 50% normalization uncertainty on the misidentified lepton background. The lower panels show the ratio of the data and predicted distributions, along with the uncertainty in the ratio. The first and last bins contain any underflow and overflow events, respectively.

Appendix E

Distributions of Kinematic Variables - $\sigma_{t\bar{t}}$ Measurement

Comparison between data and prediction for the leading jet: p_T , η and ϕ , second and third jet p_T , lepton p_T , η and ϕ , $\Delta\phi$ between the lepton and the leading jet, E_T^{miss} , and $m_T(l\nu)$ in the lepton+jets final state is shown in:

- Figures [E.1](#) and [E.2](#) for $\ell+2j \geq 1b$
- Figures [E.3](#) and [E.4](#) for $\ell+3j$ 1b
- Figures [E.5](#) and [E.6](#) for $\ell+3j$ 2b
- Figures [E.7](#) and [E.8](#) for $\ell+\geq 4j$ 1b
- Figures [E.9](#) and [E.10](#) for $\ell+4j$ 2b
- Figures [E.11](#) and [E.12](#) for $\ell+\geq 5j$ 2b

These plots show that the six analysis regions are well modelled by the MC simulation and data-driven misidentified lepton background.

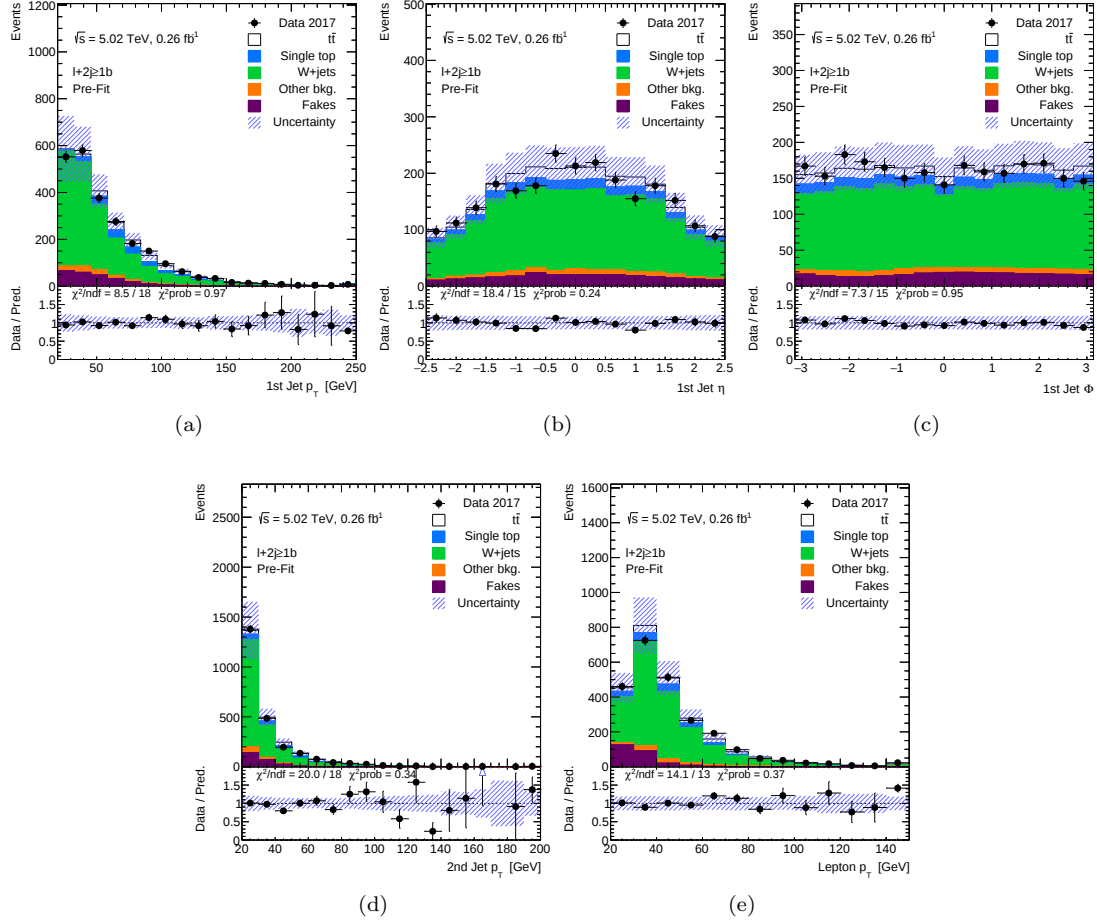


Figure E.1: The (a) leading jet p_T , (b) leading jet η , (c) leading jet Φ , (d) 2nd leading jet p_T , and (e) lepton p_T distributions for data (dots) in the $\ell+2j \geq 1b$ region. Note that the p_T of the third jet is not shown because there is no third jet in this region. The MC simulation of the signal (white histograms) and various backgrounds (represented by histograms of different colours) are also included. The error bars on the dots represent the statistical uncertainty on the data while the blue cross-hatched lines correspond to the total uncertainties on the prediction. The lower panels show the ratio of the data and predicted distributions, along with the uncertainty in the ratio. The first and last bins contain any underflow and overflow events, respectively.

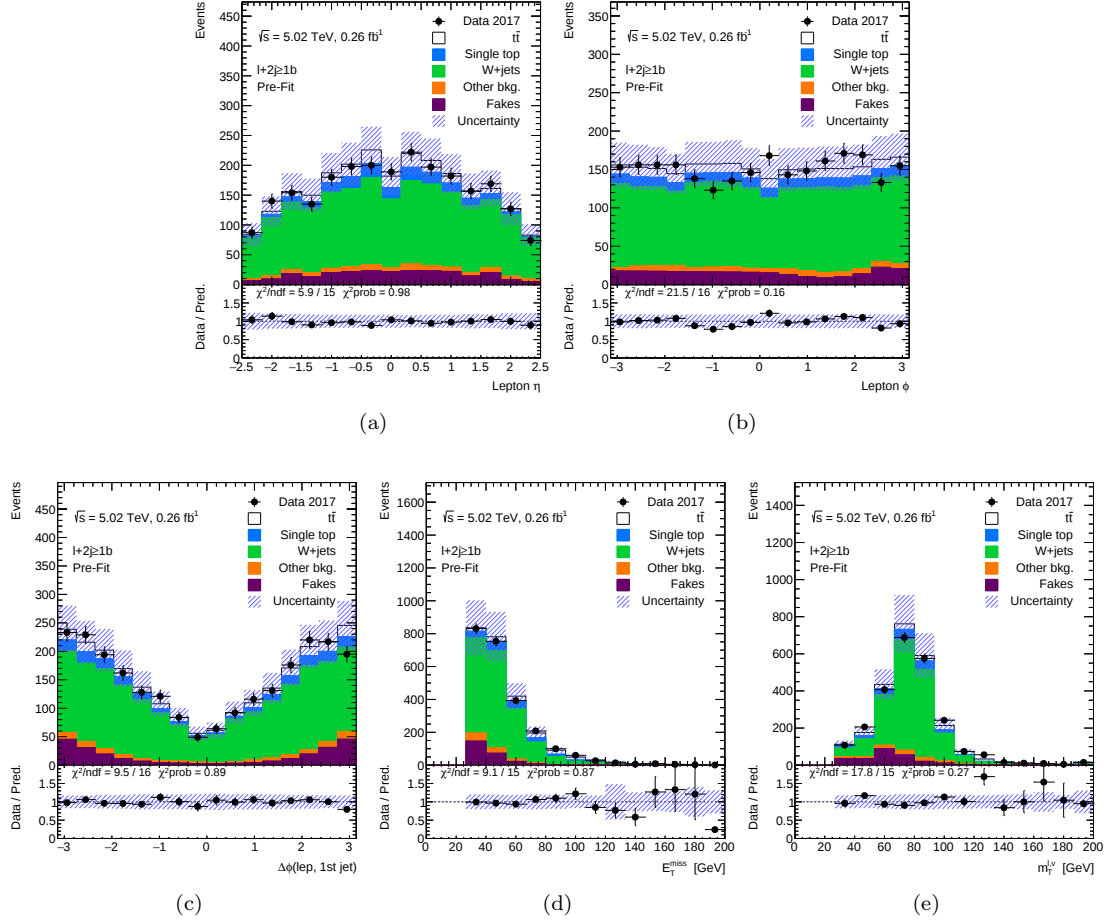


Figure E.2: The (a) lepton η , (b) lepton Φ , (c) difference in azimuthal angle between the lepton and the leading jet, (d) E_T^{miss} , and (e) m_T^W distributions for data (dots) in the $\ell+2j \geq 1b$ region. The MC simulation of the signal (white histograms) and various backgrounds (represented by histograms of different colours) are also included. The error bars on the dots represent the statistical uncertainty on the data while the blue cross-hatched lines correspond to the total uncertainties on the prediction. The lower panels show the ratio of the data and predicted distributions, along with the uncertainty in the ratio. The first and last bins contain any underflow and overflow events, respectively.

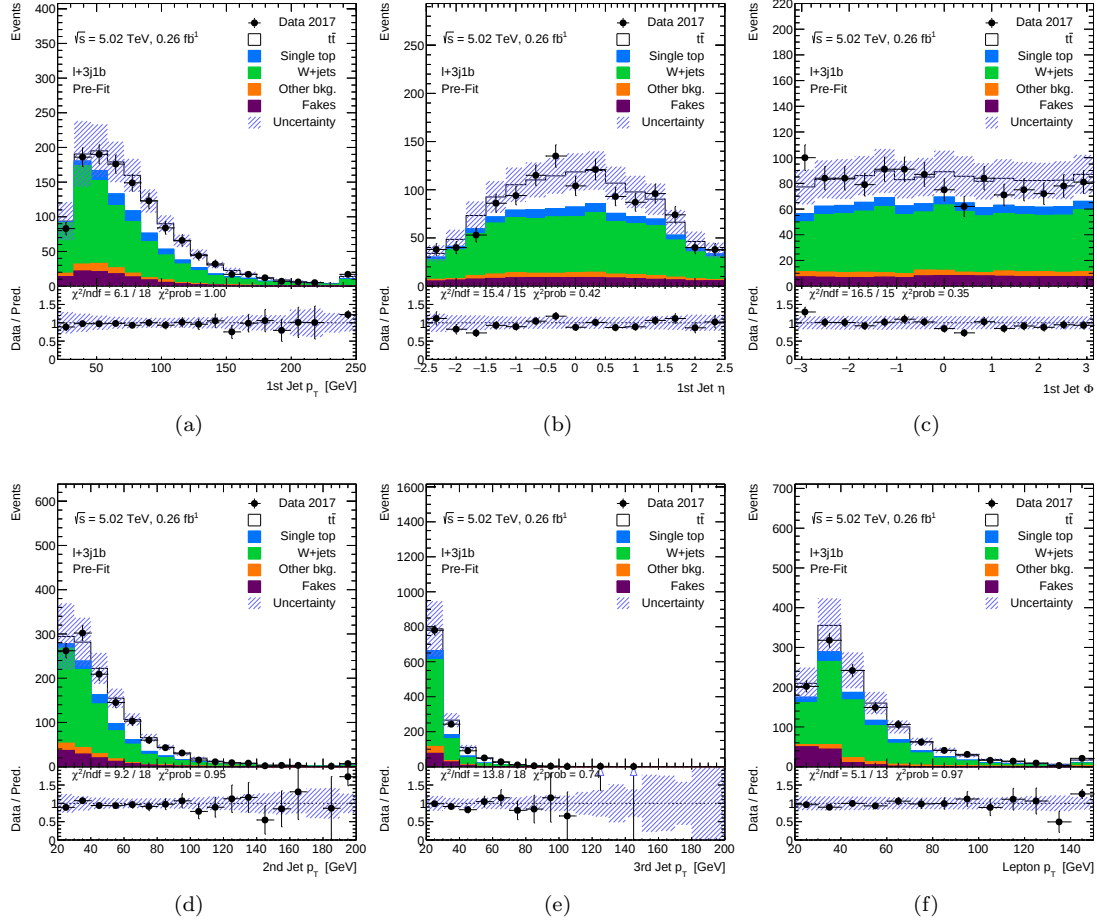


Figure E.3: The (a) leading jet p_T , (b) leading jet η , (c) leading jet Φ , (d) 2nd leading jet p_T , (e) 3rd leading jet p_T , and (f) lepton p_T distributions for data (dots) in the $\ell+3j$ 1b region. The MC simulation of the signal (white histograms) and various backgrounds (represented by histograms of different colours) are also included. The error bars on the dots represent the statistical uncertainty on the data while the blue cross-hatched lines correspond to the total uncertainties on the prediction. The lower panels show the ratio of the data and predicted distributions, along with the uncertainty in the ratio. The first and last bins contain any underflow and overflow events, respectively.

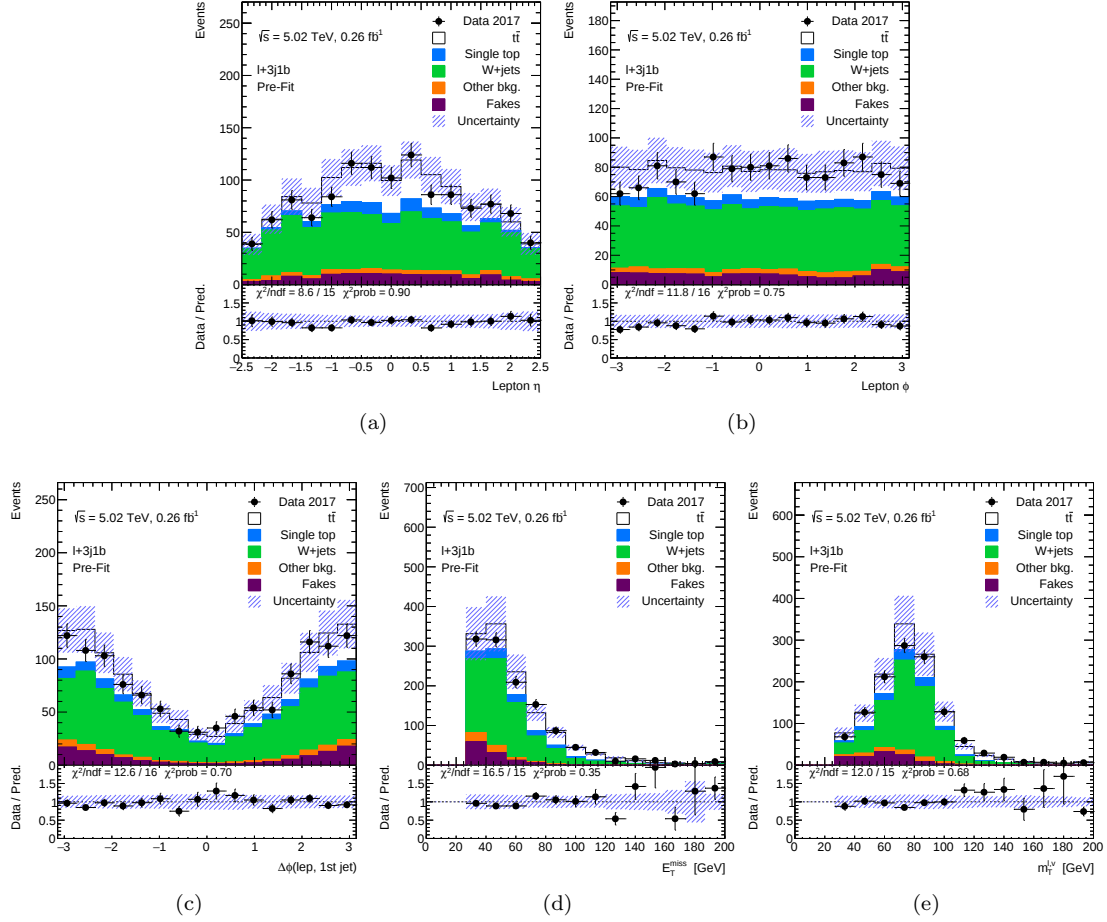


Figure E.4: The (a) lepton η , (b) lepton Φ , (c) difference in azimuthal angle between the lepton and the leading jet, (d) E_T^{miss} , and (e) m_T^W distributions for data (dots) in the $\ell+3j\ 1b$ region. The MC simulation of the signal (white histograms) and various backgrounds (represented by histograms of different colours) are also included. The error bars on the dots represent the statistical uncertainty on the data while the blue cross-hatched lines correspond to the total uncertainties on the prediction. The lower panels show the ratio of the data and predicted distributions, along with the uncertainty in the ratio. The first and last bins contain any underflow and overflow events, respectively.

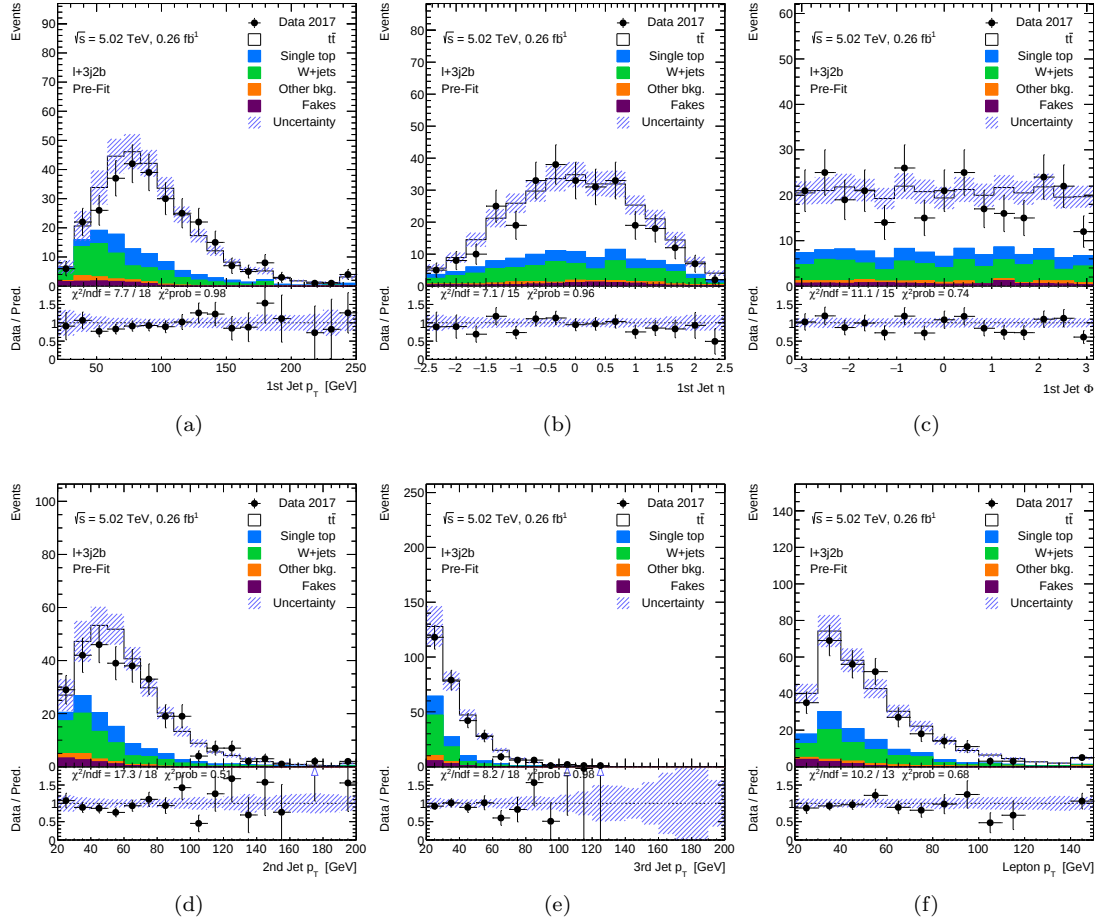


Figure E.5: The (a) leading jet p_T , (b) leading jet η , (c) leading jet Φ , (d) 2nd leading jet p_T , (e) 3rd leading jet p_T , and (f) lepton p_T distributions for data (dots) in the $\ell+3j$ 2b region. The MC simulation of the signal (white histograms) and various backgrounds (represented by histograms of different colours) are also included. The error bars on the dots represent the statistical uncertainty on the data while the blue cross-hatched lines correspond to the total uncertainties on the prediction. The lower panels show the ratio of the data and predicted distributions, along with the uncertainty in the ratio. The first and last bins contain any underflow and overflow events, respectively.

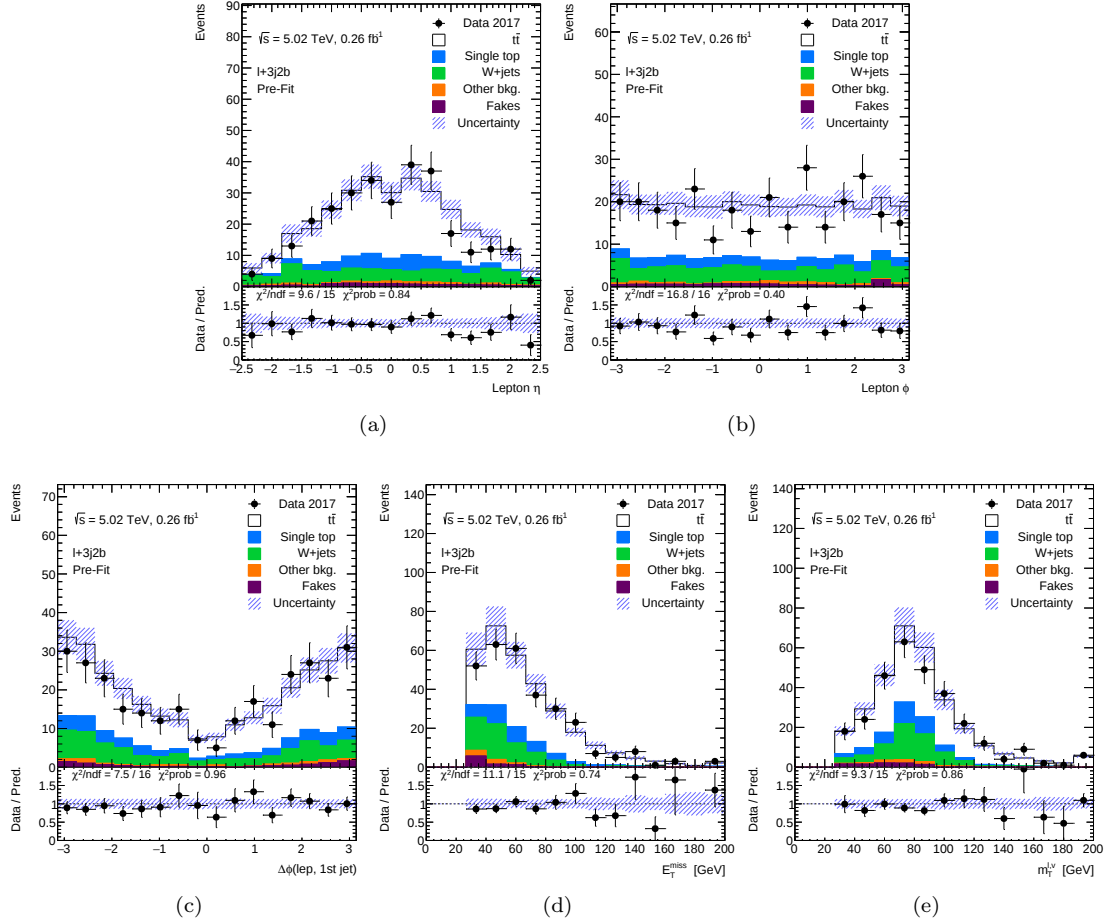


Figure E.6: The (a) lepton η , (b) lepton Φ , (c) difference in azimuthal angle between the lepton and the leading jet, (d) E_T^{miss} , and (e) m_T^W distributions for data (dots) in the $\ell+3j$ 2b region. The MC simulation of the signal (white histograms) and various backgrounds (represented by histograms of different colours) are also included. The error bars on the dots represent the statistical uncertainty on the data while the blue cross-hatched lines correspond to the total uncertainties on the prediction. The lower panels show the ratio of the data and predicted distributions, along with the uncertainty in the ratio. The first and last bins contain any underflow and overflow events, respectively.

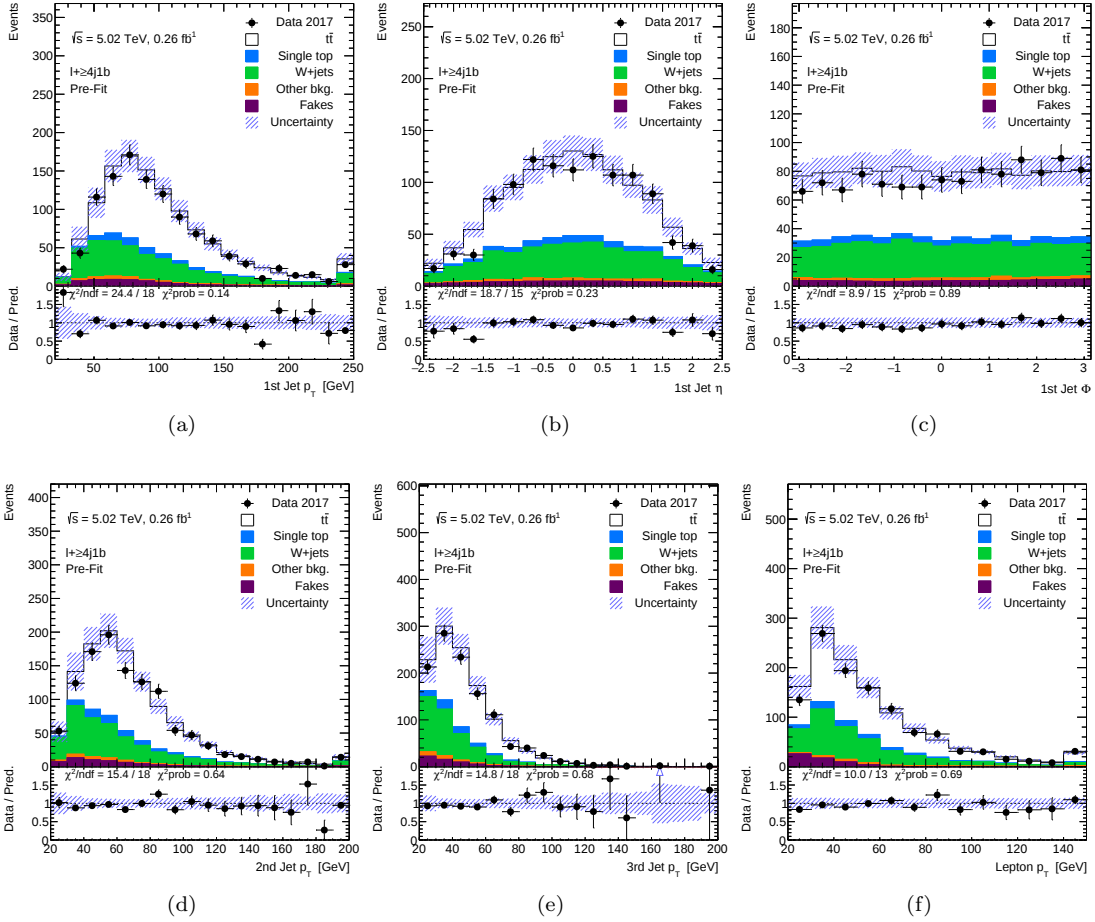


Figure E.7: The (a) leading jet p_T , (b) leading jet η , (c) leading jet Φ , (d) 2nd leading jet p_T , (e) 3rd leading jet p_T , and (f) lepton p_T distributions for data (dots) in the $\ell+\geq 4j$ 1b region. The MC simulation of the signal (white histograms) and various backgrounds (represented by histograms of different colours) are also included. The error bars on the dots represent the statistical uncertainty on the data while the blue cross-hatched lines correspond to the total uncertainties on the prediction. The lower panels show the ratio of the data and predicted distributions, along with the uncertainty in the ratio. The first and last bins contain any underflow and overflow events, respectively.

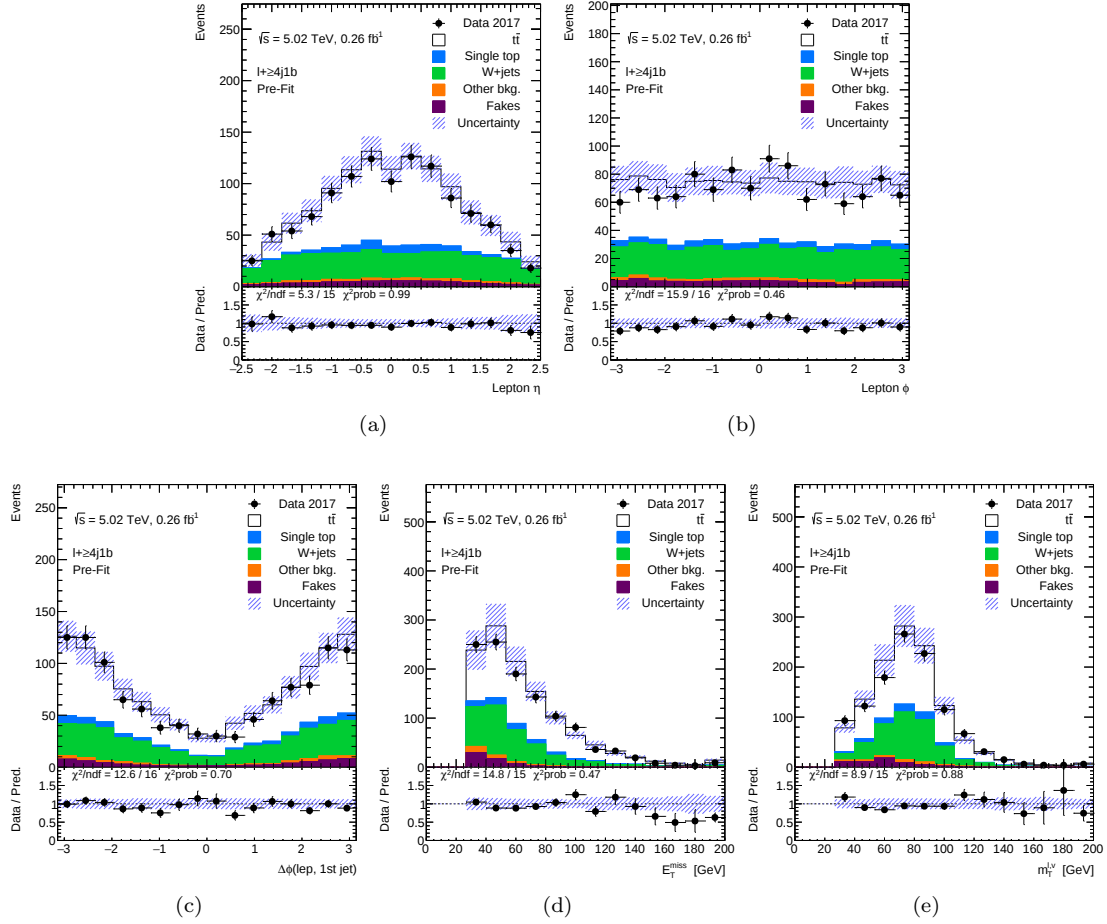


Figure E.8: The (a) lepton η , (b) lepton Φ , (c) difference in azimuthal angle between the lepton and the leading jet, (d) E_T^{miss} , and (e) $m_{\ell\ell}^W$ distributions for data (dots) in the $\ell + \geq 4j$ 1b region. The MC simulation of the signal (white histograms) and various backgrounds (represented by histograms of different colours) are also included. The error bars on the dots represent the statistical uncertainty on the data while the blue cross-hatched lines correspond to the total uncertainties on the prediction. The lower panels show the ratio of the data and predicted distributions, along with the uncertainty in the ratio. The first and last bins contain any underflow and overflow events, respectively.

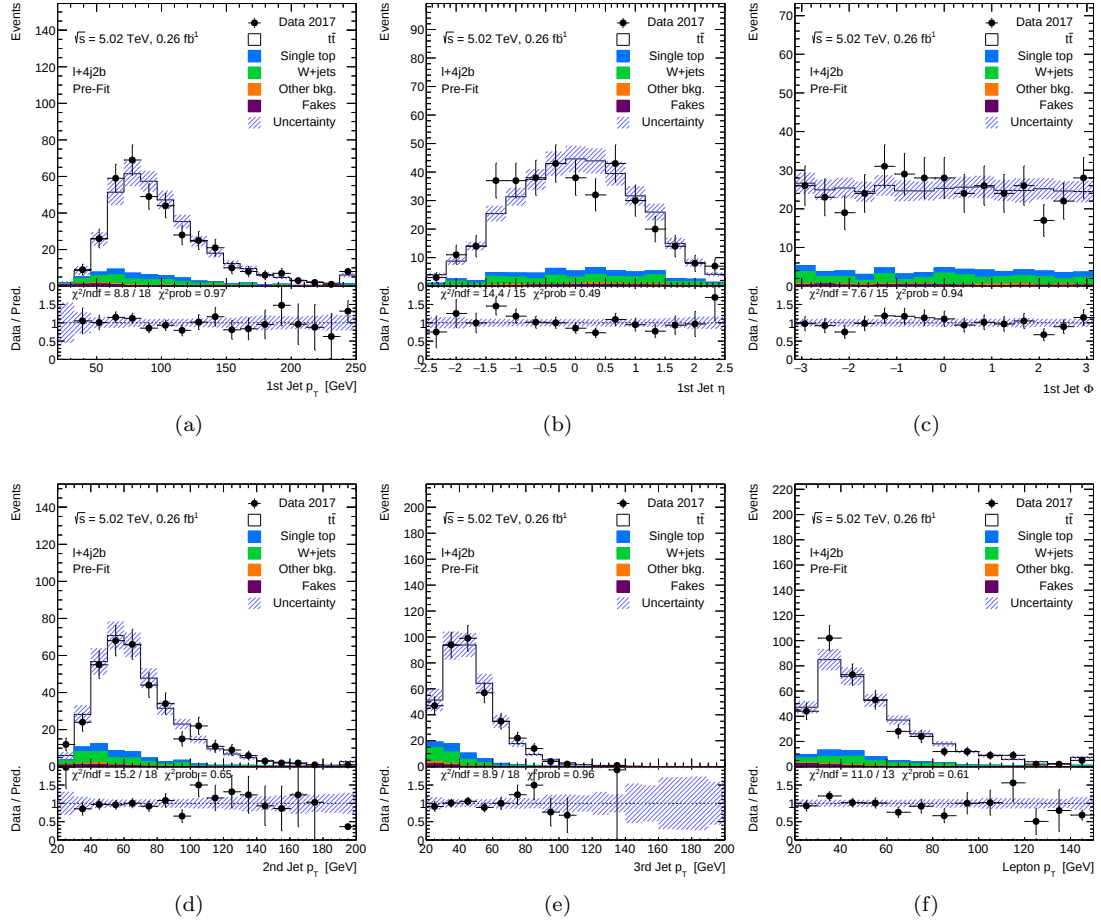


Figure E.9: The (a) leading jet p_T , (b) leading jet η , (c) leading jet Φ , (d) 2nd leading jet p_T , (e) 3rd leading jet p_T , and (f) lepton p_T distributions for data (dots) in the $\ell+4j$ 2b region. The MC simulation of the signal (white histograms) and various backgrounds (represented by histograms of different colours) are also included. The error bars on the dots represent the statistical uncertainty on the data while the blue cross-hatched lines correspond to the total uncertainties on the prediction. The lower panels show the ratio of the data and predicted distributions, along with the uncertainty in the ratio. The first and last bins contain any underflow and overflow events, respectively.

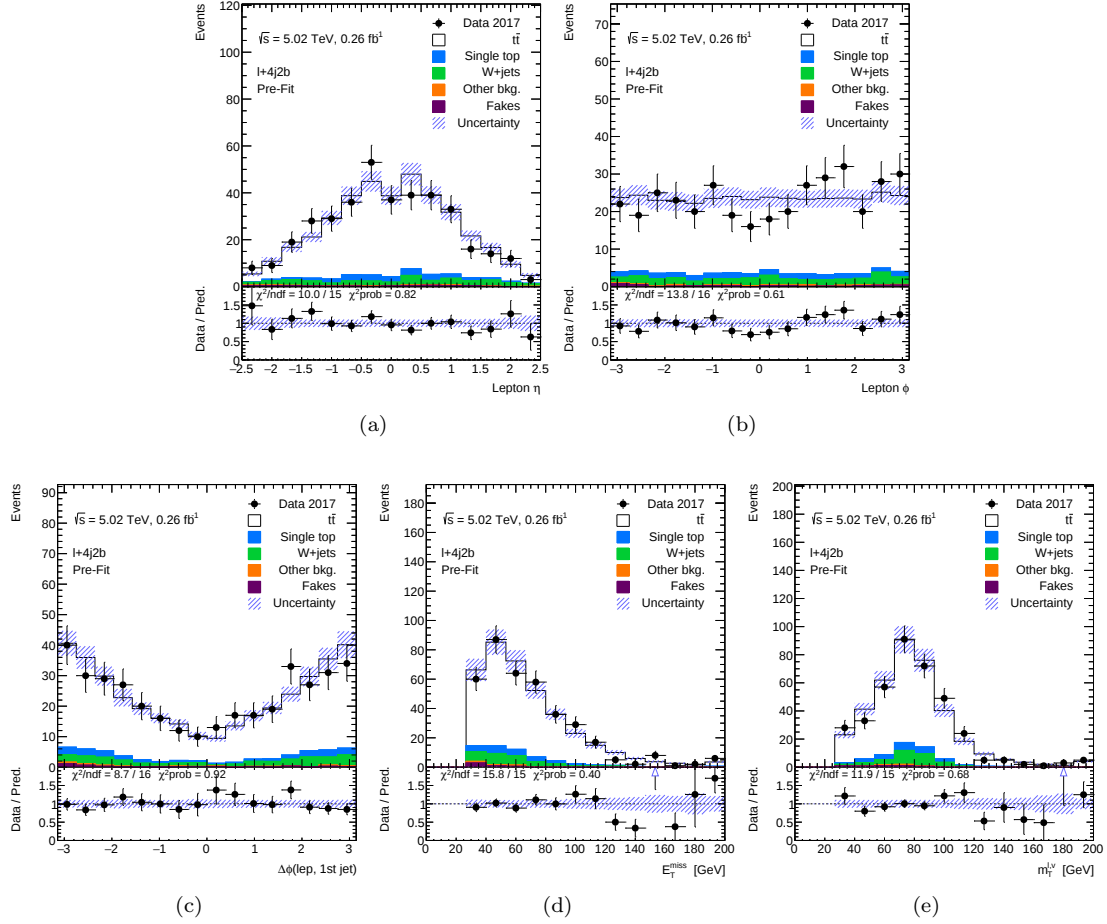


Figure E.10: The (a) lepton η , (b) lepton Φ , (c) difference in azimuthal angle between the lepton and the leading jet, (d) E_T^{miss} , and (e) m_T^W distributions for data (dots) in the $\ell+4j$ 2b region. The MC simulation of the signal (white histograms) and various backgrounds (represented by histograms of different colours) are also included. The error bars on the dots represent the statistical uncertainty on the data while the blue cross-hatched lines correspond to the total uncertainties on the prediction. The lower panels show the ratio of the data and predicted distributions, along with the uncertainty in the ratio. The first and last bins contain any underflow and overflow events, respectively.

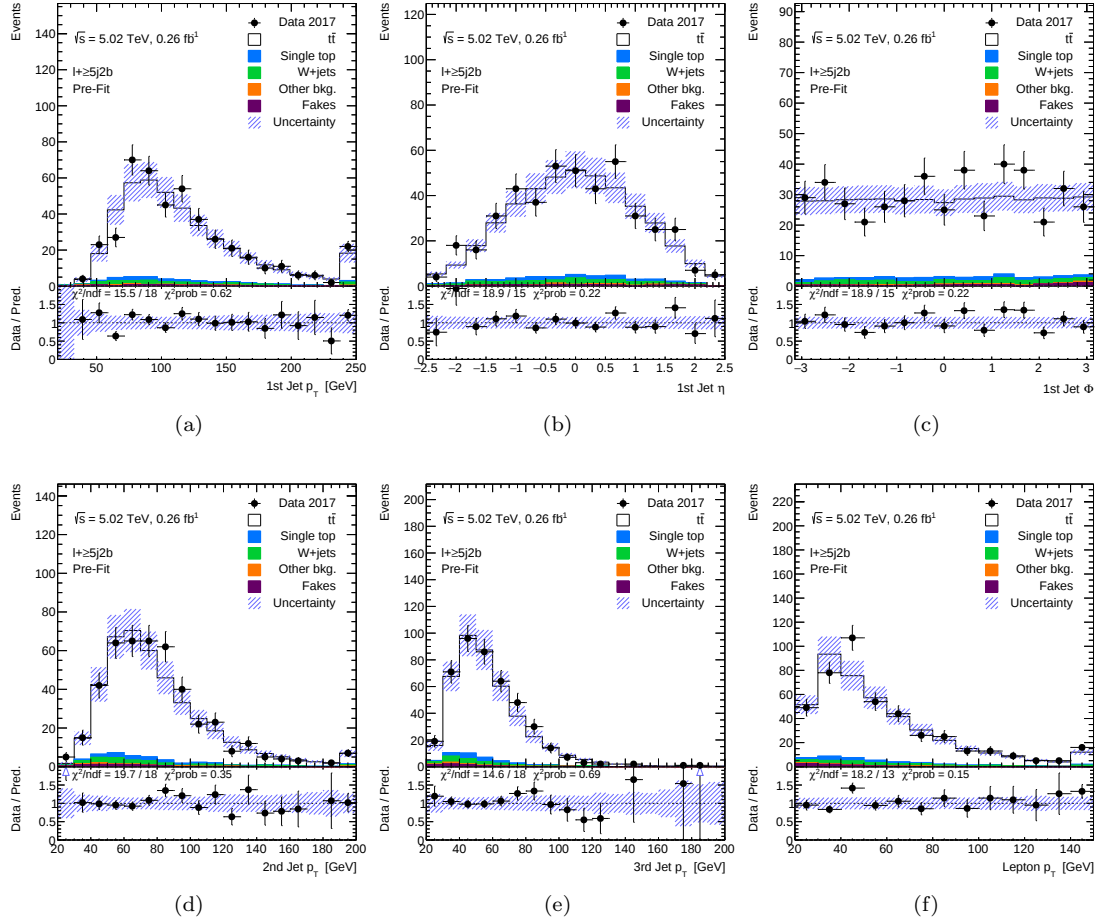


Figure E.11: The (a) leading jet p_T , (b) leading jet η , (c) leading jet Φ , (d) 2nd leading jet p_T , (e) 3rd leading jet p_T , and (f) lepton p_T distributions for data (dots) in the $\ell+\geq 5j$ 2b region. The MC simulation of the signal (white histograms) and various backgrounds (represented by histograms of different colours) are also included. The error bars on the dots represent the statistical uncertainty on the data while the blue cross-hatched lines correspond to the total uncertainties on the prediction. The lower panels show the ratio of the data and predicted distributions, along with the uncertainty in the ratio. The first and last bins contain any underflow and overflow events, respectively.

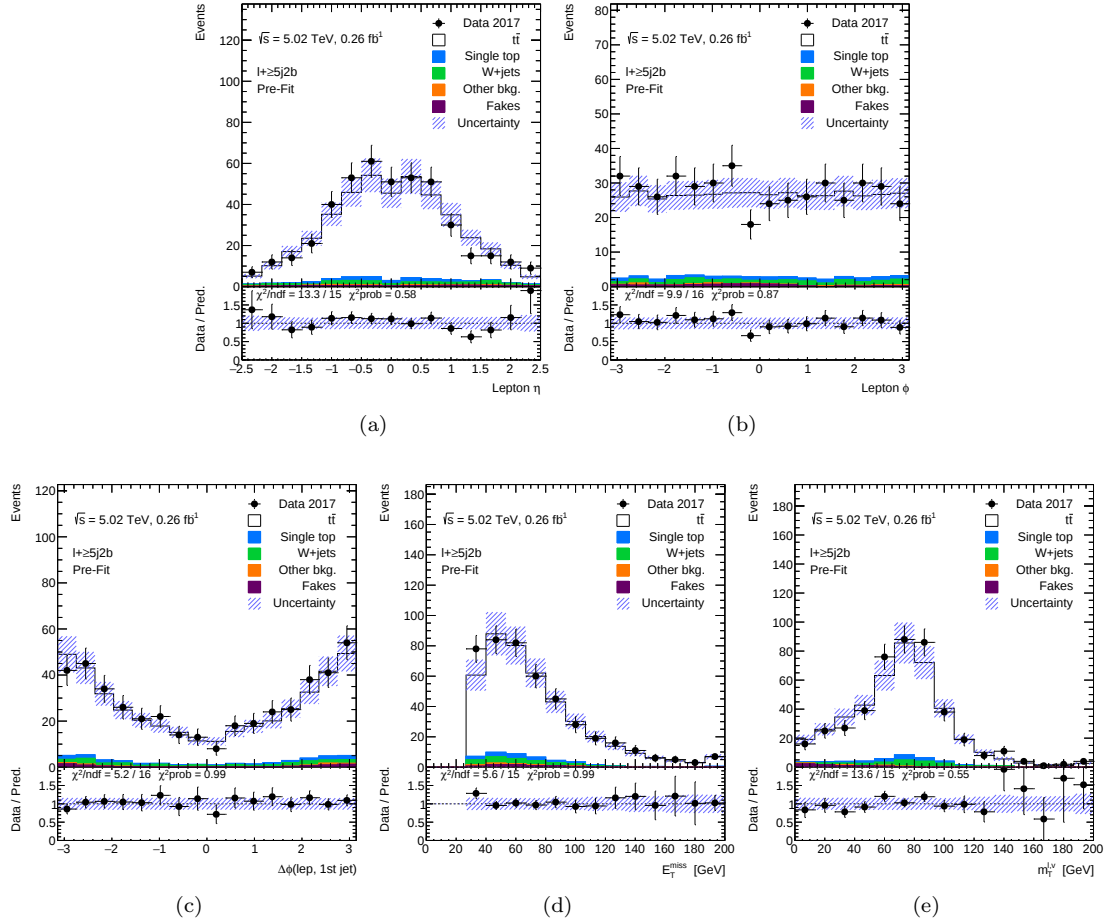


Figure E.12: The (a) lepton η , (b) lepton Φ , (c) difference in azimuthal angle between the lepton and the leading jet, (d) E_T^{miss} , and (e) m_T^W distributions for data (dots) in the $\ell + \geq 5j$ 2b region. The MC simulation of the signal (white histograms) and various backgrounds (represented by histograms of different colours) are also included. The error bars on the dots represent the statistical uncertainty on the data while the blue cross-hatched lines correspond to the total uncertainties on the prediction. The lower panels show the ratio of the data and predicted distributions, along with the uncertainty in the ratio. The first and last bins contain any underflow and overflow events, respectively.

Appendix F

Distributions of BDT Input Variables - $\sigma_{t\bar{t}}$ Measurement

Comparisons between the shapes of the signal and background alongside a comparison of the data and predicted histograms are shown for events passing the ℓ +jets preselection for the BDT input variables. The plots are shown in:

- Figure F.1 and Figure F.2 for H_T^{had}
- Figure F.3 and Figure F.4 for FW2
- Figure F.5 and Figure F.6 for lepton η
- Figure F.7 and Figure F.8 for ΔR_{bl} (med.)
- Figure F.9 and Figure F.10 for ΔR_{jj} (med.)
- Figure F.11 and Figure F.12 for $m(jj)^{\text{min.}\Delta R}$
- Figure F.13 and Figure F.14 for ΔR_{uu} (med.)
- Figure F.15 and Figure F.16 for $m(uu)^{\text{min.}\Delta R}$

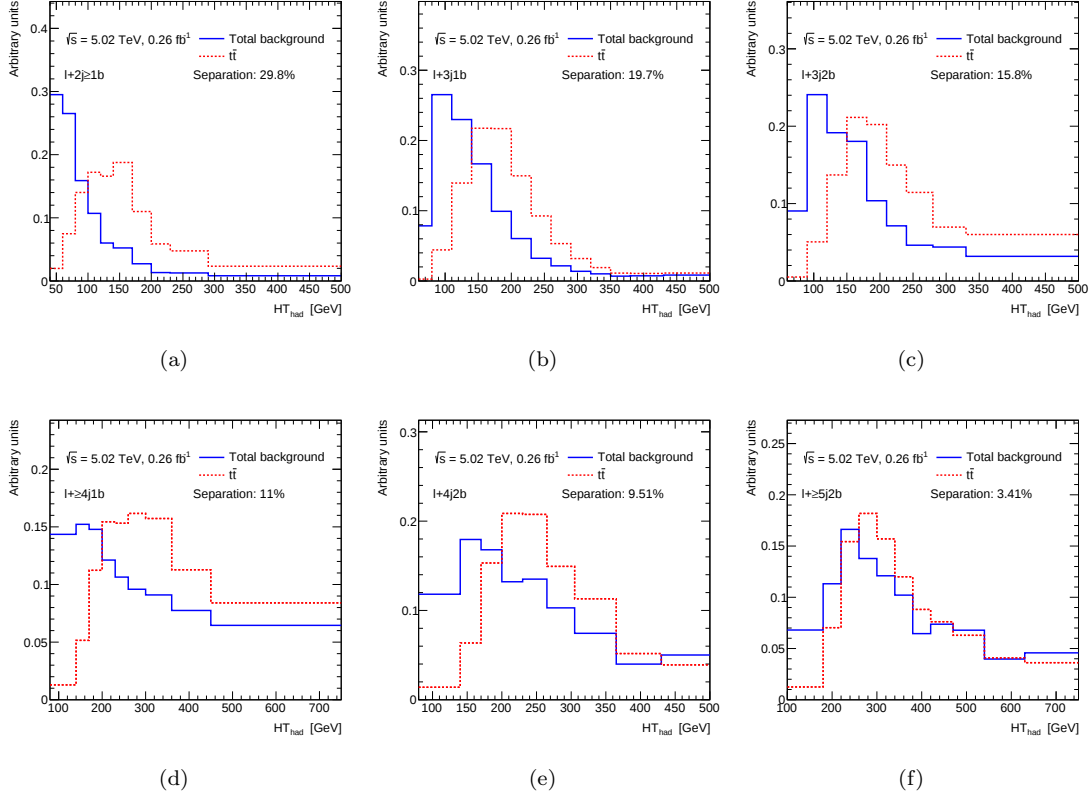


Figure F.1: Comparison between the shapes of the H_T^{had} distribution for the $t\bar{t}$ signal (red) and total background (blue) in (a) $\ell+2j\geq 1b$, (b) $\ell+3j1b$, (c) $\ell+3j2b$, (d) $\ell+\geq 4j1b$, (e) $\ell+4j2b$, and (f) $\ell+\geq 5j2b$. The distributions are normalized to unit area in order to visualize the separation in the BDT response between the two samples.

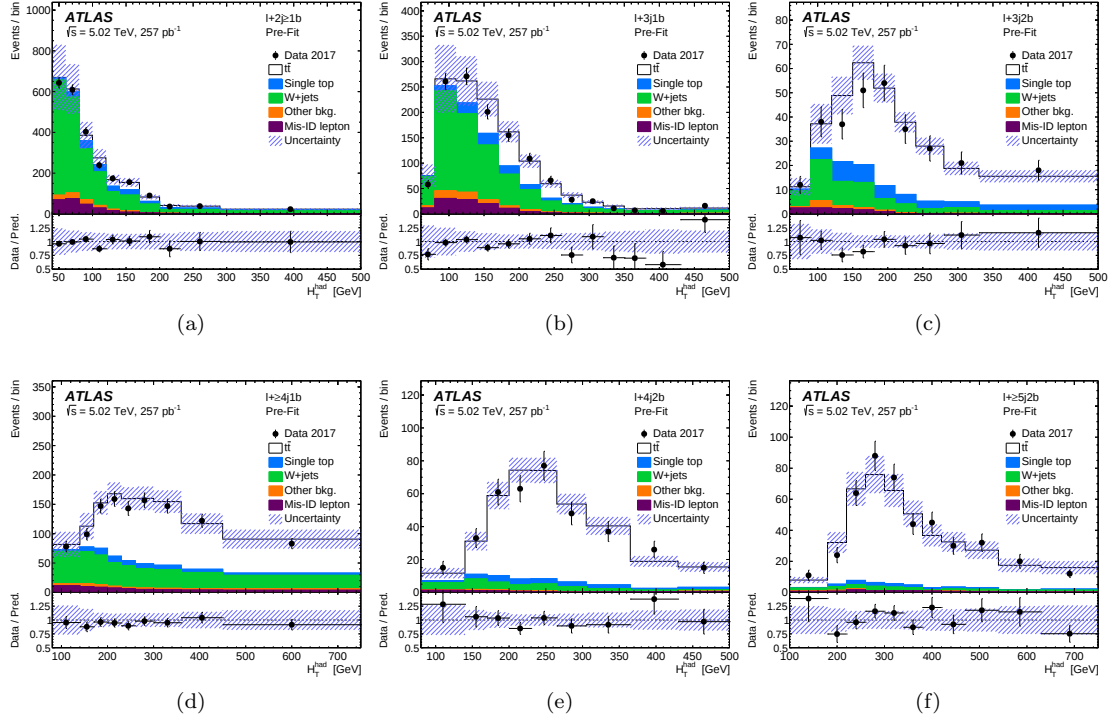


Figure F.2: The H_T^{had} distribution for data (dots) in (a) $\ell+2j \geq 1b$, (b) $\ell+3j 1b$, (c) $\ell+3j 2b$, (d) $\ell+\geq 4j 1b$, (e) $\ell+4j 2b$, and (f) $\ell+\geq 5j 2b$. The MC simulation of the signal (white histograms) and various backgrounds (represented by histograms of different colours) are also included. The error bars on the dots represent the statistical uncertainty on the data while the blue cross-hatched lines correspond to the total uncertainties on the prediction. The lower panels show the ratio of the data and predicted distributions, along with the uncertainty in the ratio.

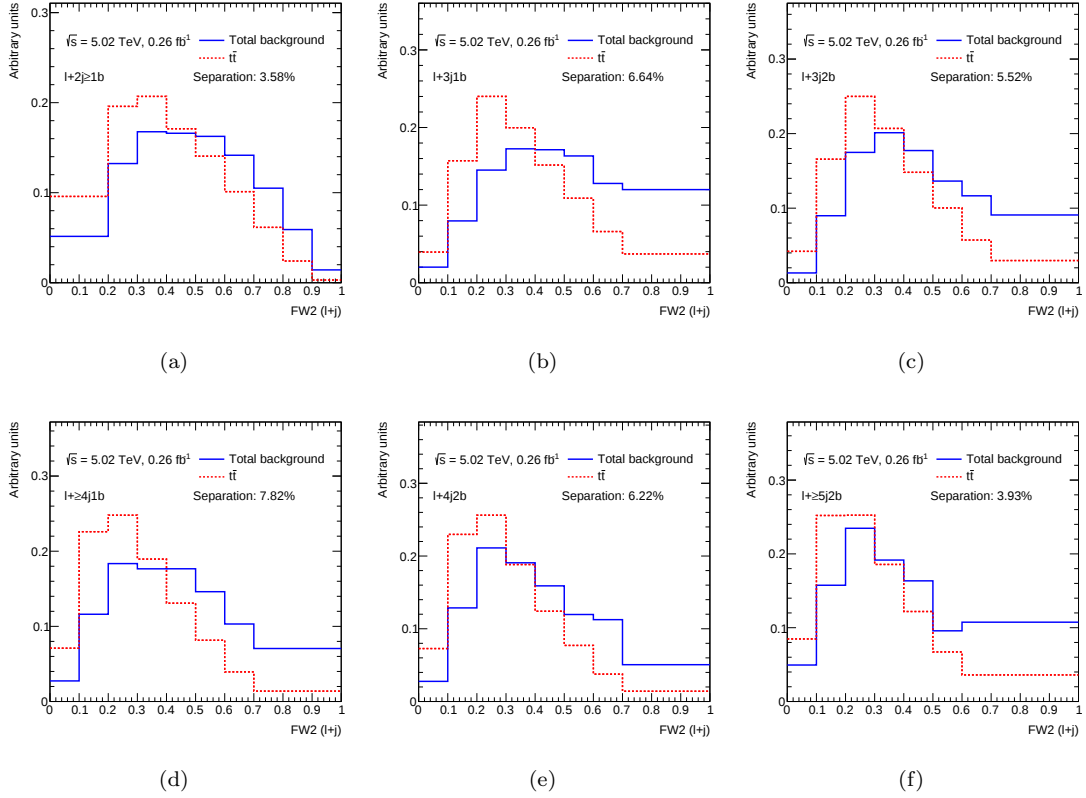


Figure F.3: Comparison between the shapes of the FW2 distribution for the $t\bar{t}$ signal (red) and total background (blue) in (a) $l+2j \geq 1b$, (b) $l+3j 1b$, (c) $l+3j 2b$, (d) $l+\geq 4j 1b$, (e) $l+4j 2b$, and (f) $l+\geq 5j 2b$. The distributions are normalized to unit area in order to visualize the separation in the BDT response between the two samples.

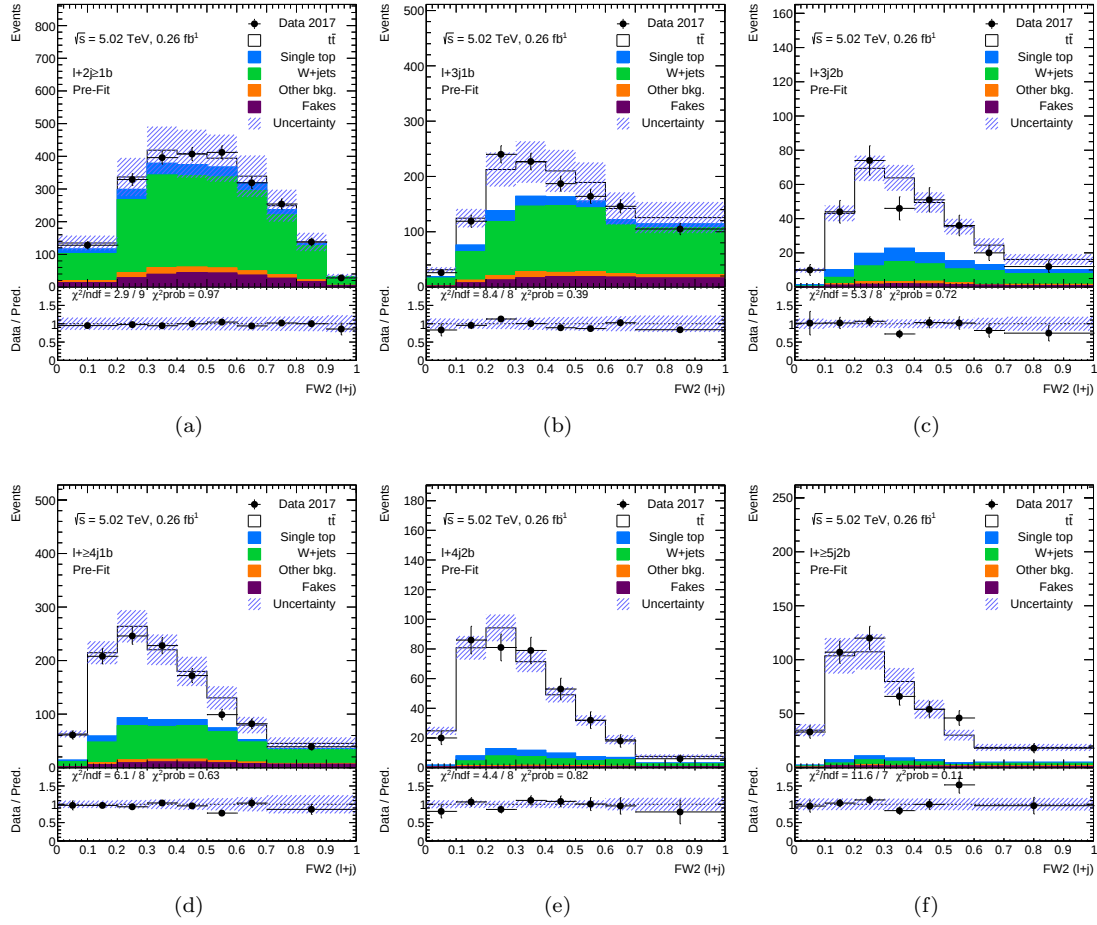


Figure F.4: The FW2 distribution for data (dots) in (a) $\ell+2j \geq 1b$, (b) $\ell+3j \geq 1b$, (c) $\ell+3j \geq 2b$, (d) $\ell+4j \geq 1b$, (e) $\ell+4j \geq 2b$, and (f) $\ell+5j \geq 2b$. The MC simulation of the signal (white histograms) and various backgrounds (represented by histograms of different colours) are also included. The error bars on the dots represent the statistical uncertainty on the data while the blue cross-hatched lines correspond to the total uncertainties on the prediction. The lower panels show the ratio of the data and predicted distributions, along with the uncertainty in the ratio.

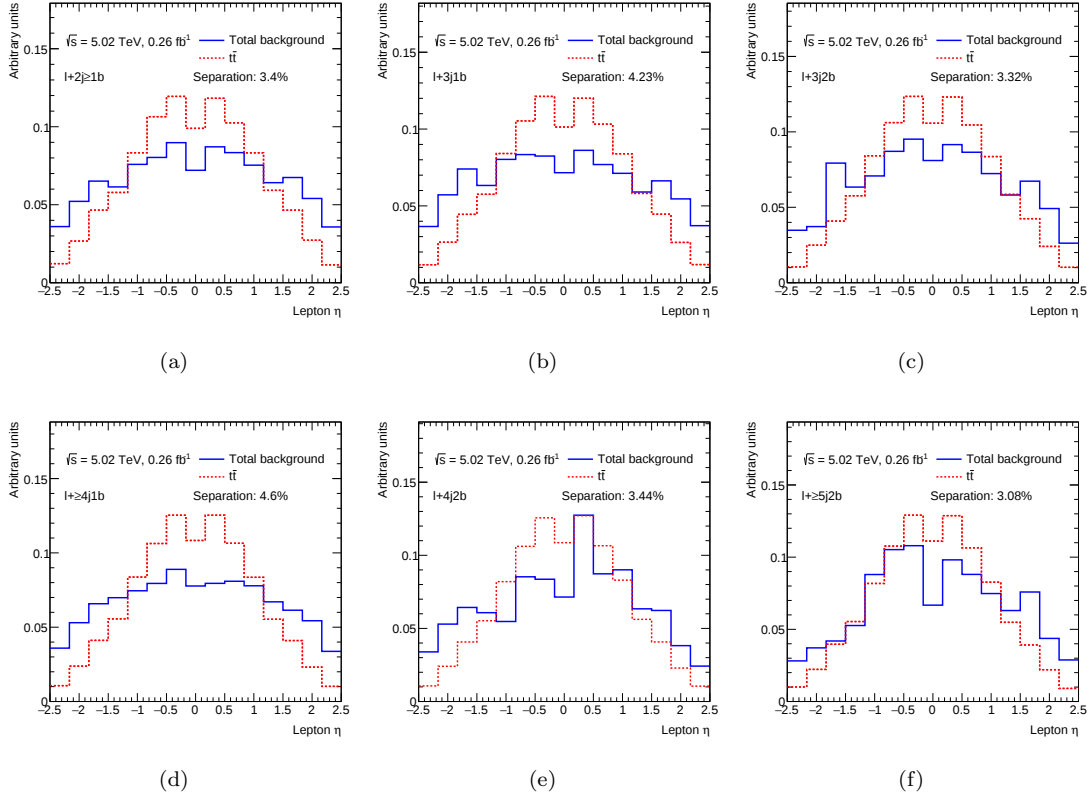


Figure F.5: Comparison between the shapes of the lepton η distribution for the $t\bar{t}$ signal (red) and total background (blue) in (a) $\ell+2j \geq 1b$, (b) $\ell+3j 1b$, (c) $\ell+3j 2b$, (d) $\ell+\geq 4j 1b$, (e) $\ell+4j 2b$, and (f) $\ell+\geq 5j 2b$. The distributions are normalized to unit area in order to visualize the separation in the BDT response between the two samples.

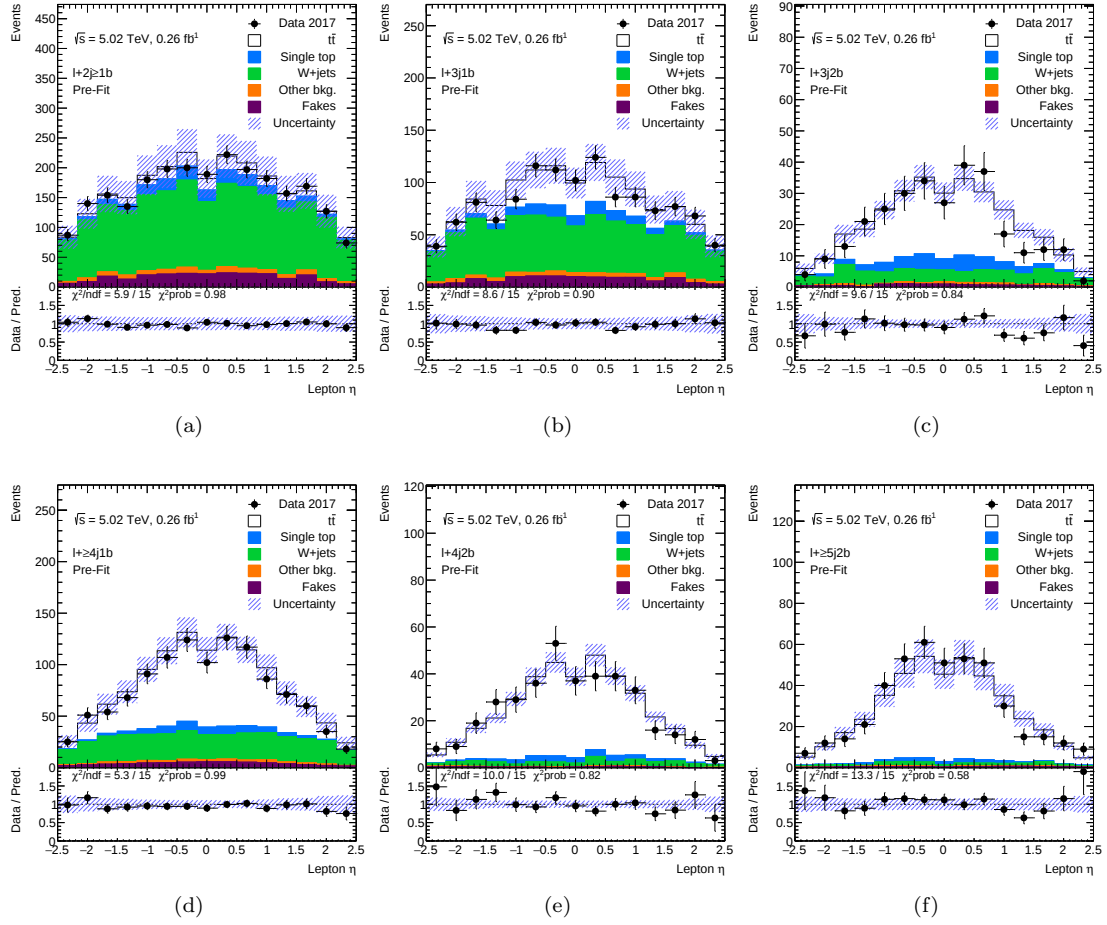


Figure F.6: The lepton η distribution for data (dots) in (a) $\ell+2j\geq 1b$, (b) $\ell+3j1b$, (c) $\ell+3j2b$, (d) $\ell+\geq 4j1b$, (e) $\ell+4j2b$, and (f) $\ell+\geq 5j2b$. The MC simulation of the signal (white histograms) and various backgrounds (represented by histograms of different colours) are also included. The error bars on the dots represent the statistical uncertainty on the data while the blue cross-hatched lines correspond to the total uncertainties on the prediction. The lower panels show the ratio of the data and predicted distributions, along with the uncertainty in the ratio.

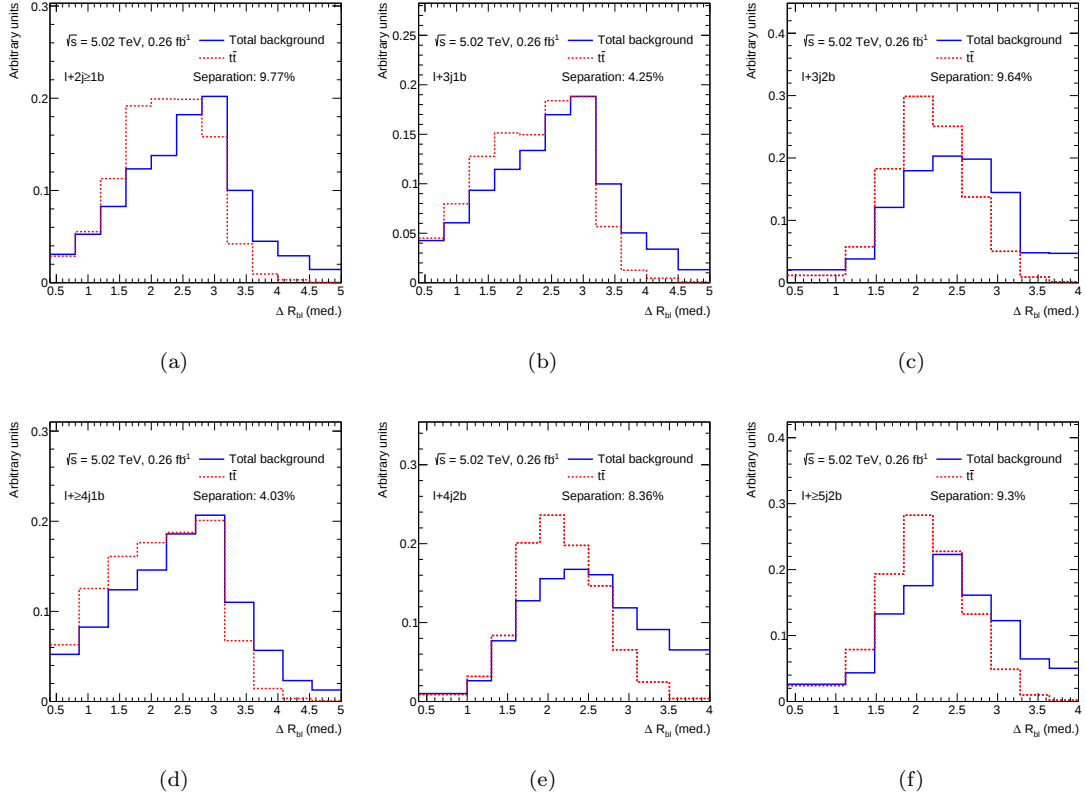


Figure F.7: Comparison between the shapes of the median ΔR_{bl} distribution for the $t\bar{t}$ signal (red) and total background (blue) in (a) $\ell+2j \geq 1b$, (b) $\ell+3j \geq 1b$, (c) $\ell+3j \geq 2b$, (d) $\ell+\geq 4j \geq 1b$, (e) $\ell+4j \geq 2b$, and (f) $\ell+\geq 5j \geq 2b$. The distributions are normalized to unit area in order to visualize the separation in the BDT response between the two samples.

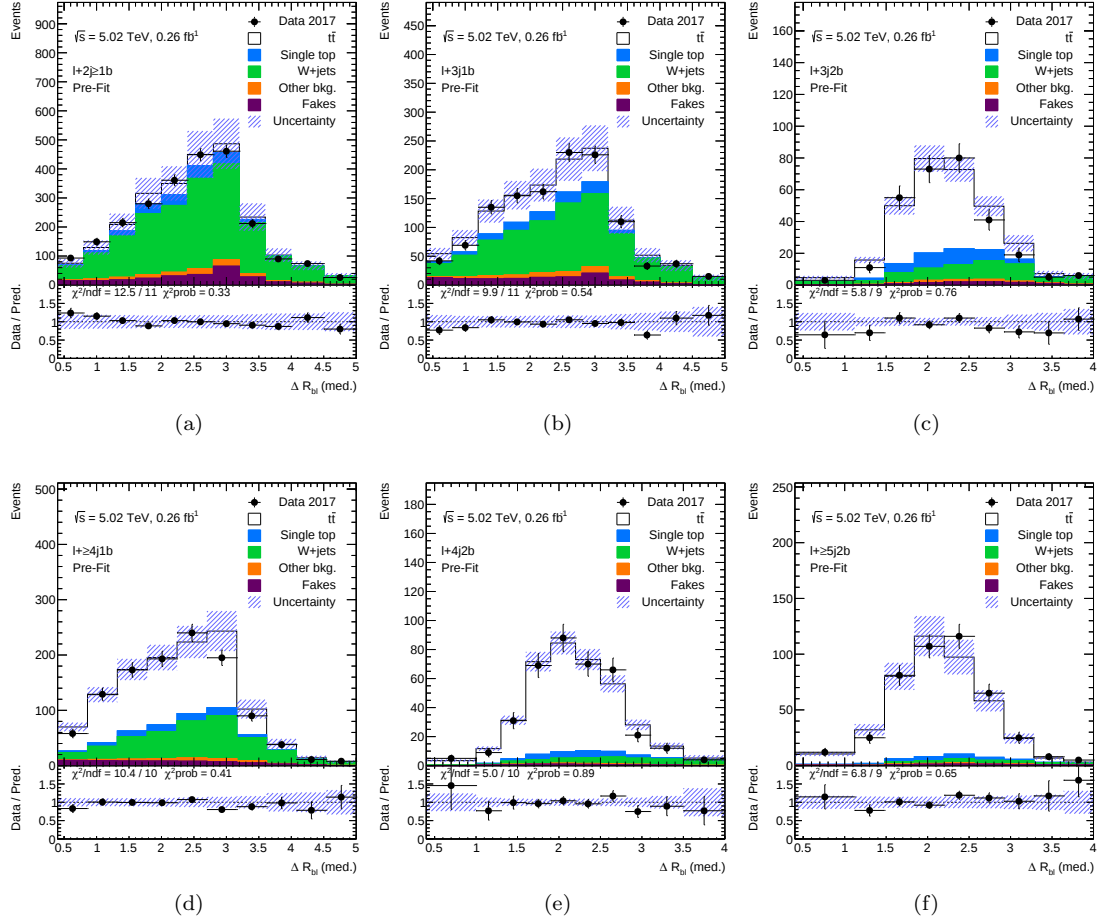


Figure F.8: The median ΔR_{bl} distribution for data (dots) in (a) $\ell+2j\geq 1b$, (b) $\ell+3j$ 1b, (c) $\ell+3j$ 2b, (d) $\ell+\geq 4j$ 1b, (e) $\ell+4j$ 2b, and (f) $\ell+\geq 5j$ 2b. The MC simulation of the signal (white histograms) and various backgrounds (represented by histograms of different colours) are also included. The error bars on the dots represent the statistical uncertainty on the data while the blue cross-hatched lines correspond to the total uncertainties on the prediction. The lower panels show the ratio of the data and predicted distributions, along with the uncertainty in the ratio.

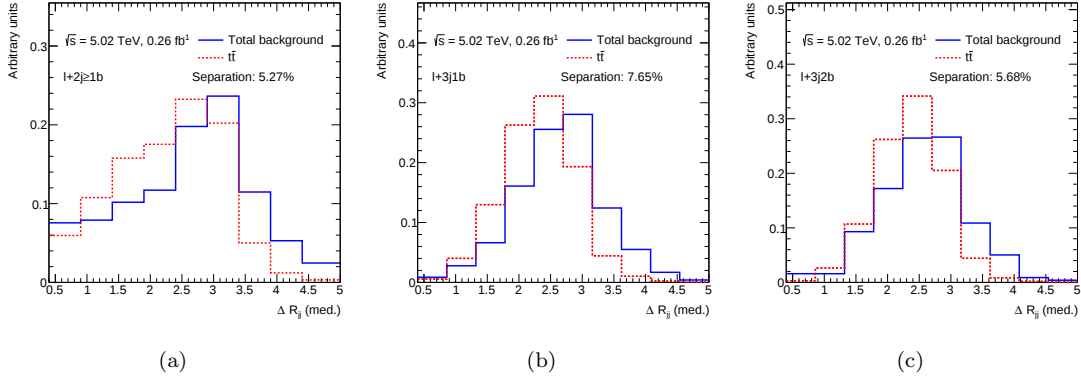


Figure F.9: Comparison between the shapes of the median ΔR_{jj} distribution for the $t\bar{t}$ signal (red) and total background (blue) in (a) $\ell+2j\geq 1b$, (b) $\ell+3j$ 1b, (c) $\ell+3j$ 2b. The distributions are normalized to unit area in order to visualize the separation in the BDT response between the two samples.

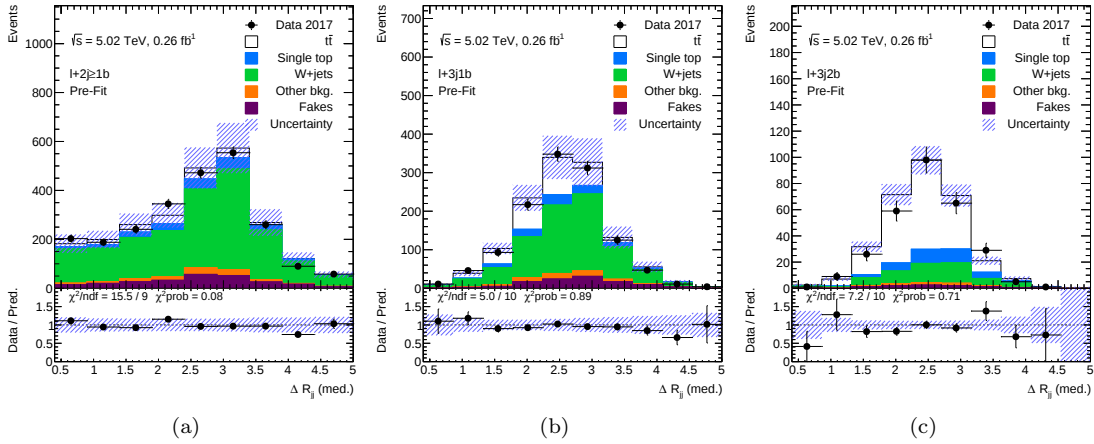


Figure F.10: The median ΔR_{jj} distribution for data (dots) in (a) $\ell+2j\geq 1b$, (b) $\ell+3j$ 1b, (c) $\ell+3j$ 2b. The MC simulation of the signal (white histograms) and various backgrounds (represented by histograms of different colours) are also included. The error bars on the dots represent the statistical uncertainty on the data while the blue cross-hatched lines correspond to the total uncertainties on the prediction. The lower panels show the ratio of the data and predicted distributions, along with the uncertainty in the ratio.

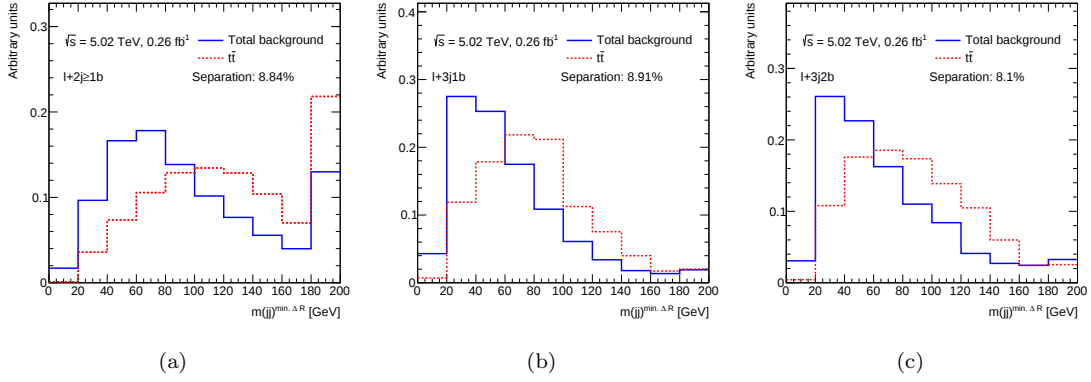


Figure F.11: Comparison between the shapes of the $m(jj)^{\min, \Delta R}$ distribution for the $t\bar{t}$ signal (red) and total background (blue) in (a) $\ell+2j \geq 1b$, (b) $\ell+3j 1b$, (c) $\ell+3j 2b$. The distributions are normalized to unit area in order to visualize the separation in the BDT response between the two samples.

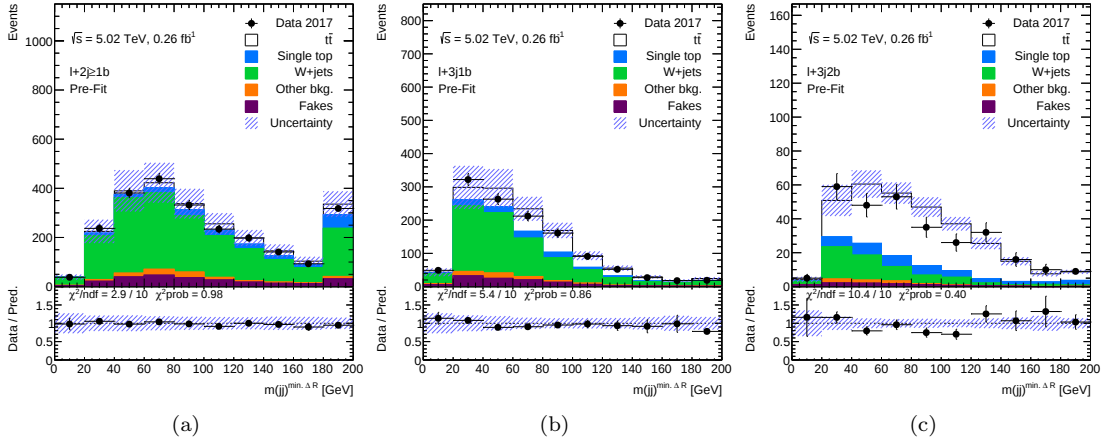


Figure F.12: The $m(jj)^{\min, \Delta R}$ distribution for data (dots) in (a) $\ell+2j \geq 1b$, (b) $\ell+3j 1b$, (c) $\ell+3j 2b$. The MC simulation of the signal (white histograms) and various backgrounds (represented by histograms of different colours) are also included. The error bars on the dots represent the statistical uncertainty on the data while the blue cross-hatched lines correspond to the total uncertainties on the prediction. The lower panels show the ratio of the data and predicted distributions, along with the uncertainty in the ratio.

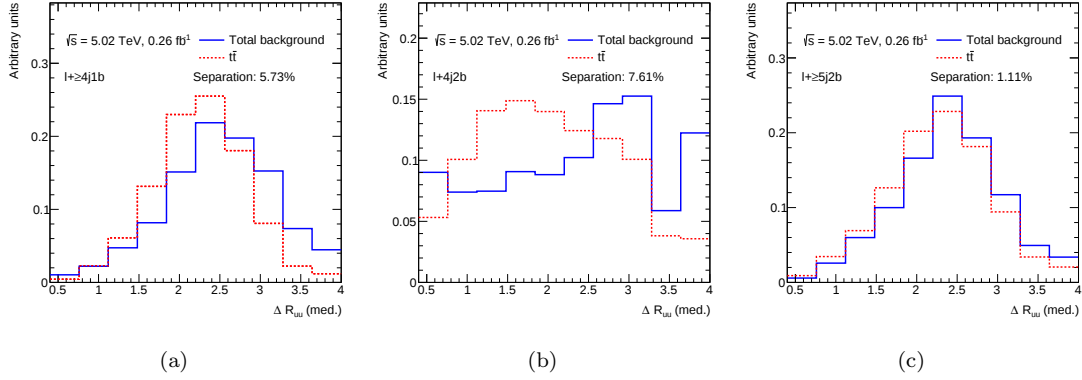


Figure F.13: Comparison between the shapes of the median ΔR_{uu} distribution for the $t\bar{t}$ signal (red) and total background (blue) in (a) $\ell+\geq 4j$ 1b, (b) $\ell+4j$ 2b, (c) $\ell+\geq 5j$ 2b. The distributions are normalized to unit area in order to visualize the separation in the BDT response between the two samples.

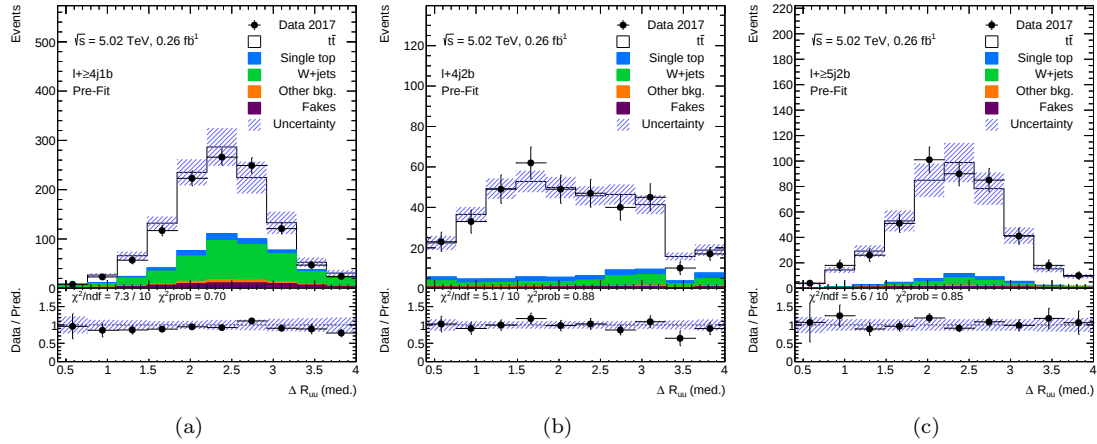


Figure F.14: The median ΔR_{uu} distribution for data (dots) in (a) $\ell+\geq 4j$ 1b, (b) $\ell+4j$ 2b, (c) $\ell+\geq 5j$ 2b. The MC simulation of the signal (white histograms) and various backgrounds (represented by histograms of different colours) are also included. The error bars on the dots represent the statistical uncertainty on the data while the blue cross-hatched lines correspond to the total uncertainties on the prediction. The lower panels show the ratio of the data and predicted distributions, along with the uncertainty in the ratio.

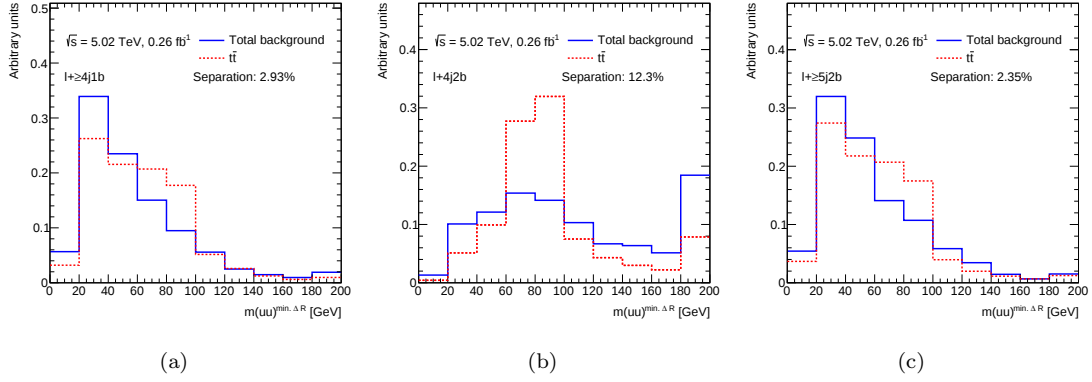


Figure F.15: Comparison between the shapes of the $m(uu)^{\min, \Delta R}$ distribution for the $t\bar{t}$ signal (red) and total background (blue) in (a) $\ell+\ge 4j$ 1b, (b) $\ell+4j$ 2b, (c) $\ell+\ge 5j$ 2b. The distributions are normalized to unit area in order to visualize the separation in the BDT response between the two samples.

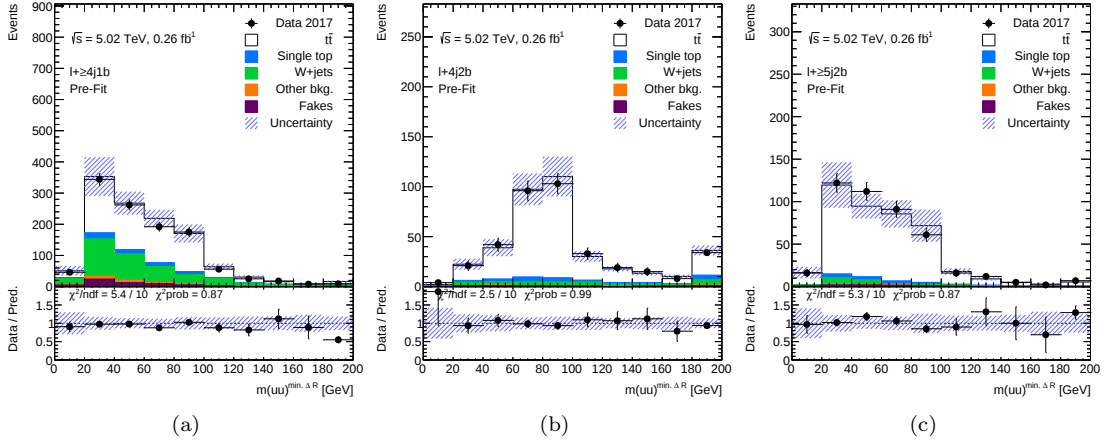


Figure F.16: The $m(uu)^{\min, \Delta R}$ distribution for data (dots) in (a) $\ell+\ge 4j$ 1b, (b) $\ell+4j$ 2b, (c) $\ell+\ge 5j$ 2b. The MC simulation of the signal (white histograms) and various backgrounds (represented by histograms of different colours) are also included. The error bars on the dots represent the statistical uncertainty on the data while the blue cross-hatched lines correspond to the total uncertainties on the prediction. The lower panels show the ratio of the data and predicted distributions, along with the uncertainty in the ratio.

Appendix G

JES Flavour Composition and Response Uncertainties

This appendix documents the derivation of the JES flavour composition and flavour response uncertainties. Since the flavour composition and response are analysis dependent, the corresponding uncertainties can be improved by estimating the jet composition for the analysis using the MC samples. According to Ref. [134], the flavour response (σ_{response}) and flavour composition ($\sigma_{\text{composition}}$) uncertainties in bins of p_T and η can be written as

$$\sigma_{\text{response}} = \sigma_g^f \frac{|\mathcal{R}_q^{\text{Pythia}} - \mathcal{R}_g^{\text{Pythia}}|}{f_g \mathcal{R}_g^{\text{Pythia}} + (1 - f_g) \mathcal{R}_q^{\text{Pythia}}} \quad (\text{G.1})$$

$$\sigma_{\text{composition}} = f_g \left(\mathcal{R}_g^{\text{Pythia}} - \mathcal{R}_g^{\text{Herwig}} \right) \quad (\text{G.2})$$

Here, f_g is the fraction of gluon initiated jets, σ_g^f is the uncertainty on this fraction, $\mathcal{R}_q^X$ is the response of light quark jets with a given model X , and $\mathcal{R}_g^X$ is the response of gluon jets for a given model X .

By default, ATLAS JES uncertainties assume $f_g = 50\%$ and this can lead to larger than expected uncertainties from flavour response and flavour composition. Considering that the fraction of $t\bar{t}$ events produced via quark-antiquark annihilation is larger at lower centre-of-mass energies, the $\sqrt{s} = 5.02$ TeV measurement overestimates the effect of these uncertainties if using the default scheme. The two flavour uncertainties can be reduced by extracting f_g using truth MC information. Figure G.1 shows the fractions of gluon initiated jets for the nominal $t\bar{t}$ sample as a 2D histogram in bins of jet $|\eta|$ and jet p_T .

Figure G.2 shows the effects of recalculating the quark-gluon fractions by comparing the ranking plot of an Asimov fit using JES uncertainties based on the default and recalculated f_g . The JES flavour

composition and flavour response uncertainties do not show up in the list of top 15 uncertainties when using the recalculated quark-gluon fractions since the post-fit impact on μ drops by a factor of 1/10, 1/3, and 1/2 for the b -jet energy scale, JES flavour composition, and JES flavour response uncertainties, respectively.

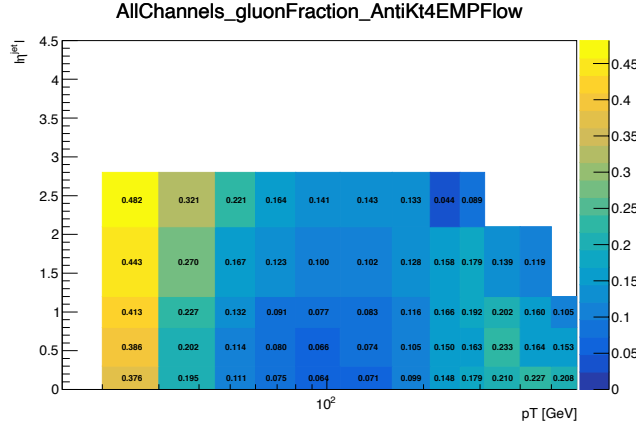


Figure G.1: The fraction of gluon initiated jets in the nominal $t\bar{t}$ sample shown in bins of jet $|\eta|$ and jet p_T . The gluon fractions are almost 10% lower than the default fraction at low p_T , and are much lower than the default at higher p_T .

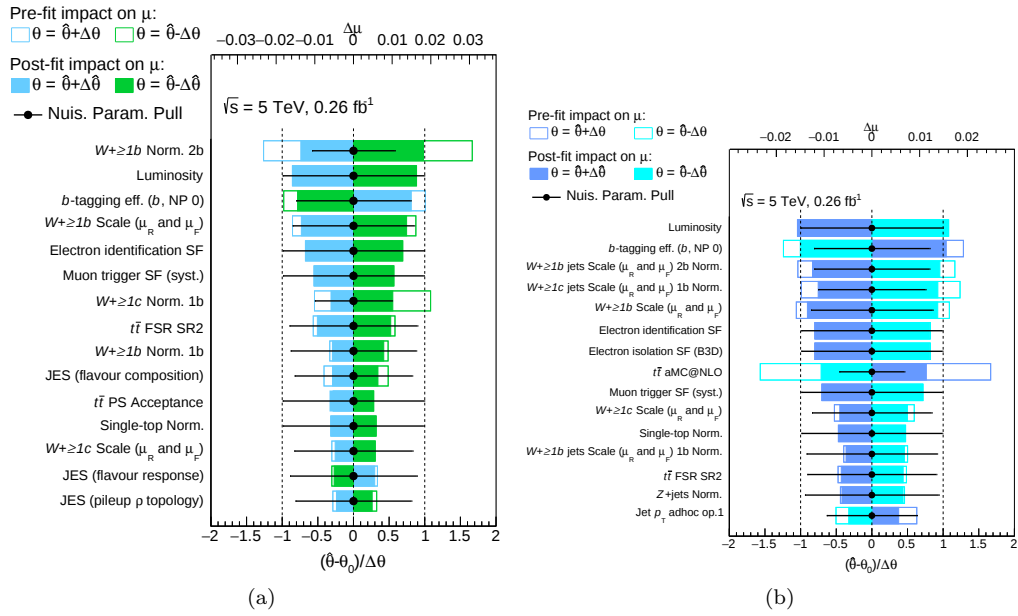


Figure G.2: Ranking plot for a fit to Asimov data using: (a) JES uncertainties based on $f_g = 50\%$ and (b) JES uncertainties based on the recalculated gluon fraction.

Appendix H

Convino studies

Two studies were performed to understand the sensitivity of the combined uncertainty given by Convino with respect to the "input correlation values". In this context, input correlation value is used to refer to the Convino input that defines the correlation between the systematic uncertainties of two different measurements. These values are the off-diagonal values of the correlation matrix used by the χ^2 fit, as presented in Equation 6.9. The study to quantify the sensitivity of the correlation value in the case of one-to-one uncertainties is presented in Section H.1 whereas the second study on one-to-many uncertainties is discussed in Section H.2. The results of the two studies justify the three principles defined in Section 6.9.2. In both studies, a test combination is emulated by performing Asimov fits to the e +jets and μ +jets channels using some variation of the nominal single lepton fitting scheme. The two individual channels are then combined using Convino and the `TRExFitter` package (denoted as `multifit`) to allow for an independent validation since the `TRExFitter` package combines the actual likelihoods used to define the individual fits while Convino emulates the likelihood function.

Finally, Section H.3 provides an additional cross-check of the combination scheme by comparing the pre- and post-Convino-fit correlation matrices in a pseudo Asimov fit.

H.1 One-to-one Systematics

In this study, an Asimov fit to the BDT response distribution is performed using the nominal single lepton fitting scheme while excluding the MC statistical uncertainty (denoted as γ). The post-fit results are as follows:

- e +jets fit: $\mu = 1.0 \pm 0.0570$
- μ +jets fit: $\mu = 1.0 \pm 0.0529$

- TRexFitter combined fit (multifit): $\mu = 1.0 \pm 0.0445$

Figures [H.1](#) and [H.2](#) show the pulls and constraints for the fitted nuisance parameters, for the e +jets and μ +jets fits, respectively. Note that all NPs between the e +jets and μ +jets fits are shared except the ones representing the lepton objects and misidentified lepton background uncertainties.

For this study, the sensitivity of the Convino results is tested by scanning the input correlation value for all shared uncertainties from 0 to 1 and identifying the corresponding change in the combined uncertainty. The combined central value is always 1.0 no matter the input correlation value. To first-order, two different NPs in the two measurements are considered to be completely uncorrelated and so the correlation value in such a case is always set to 0. For example, the $t\bar{t}$ matrix element normalization uncertainty in the e +jets channel is considered to be uncorrelated to the $t\bar{t}$ parton shower normalization uncertainty in μ +jets channel. Furthermore, if the uncertainty is unique to a single measurement then it is considered to be uncorrelated with all the systematic uncertainties in the other measurement. This study is summarized in Table [H.1](#) and the final combined uncertainty is found to be highly dependent on the overall input correlation value and as expected, a correlation value near 1.0 provides perfect agreement with the multifit post-fit uncertainty. A correlation value of 1.0 cannot be used because the matrix in Equation [6.9](#) becomes non-invertible. Thus, a value of 0.99 is used instead for such uncertainties in the combination between the single lepton and dilepton results.

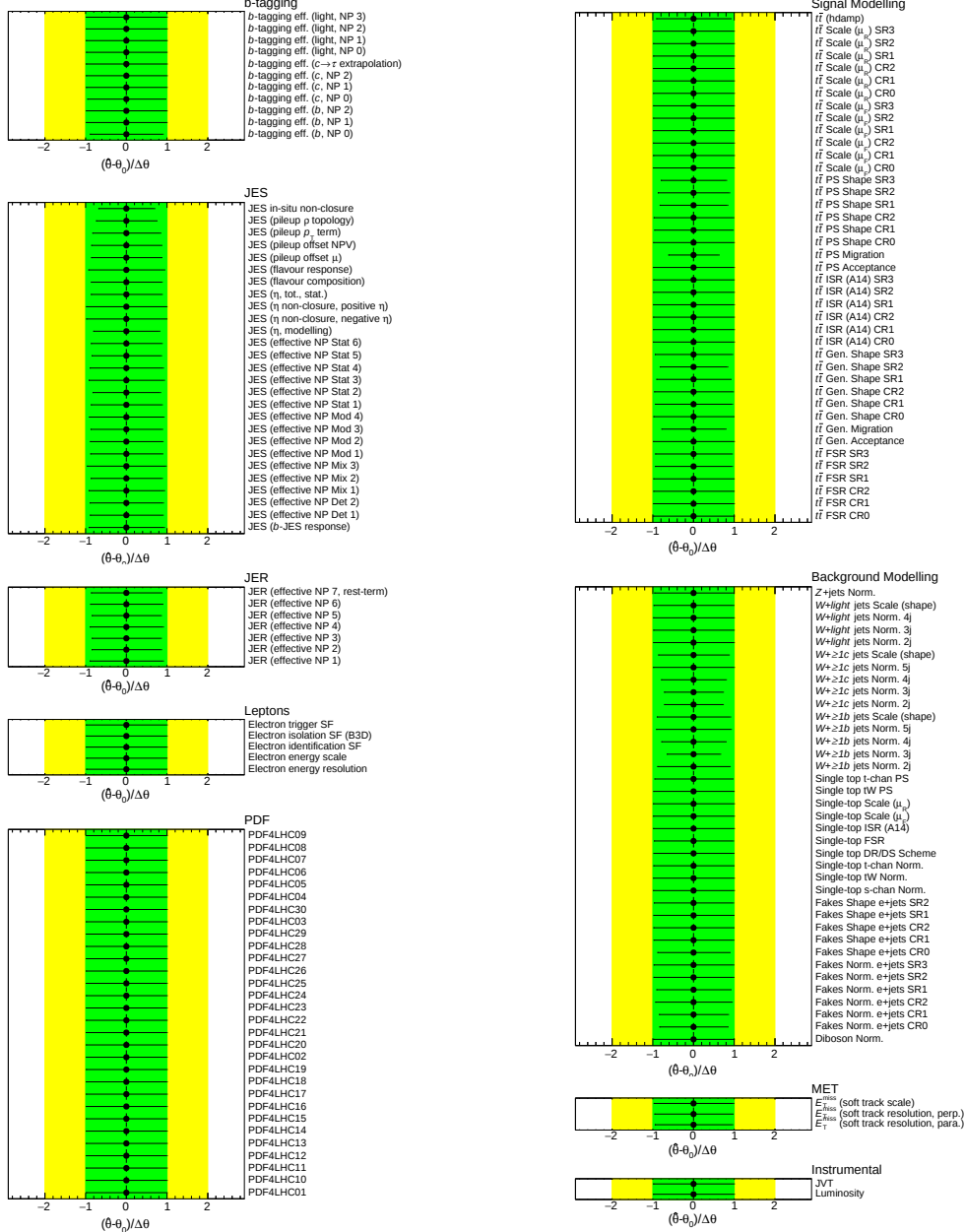


Figure H.1: Nuisance parameters after a fit to Asimov data using the BDT response distributions in the six analysis regions. The six analysis regions only contain events in the e +jets channel. NPs are arranged in different groups.

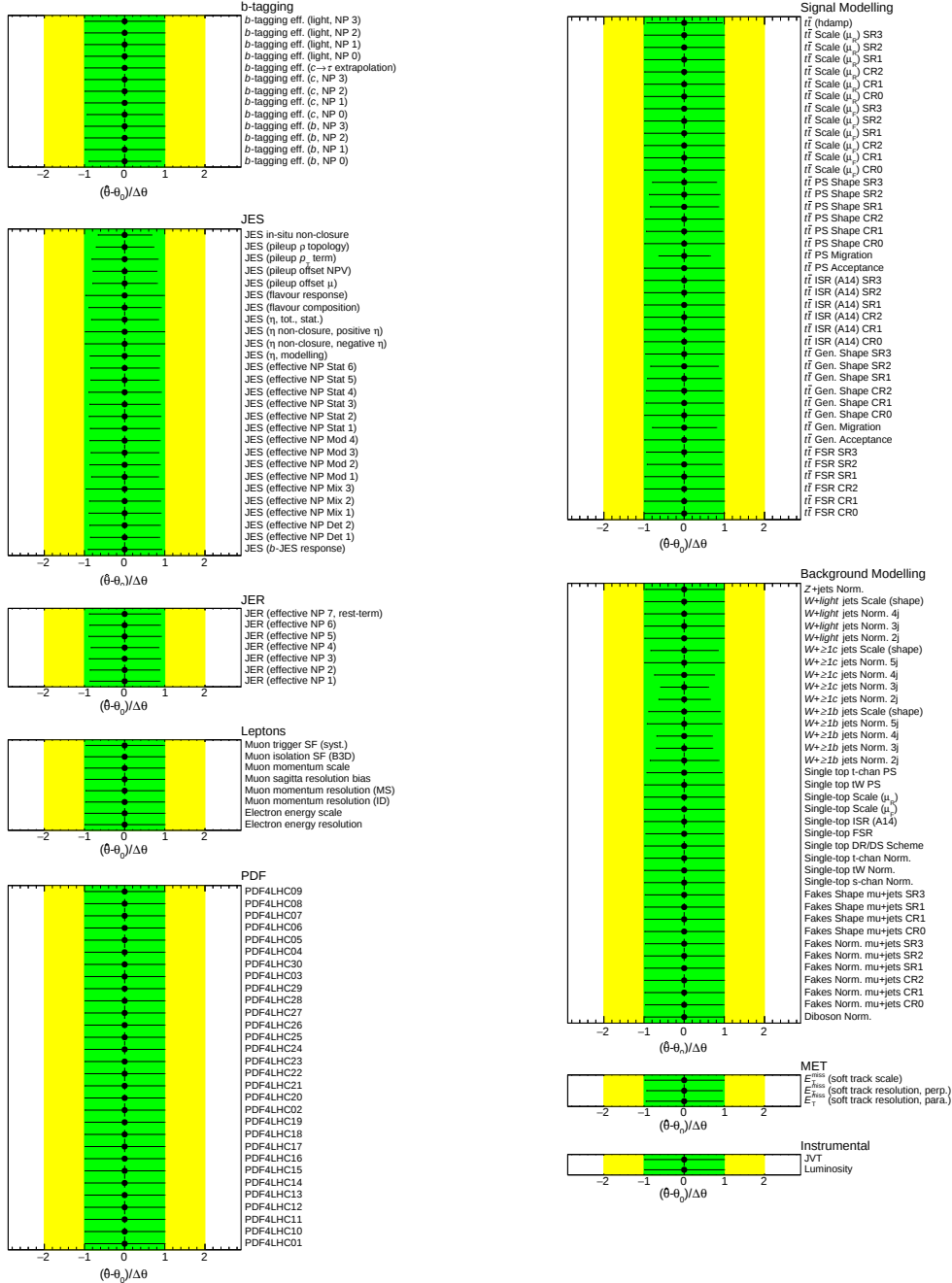


Figure H.2: Nuisance parameters after a fit to Asimov data using the BDT response distributions in the six analysis regions. The six analysis regions only contain events in the μ +jets channel. NPs are arranged in different groups.

Table H.1: Table listing the Convino results for various correlation values between one-to-one NPs. Note that the final uncertainty is highly dependent on the correlation value used and that a correlation value of 0.99 provides an exact match to the uncertainty from the multifit option, (1.0 ± 0.0445) with differences arising in the fifth decimal point.

Input Correlation Value	Convino Result
0	1.0 ± 0.0388
0.5	1.0 ± 0.0420
0.99	1.0 ± 0.0445

H.2 One-to-many Systematics

This study is used to assess the effect of the input correlation value in the case of a one-to-many uncertainty. Similar to the previous study, an Asimov fit to the BDT variable is performed excluding the MC statistical uncertainties. To simulate a one-to-many situation, the normalization and six shape components of the $t\bar{t}$ matrix element uncertainty are fully correlated into a single NP in the μ +jets fit while the e +jets fit follows the nominal decorrelation scheme. The post-fit results are as follows:

- e +jets fit: $\mu = 1.0 \pm 0.0570$
- μ +jets fit: $\mu = 1.0 \pm 0.0541$
- TRexFitter combined fit (multifit): $\mu = 1.0 \pm 0.0445$

Figures H.1 and H.2 show the pulls and constraints for the fitted nuisance parameters, for the e +jets and μ +jets fits, respectively. Note the " $t\bar{t}$ aMCCorrelated" NP in the μ +jets plots.

Various combinations of input correlation values for the correlation between the normalization and the six shape components are scanned and the combined uncertainties are shown in Table H.2. In Table H.2, the correlation values are presented as a tuple (X, Y) where X is the input correlation value applied between the matrix element normalization and the $t\bar{t}$ aMCCorrelated NP while Y is the input correlation value applied between all six shape NPs and the $t\bar{t}$ aMCCorrelated NP. Note that many combinations of (X, Y) fail (especially with large correlations) because of the invertibility requirement of the matrix in the χ^2 . The final uncertainty is found to be insensitive to the input correlation values since the input set of (0, 0) provides exactly the same uncertainty as the multifit option and the other successful combinations have negligible differences. This is further validated by comparing the relevant post-fit correlations to the $t\bar{t}$ aMCCorrelated NP in the multifit and Convino as seen in Table H.3, wherein the Convino result using the (0, 0) scheme gives almost the same post-fit correlations as the multifit.

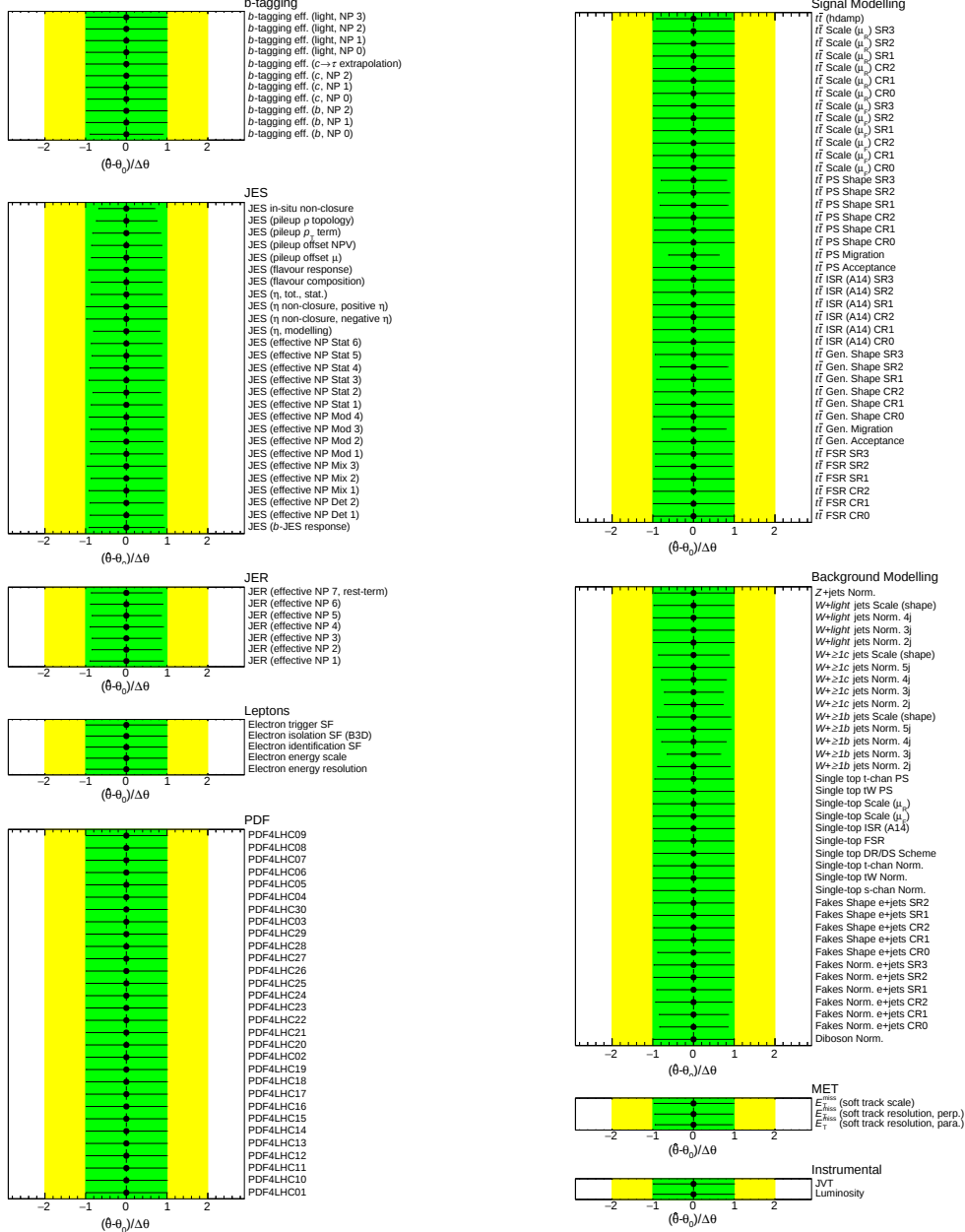


Figure H.3: Nuisance parameters after a fit to Asimov data using the BDT response distributions in the six analysis regions. The six analysis regions only contain events in the e +jets channel. NPs are arranged in different groups.

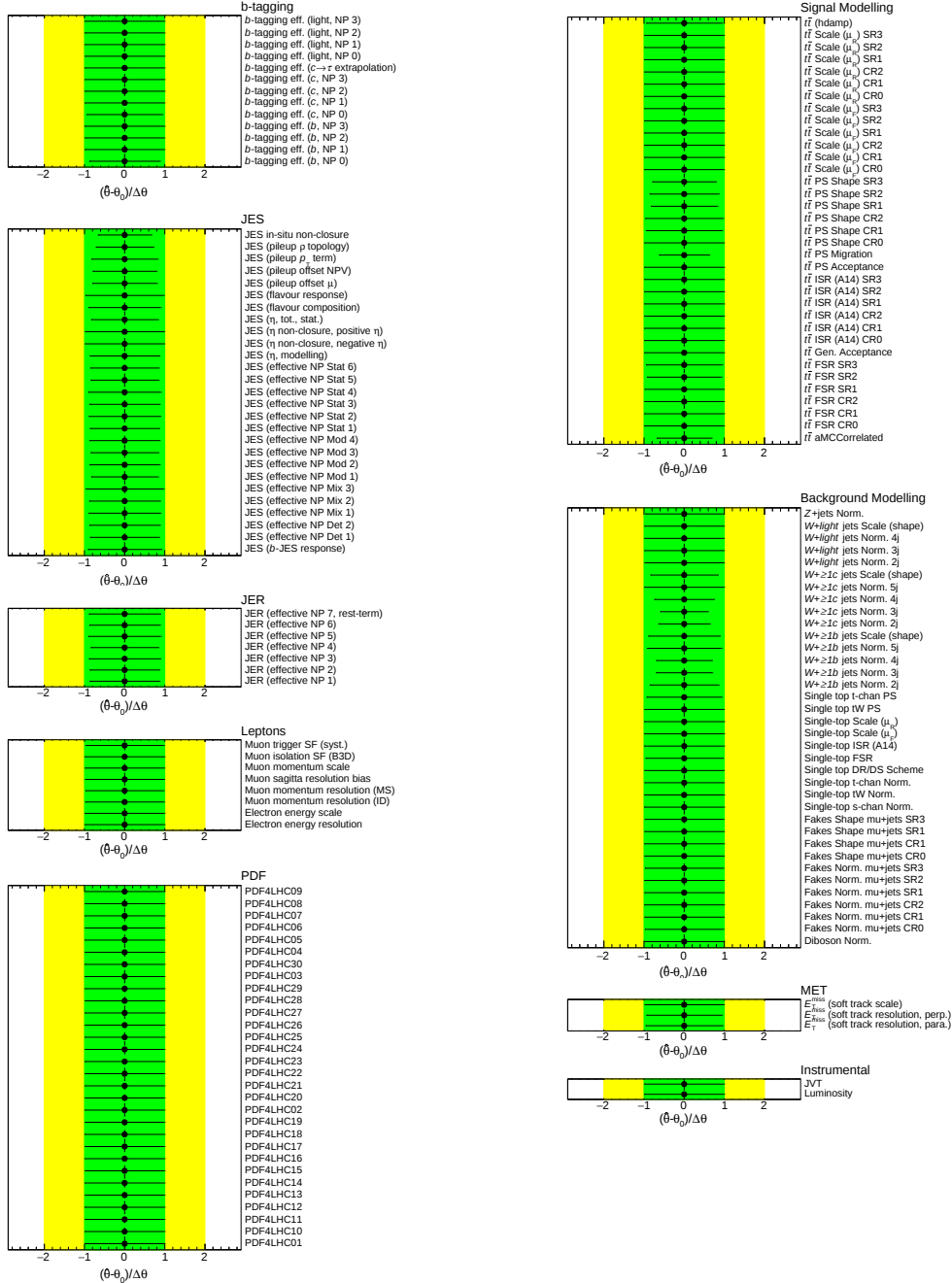


Figure H.4: Nuisance parameters after a fit to Asimov data using the BDT response distributions in the six analysis regions. The six analysis regions only contain events in the μ +jets channel. NPs are arranged in different groups. Note the " $t\bar{t}$ aMCCorrelated" NP

Table H.2: Table listing the Convino results for various combinations of correlation values. Note that the correlation values are presented as a tuple (X, Y) where X is the input correlation value applied between the matrix element normalization and the $t\bar{t}$ aMCCorrelated NP while Y is the input correlation value applied between all six shape NPs and the $t\bar{t}$ aMCCorrelated NP. Results where the χ^2 correlation matrix failed to invert due to large off-diagonal terms are denoted as "Failed". The correlation value scheme of (0.0, 0.0) provides the exact same result as the multifit option (1.0 ± 0.0445) with differences visible in the 5th decimal place.

Input Correlation Value	Convino Result Uncertainty
(0.99, 0.99)	Failed
(0.99, 0.5)	Failed
(0.99, 0.25)	Failed
(0.99, 0.0)	1.0 ± 0.0447
(0.5, 0.99)	Failed
(0.5, 0.5)	Failed
(0.5, 0.25)	1.0 ± 0.0445
(0.5, 0.0)	1.0 ± 0.0448
(0.25, 0.99)	Failed
(0.25, 0.5)	Failed
(0.25, 0.25)	1.0 ± 0.0448
(0.25, 0.0)	1.0 ± 0.0447
(0.0, 0.99)	Failed
(0.0, 0.5)	Failed
(0.0, 0.25)	1.0 ± 0.0447
(0.0, 0.0)	1.0 ± 0.0445

Table H.3: Table listing the post-fit correlations of the decorrelated matrix element NPs in the e +jets fit to the $t\bar{t}$ aMCCorrelated NP in the μ +jets fit. The post-fit correlations shown are the multifit and Convino results, both of which are in good agreement. Note that the Convino result used a (0, 0) as the input correlation value.

NP Name	Multifit Result (%)	Convino Result (%)
Normalization	26.8	25.8
Shape CR0	0.7	0.7
Shape CR1	0.3	0.3
Shape CR2	0.6	0.6
Shape SR1	6.0	5.8
Shape SR2	10.1	9.9
Shape SR3	1.7	1.6

Another study was performed to validate the insensitivity of the input correlation value in the "1-many" case. In this study, the shape and normalization components of the matrix element uncertainty in the single lepton likelihood fit to Asimov data are combined into a single NP before being combined with the dilepton measurement using Convino. By the principles defined in Section 6.9.2, an input correlation value of 0.99 must be used between the two matrix element NPs as they are now "one-to-one" NPs. Table H.4 shows that the total combined uncertainty in such a fit is insensitive to the input correlation. This further reinforces the choice to use the three principles defined in Section 6.9.2.

Table H.4: Table listing the total combined uncertainty for various input correlation values where the matrix element NP is fully correlated in the single lepton profile likelihood fit to Asimov data. This fit to Asimov data is combined with the dilepton measurement. The combined uncertainty is found to be insensitive to the input correlation value between the matrix element NP of the two individual measurements.

Input Correlation Value	Combined Uncertainty
0.0	0.0398
0.25	0.0399
0.50	0.0400
0.99	0.0402

H.3 Correlation Matrix Consistency Check

A consistency check on the Convino output is performed by comparing the pre- and post-Convino-fit correlation matrices after a combination between the single lepton measurement using Asimov data and the dilepton measurement. Note that the pre-Convino-fit correlation matrix is used as an input to Convino and can be expressed in the form of Equation 6.9. The block diagonals for the dilepton and single lepton measurements are thus represented by an identity matrix (D) and the post-fit correlation matrix from the single lepton fit to data (S), respectively. The off diagonal terms are determined by the three principles defined in Section 6.9.2.

Figure H.5 shows a histogram of the difference between the pre- and post-Convino-fit sub-matrices D and S . Note that both histograms are centred around zero and the histogram showing the difference in the dilepton measurement has a larger spread than the single-lepton. The largest differences in both cases were studied and found to be arising from nuisance parameters with negligible uncertainties. Thus, differences in the tails are attributed to numerical instabilities. This study shows that the correlation structure between nuisance parameters in a single measurement is preserved when running a fit with Convino and following the rules in Section 6.9.2.

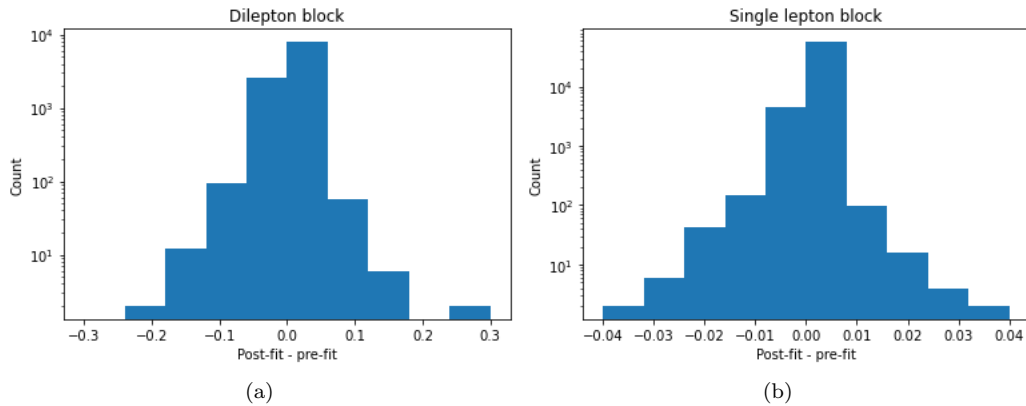


Figure H.5: Histograms showing the difference between the pre- and post-Convino-fit correlation matrix for the block matrices representing the individual (a) dilepton and (b) single lepton measurements.

Appendix I

Misidentified Lepton Background Validation - t -channel Measurement

I.1 Nominal Samples

The nominal and alternate parameterizations used to estimate the misidentified lepton background are validated by constructing two control regions enriched in misidentified leptons. This section focuses on the nominal parametrization in lepton $|\phi|$ and the $\geq 1j, \geq 1b$ region (denoted in this appendix as “nominal sample”) used to calculate the fake efficiencies.

The validation regions require events to first pass a subset of the nominal selection with the following cuts:

- Single-electron or single-muon trigger satisfied
- Exactly one lepton candidate (electron or muon) with $p_T > 18 \text{ GeV}$
- Electron candidates satisfy $|\eta_{cl}| < 2.47$ but candidates with $1.37 < |\eta_{cl}| < 1.52$ are excluded
- Muon candidates satisfy $|\eta| < 2.5$
- Exactly two jets with $p_T > 23 \text{ GeV}$ and $|\eta| < 4.0$, with exactly one b -tagged jet based on the DL1r algorithm at 60% working point

Events passing this selection were then split into two orthogonal regions according to the lepton flavour, an e +jets channel and a μ +jets” channel. The E_T^{miss} and m_T^W cuts are inverted in order to increase the fraction of misidentified lepton background.

For the e +jets channel, events are required to have $(E_T^{\text{miss}} + m_T^W) < 70 \text{ GeV}$ in order to remain orthogonal to the analysis region, $E_T^{\text{miss}} > 15 \text{ GeV}$, and $m_T^W > 25 \text{ GeV}$. The observed and predicted distributions for the electron p_T , electron η , H_T , and the absolute minimum azimuthal angle between the electron and jets in the e +jets region are shown in Figure I.1.

For the μ +jets channel, events are required to have $m_T^W < 35 \text{ GeV}$ in order to remain orthogonal to the analysis region, $E_T^{\text{miss}} > 10 \text{ GeV}$ and $(E_T^{\text{miss}} + m_T^W) < 40 \text{ GeV}$. The observed and predicted distributions for the muon p_T , muon η , H_T , and the absolute minimum azimuthal angle between the muon and jets in the μ +jets region are shown in Figure I.2.

The uncertainty bands in these plots represent only the statistical uncertainty on the prediction and the 50% normalization uncertainty on the misidentified lepton background. Good agreement between data and the predicted distributions is seen in both control regions and the 50% normalization uncertainty accounts for any mis-modelling that might be present.

I.2 Alternate Samples

Two alternate calculations for the fake lepton efficiencies were also studied in the two control regions. One calculation is parametrized in lepton $|\phi|$ but with the $\geq 1j$ region (denoted as the “alternate region sample”) whereas the other calculation is parametrized in lepton $|\eta|$ in the $\geq 1j, \geq 1b$ region (denoted as the “alternate η sample”). The same control regions defined in Section I.1 were built for the two alternate samples.

Figures I.3 and I.4 show the observed and predicted distributions for the electron p_T , electron η , H_T , and the absolute minimum azimuthal angle between the electron and jets in the e +jets region, while using the alternate region and alternate η samples, respectively.

Figures I.5 and I.6 show the observed and predicted distributions for the muon p_T , muon η , H_T , and the absolute minimum azimuthal angle between the muon and jets in the μ +jets region, while using the alternate region and alternate η samples, respectively.

Overall, the agreement between data and the predicted distributions in the validation regions is worse when using the alternate samples as opposed to the nominal samples. The discrepancy in the μ +jets channel is found to be significantly worse and a modification to the validation is considered.

Figures I.7 and I.8 show the observed and predicted distributions for the muon p_T , muon η , H_T , and the absolute minimum azimuthal angle between the muon and jets in the modified μ +jets region, while using the alternate region and alternate η samples, respectively. The events in these two samples are required to have $m_T^W < 35 \text{ GeV}$, $E_T^{\text{miss}} > 20 \text{ GeV}$, and $(E_T^{\text{miss}} + m_T^W) < 45 \text{ GeV}$. Although the discrepancy between data and prediction is improved when considering this modified μ +jets region and alternate samples, the nominal samples are still found to perform better overall.

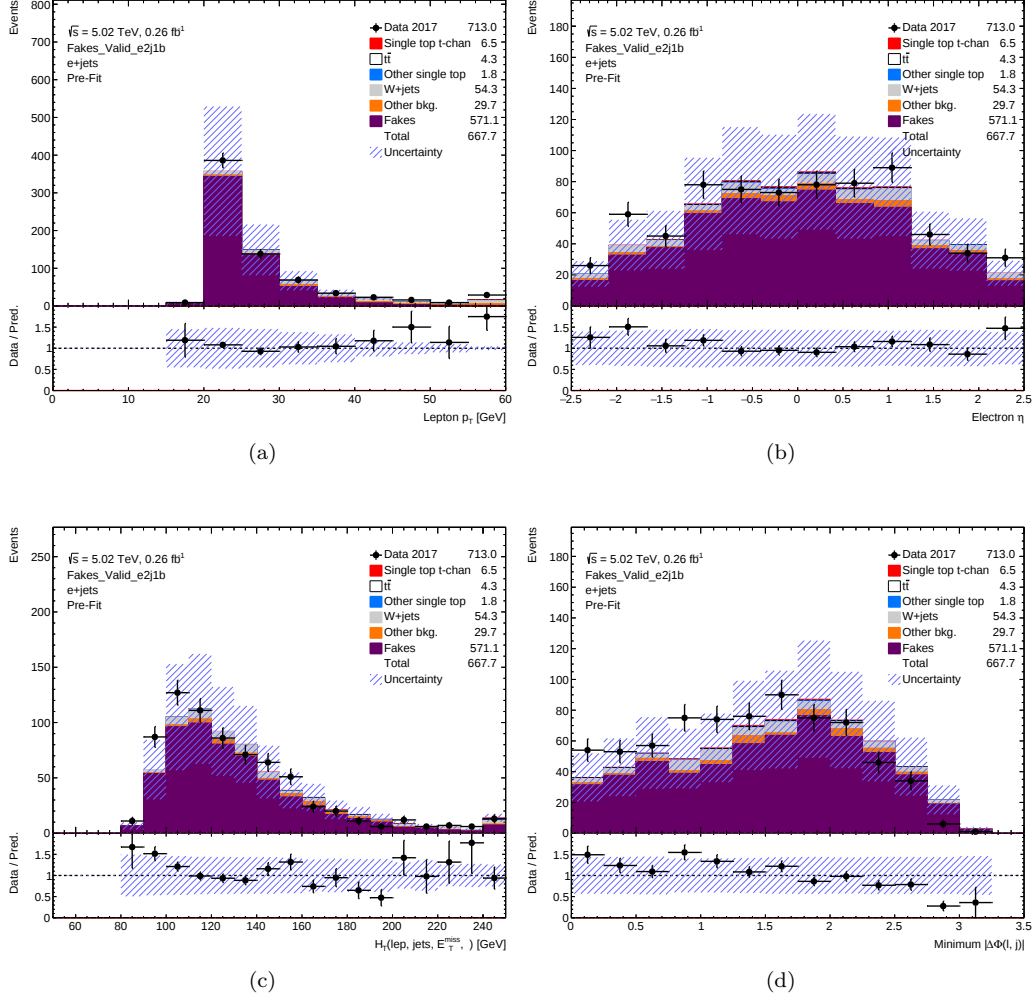


Figure I.1: The (a) electron p_T , (b) electron η , (c) H_T , and (d) minimum $|\Delta\phi(e, j)|$ distributions for data (dots) in the e +jets misidentified lepton enriched control region. The misidentified lepton background shown is the nominal sample. The MC simulation of the signal (white histograms) and various backgrounds (represented by histograms of different colours) including the misidentified lepton background (purple histograms) are also included. The error bars on the dots represent the statistical uncertainty on the data while the blue cross-hatched lines correspond to the sum in quadrature between the statistical uncertainties on the prediction and the 50% normalization uncertainty on the misidentified lepton background. The lower panels show the ratio of the data and predicted distributions, along with the uncertainty in the ratio. The first and last bins contain any underflow and overflow events, respectively.

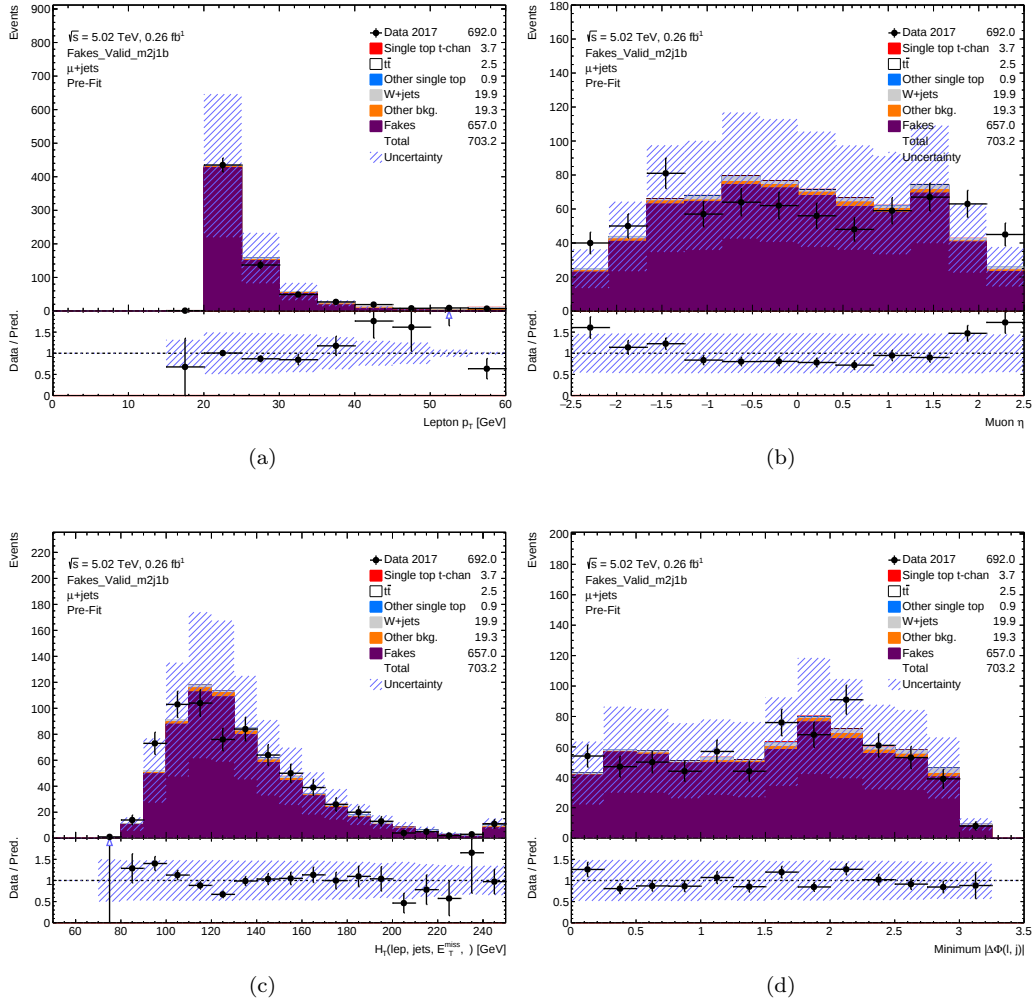


Figure I.2: The (a) muon p_T , (b) muon η , (c) H_T , and (d) minimum $|\Delta\phi(\mu, j)|$ distributions for data (dots) in the μ +jets misidentified lepton enriched control region. The misidentified lepton background shown is the nominal sample. The MC simulation of the signal (white histograms) and various backgrounds (represented by histograms of different colours) including the misidentified lepton background (purple histograms) are also included. The error bars on the dots represent the statistical uncertainty on the data while the blue cross-hatched lines correspond to the sum in quadrature between the statistical uncertainties on the prediction and the 50% normalization uncertainty on the misidentified lepton background. The lower panels show the ratio of the data and predicted distributions, along with the uncertainty in the ratio. The first and last bins contain any underflow and overflow events, respectively.

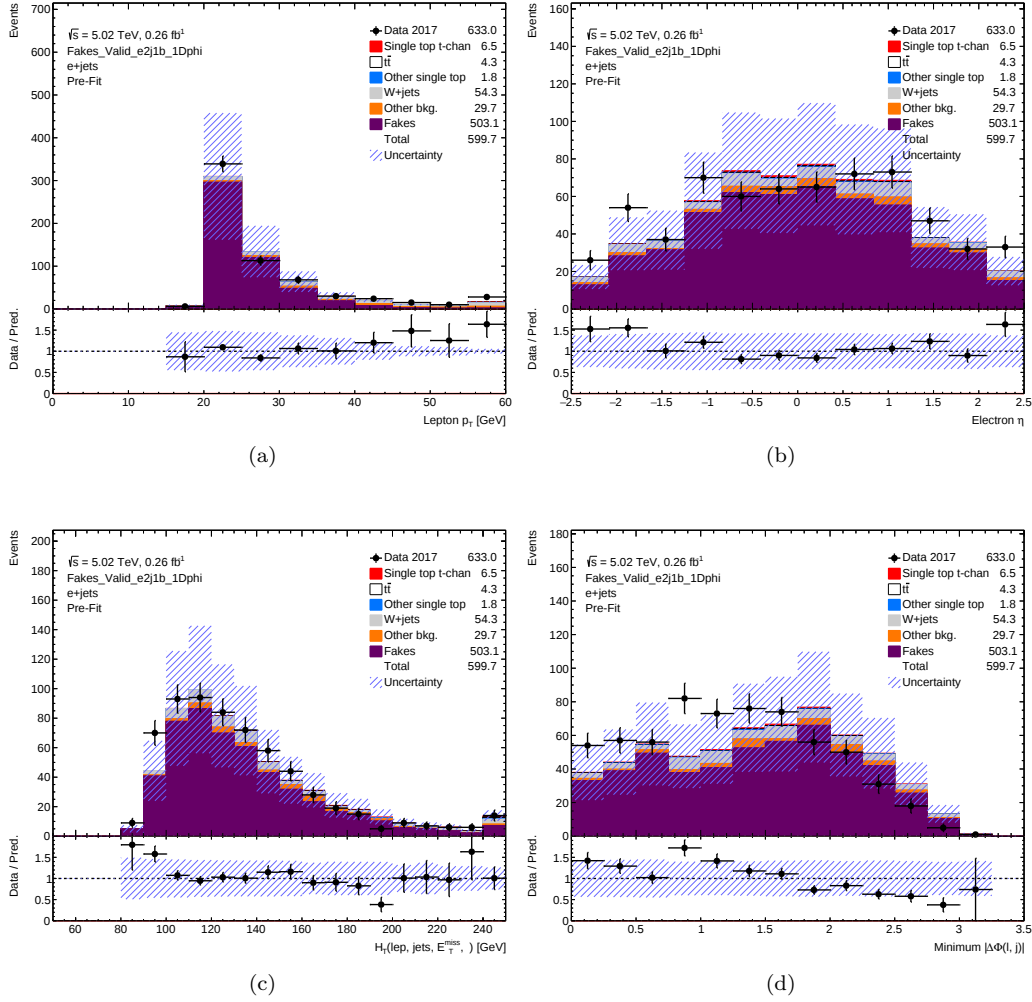


Figure I.3: The (a) electron p_T , (b) electron η , (c) H_T , and (d) minimum $|\Delta\phi(e, j)|$ distributions for data (dots) in the e +jets misidentified lepton enriched control region. The misidentified lepton background shown is the alternate region sample. The MC simulation of the signal (white histograms) and various backgrounds (represented by histograms of different colours) including the misidentified lepton background (purple histograms) are also included. The error bars on the dots represent the statistical uncertainty on the data while the blue cross-hatched lines correspond to the sum in quadrature between the statistical uncertainties on the prediction and the 50% normalization uncertainty on the misidentified lepton background. The lower panels show the ratio of the data and predicted distributions, along with the uncertainty in the ratio. The first and last bins contain any underflow and overflow events, respectively.

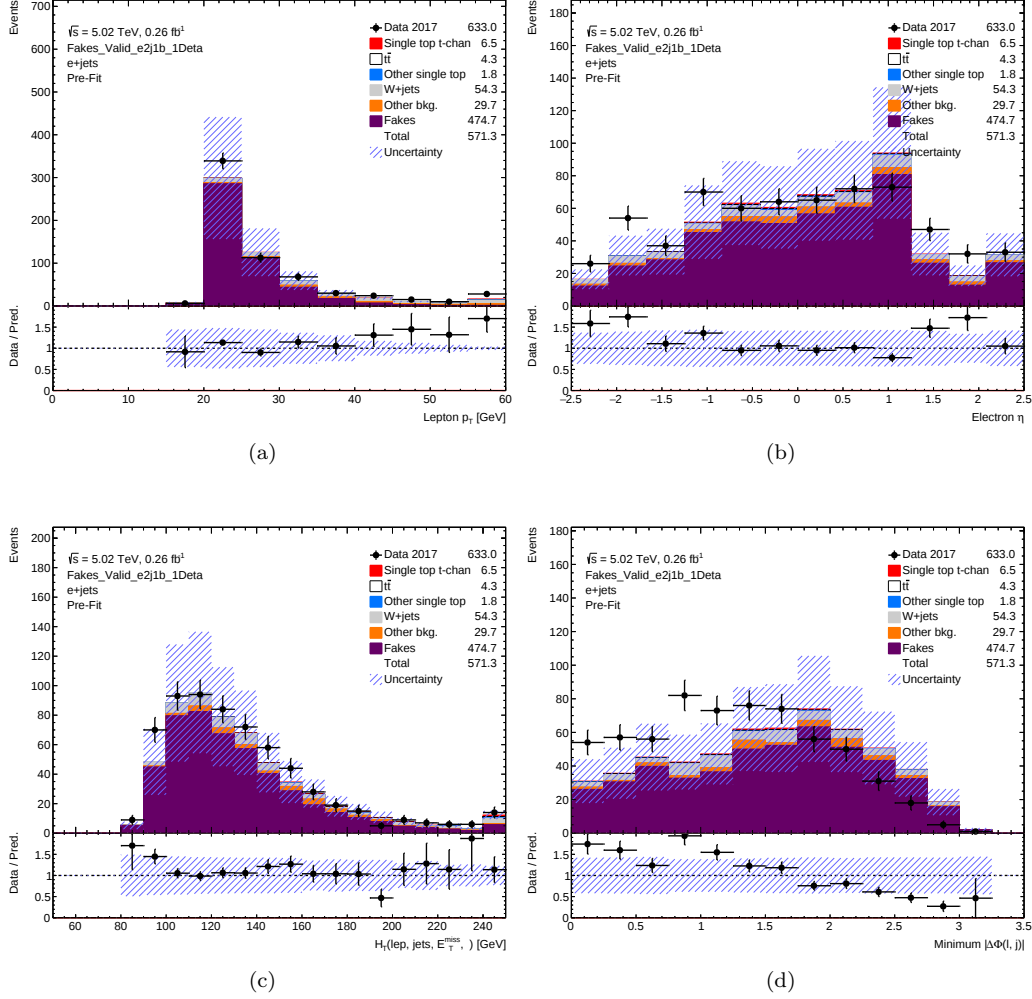


Figure I.4: The (a) electron p_T , (b) electron η , (c) H_T , and (d) minimum $|\Delta\phi(e, j)|$ distributions for data (dots) in the e +jets misidentified lepton enriched control region. The misidentified lepton background shown is the alternate η sample. The MC simulation of the signal (white histograms) and various backgrounds (represented by histograms of different colours) including the misidentified lepton background (purple histograms) are also included. The error bars on the dots represent the statistical uncertainty on the data while the blue cross-hatched lines correspond to the sum in quadrature between the statistical uncertainties on the prediction and the 50% normalization uncertainty on the misidentified lepton background. The lower panels show the ratio of the data and predicted distributions, along with the uncertainty in the ratio. The first and last bins contain any underflow and overflow events, respectively.

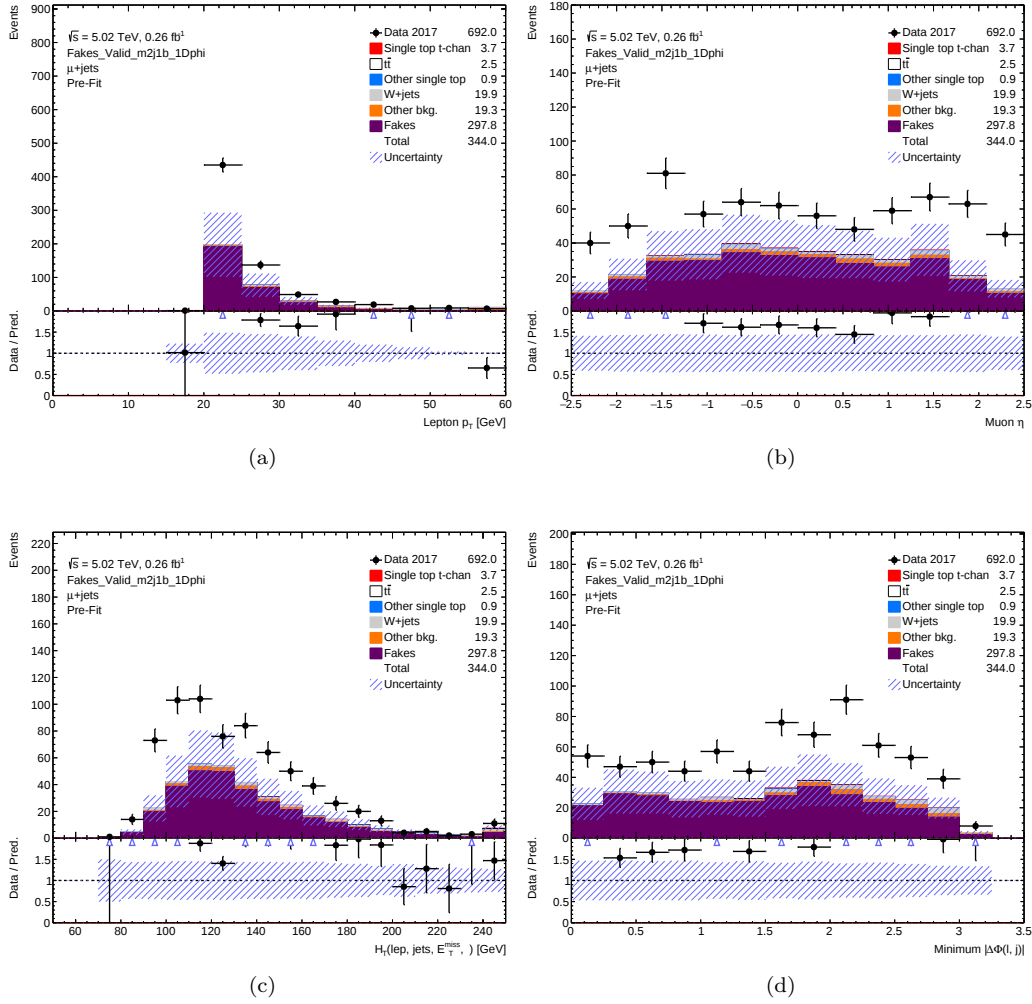


Figure I.5: The (a) muon p_T , (b) muon η , (c) H_T , and (d) minimum $|\Delta\phi(\mu, j)|$ distributions for data (dots) in the μ +jets misidentified lepton enriched control region. The misidentified lepton background shown is the alternate region sample. The MC simulation of the signal (white histograms) and various backgrounds (represented by histograms of different colours) including the misidentified lepton background (purple histograms) are also included. The error bars on the dots represent the statistical uncertainty on the data while the blue cross-hatched lines correspond to the sum in quadrature between the statistical uncertainties on the prediction and the 50% normalization uncertainty on the misidentified lepton background. The lower panels show the ratio of the data and predicted distributions, along with the uncertainty in the ratio. The first and last bins contain any underflow and overflow events, respectively.

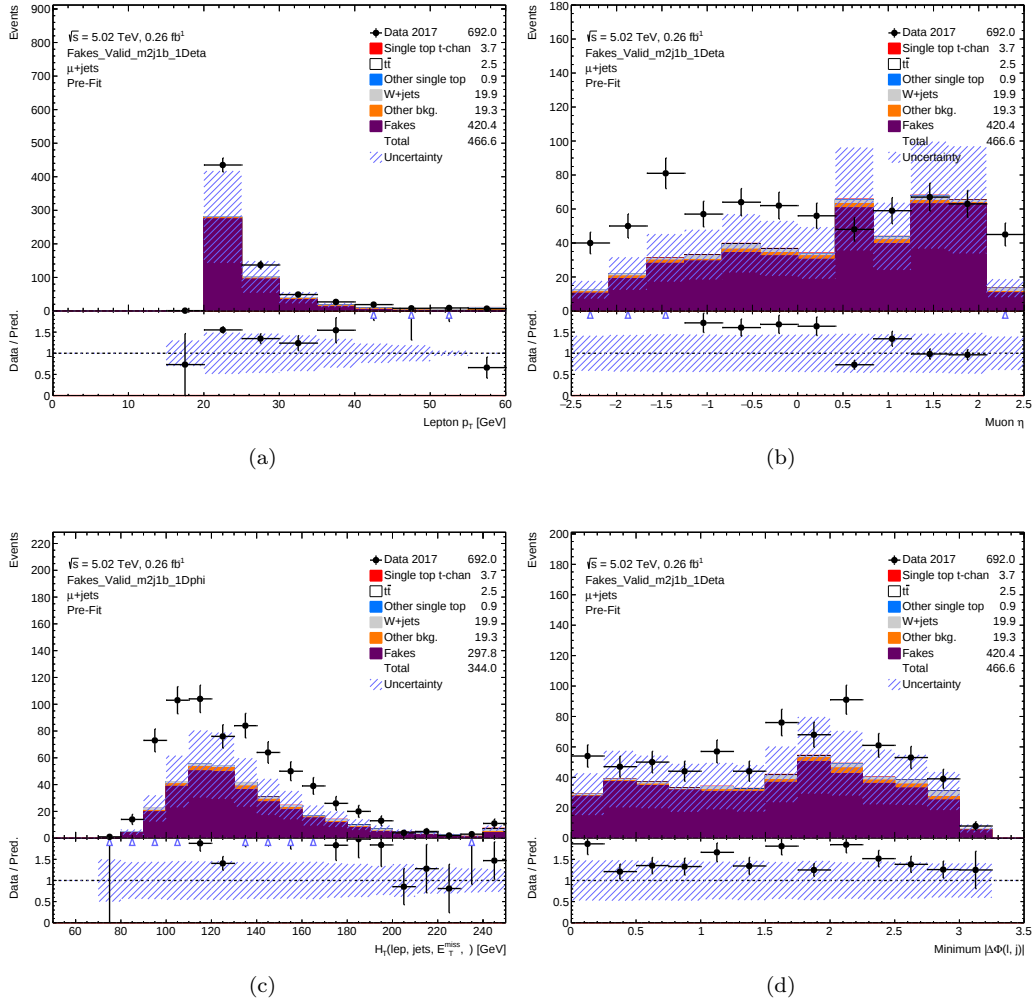


Figure I.6: The (a) muon p_T , (b) muon η , (c) H_T , and (d) minimum $|\Delta\phi(\mu, j)|$ distributions for data (dots) in the μ +jets misidentified lepton enriched control region. The misidentified lepton background shown is the alternate η sample. The MC simulation of the signal (white histograms) and various backgrounds (represented by histograms of different colours) including the misidentified lepton background (purple histograms) are also included. The error bars on the dots represent the statistical uncertainty on the data while the blue cross-hatched lines correspond to the sum in quadrature between the statistical uncertainties on the prediction and the 50% normalization uncertainty on the misidentified lepton background. The lower panels show the ratio of the data and predicted distributions, along with the uncertainty in the ratio. The first and last bins contain any underflow and overflow events, respectively.

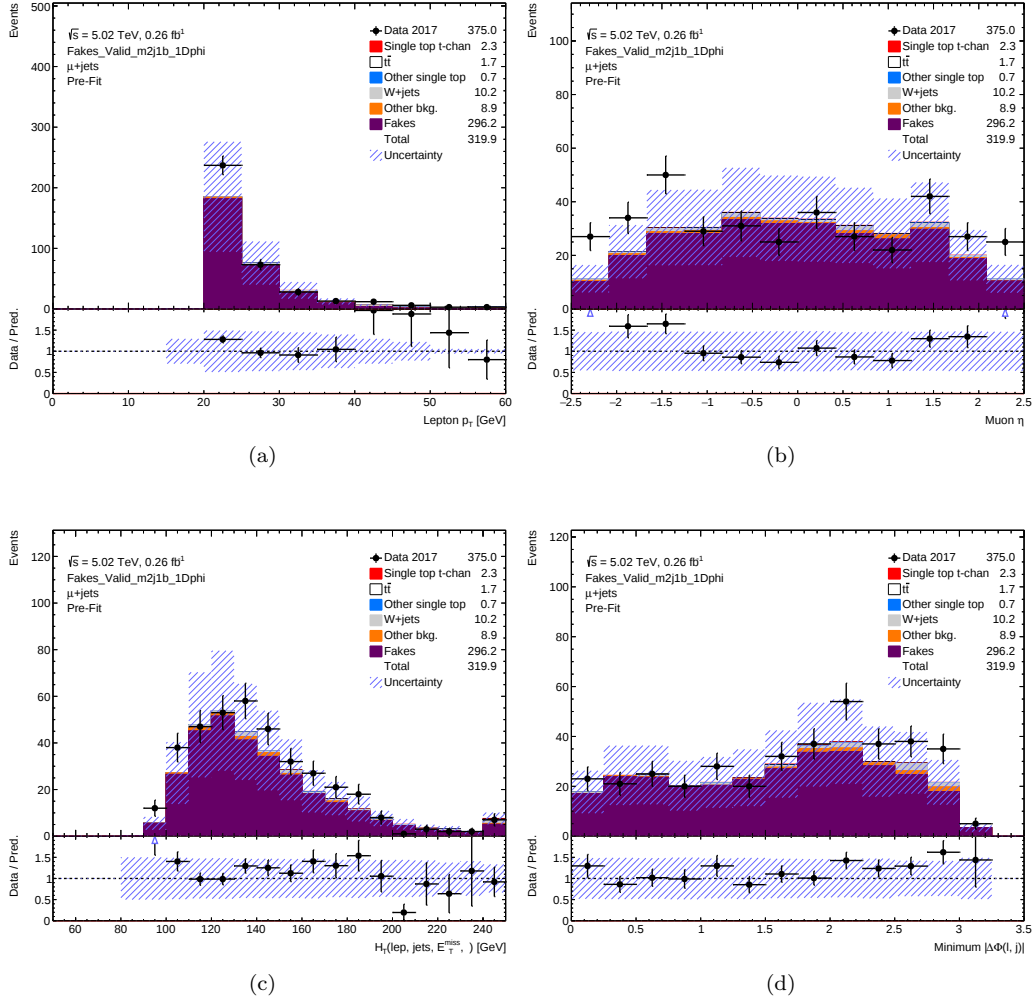


Figure I.7: The (a) muon p_T , (b) muon η , (c) H_T , and (d) minimum $|\Delta\phi(\mu, j)|$ distributions for data (dots) in the modified μ +jets misidentified lepton enriched control region. The misidentified lepton background shown is the alternate region sample. The MC simulation of the signal (white histograms) and various backgrounds (represented by histograms of different colours) including the misidentified lepton background (purple histograms) are also included. The error bars on the dots represent the statistical uncertainty on the data while the blue cross-hatched lines correspond to the sum in quadrature between the statistical uncertainties on the prediction and the 50% normalization uncertainty on the misidentified lepton background. The lower panels show the ratio of the data and predicted distributions, along with the uncertainty in the ratio. The first and last bins contain any underflow and overflow events, respectively.

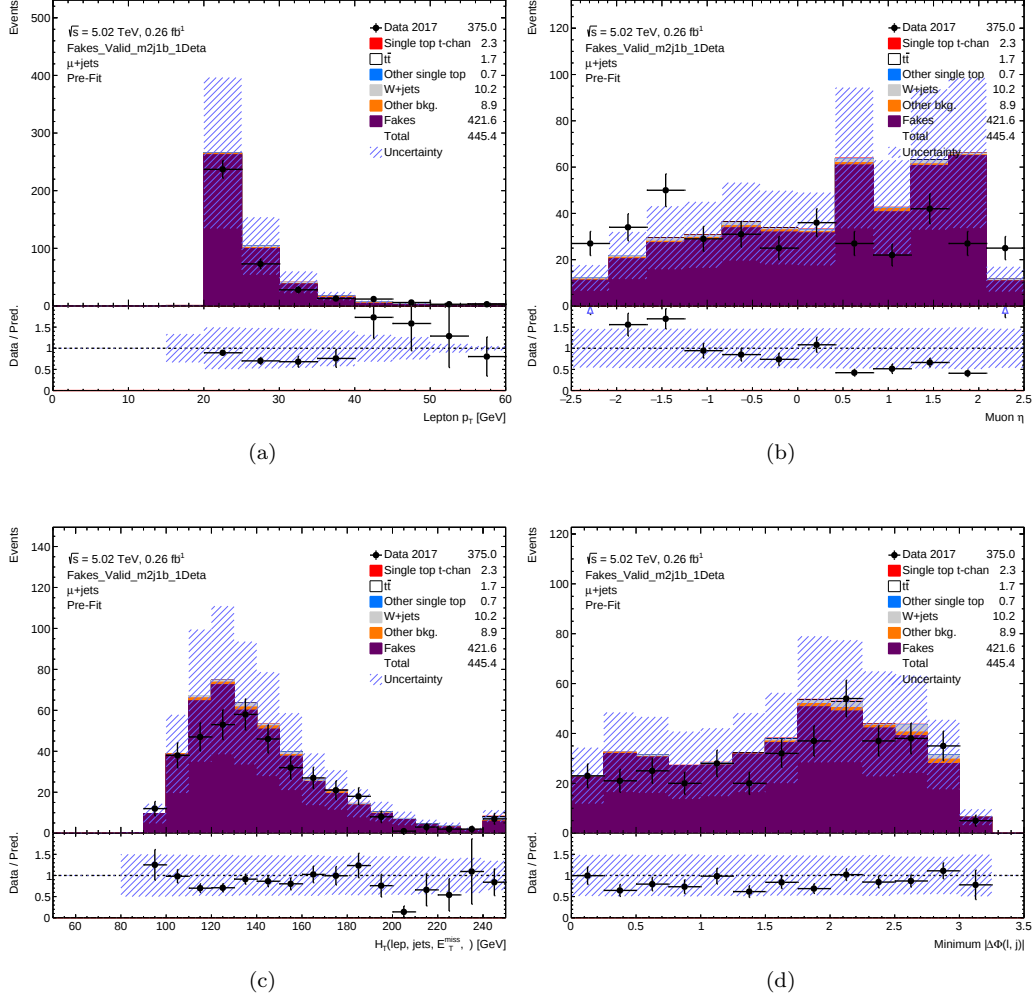


Figure I.8: The (a) muon p_T , (b) muon η , (c) H_T , and (d) minimum $|\Delta\phi(\mu, j)|$ distributions for data (dots) in the modified μ +jets misidentified lepton enriched control region. The misidentified lepton background shown is the alternate η sample. The MC simulation of the signal (white histograms) and various backgrounds (represented by histograms of different colours) including the misidentified lepton background (purple histograms) are also included. The error bars on the dots represent the statistical uncertainty on the data while the blue cross-hatched lines correspond to the sum in quadrature between the statistical uncertainties on the prediction and the 50% normalization uncertainty on the misidentified lepton background. The lower panels show the ratio of the data and predicted distributions, along with the uncertainty in the ratio. The first and last bins contain any underflow and overflow events, respectively.

Appendix J

Study of the Reconstructed Top Quark Mass

This appendix documents a study to determine the optimal reconstruction algorithm for the top quark. This study was done with central jets only and a different selection than the nominal fit. Events are required to pass the following cuts:

- Lepton $pt > 20 \text{ GeV}$
- Jet $p_T > 20 \text{ GeV}$
- $E_T^{\text{miss}} > 20 \text{ GeV}$
- $m_T^W > 35 \text{ GeV}$
- $m_T^W + E_T^{\text{miss}} > 65 \text{ GeV}$
- $H_T > 185 \text{ GeV}$
- $m_{lb} < 165 \text{ GeV}$

J.1 Top-quark Reconstruction

By requiring the invariant mass of the lepton and E_T^{miss} vector to be equal to the W boson mass (80.399 GeV), one is able to solve a quadratic equation for the neutrino p^z (p_ν^z), as discussed in Section 7.3.1. The W boson's four vector can then be reconstructed by summing the neutrino and lepton four vectors. Finally, the top quark's four vector is determined by summing the W boson's four vector with the b -jet's four vector.

J.2 Multiple Solutions

Various treatments were studied in order to deal with the multiple real and imaginary solutions encountered in a quadratic equation. Three treatments for multiple solutions were studied, such as using the solution: with the largest $|p_\nu^z|$, randomly choosing a p_ν^z , or choosing the p_ν^z that gives a reconstructed top quark mass closest to 172.5 GeV (or ~ 6.6 nanocalories). For imaginary solutions, it is assumed that the imaginary component is negligible and can be ignored. Figure J.1, J.2, and J.3 show the reconstructed W boson and top quark mass distributions for the largest p_ν^z scheme, the random p_ν^z scheme, and the top quark mass constraint scheme, respectively.

In all cases, there are tails with significant background contributions that can be mitigated by applying a cut on the reconstructed masses. The most optimal algorithm was selected after applying cuts of $m_W < 102$ GeV and $140 \text{ GeV} < m_{\text{top}} < 225$ GeV. Table J.1 summarizes the signal-to-background ratio, $\frac{S}{\sqrt{S+B}}$, and the significance calculated from a statistics only fit to Asimov data in the m_{lb} distribution. From this table, one can see that the top quark mass constraint scheme has the largest $\frac{S}{\sqrt{S+B}}$ and significance from a fit to Asimov data.

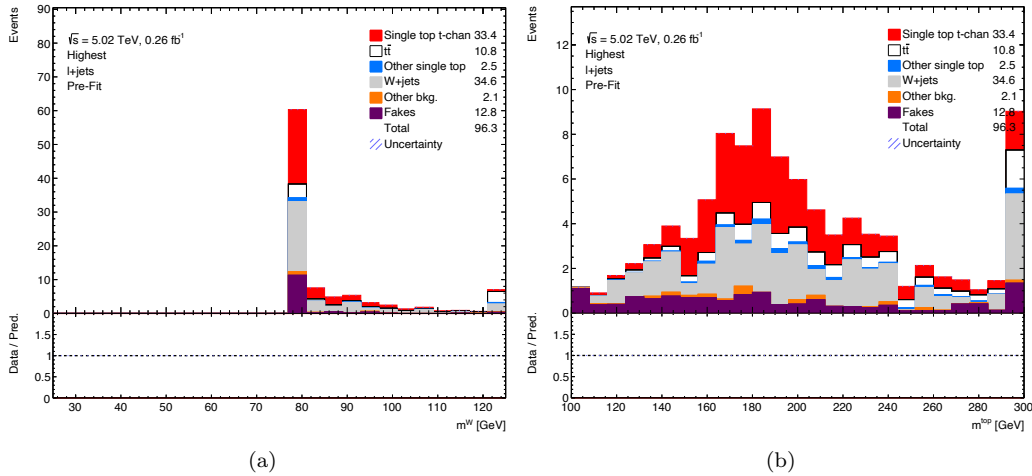


Figure J.1: The (a) reconstructed W boson mass and (b) reconstructed top quark mass distributions passing the selection and using the highest $|p_\nu^z|$ scheme for the W boson and top-quark reconstruction. Only the MC simulation of the signal (red histograms) and various backgrounds (represented by histograms of different colours) are shown. No uncertainties are shown in this plot.

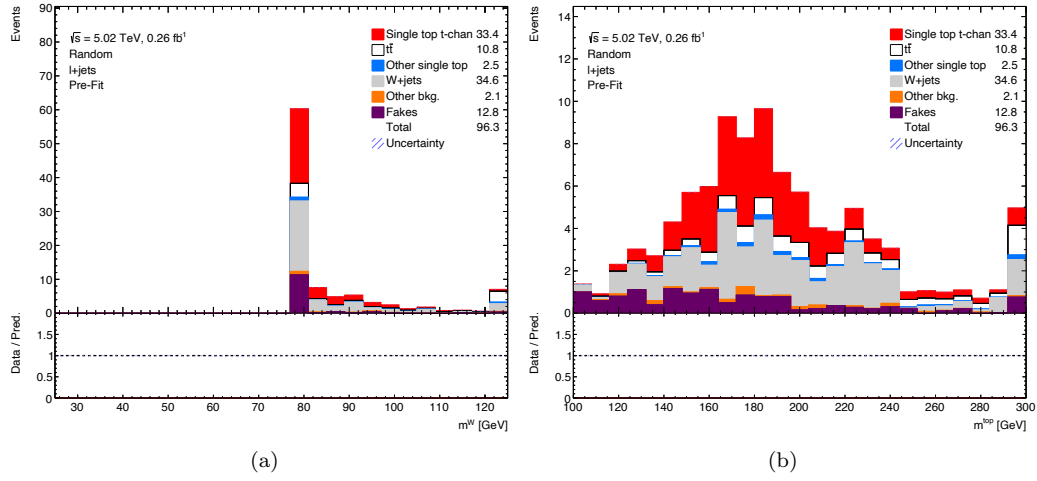


Figure J.2: The (a) reconstructed W boson mass and (b) reconstructed top quark mass distributions passing the selection and using the random p_ν^z scheme for the W boson and top-quark reconstruction. Only the MC simulation of the signal (red histograms) and various backgrounds (represented by histograms of different colours) are shown. No uncertainties are shown in this plot.

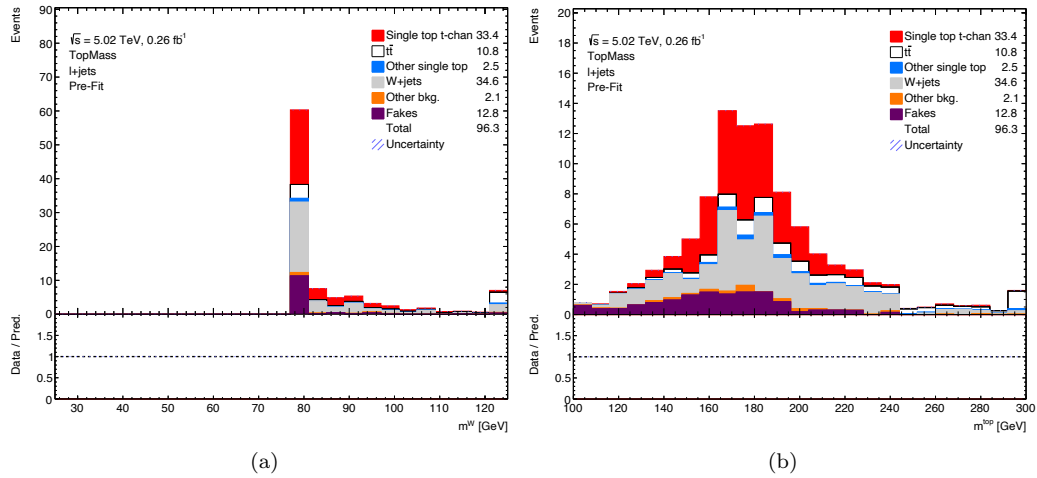


Figure J.3: The (a) reconstructed W boson mass and (b) reconstructed top quark mass distributions passing the selection and using the top quark mass constraint scheme for the W boson and top-quark reconstruction. Only the MC simulation of the signal (red histograms) and various backgrounds (represented by histograms of different colours) are shown. No uncertainties are shown in this plot.

Table J.1: A summary of the results for the three schemes used to treat multiple solutions. Note that only the real component of imaginary solutions is used for the results shown.

Scheme	$\frac{S}{B}$	$\frac{S}{\sqrt{S+B}}$	Significance from Asimov fit
Largest $ p_\nu^z $	0.73	3.3	4.2
Random p_ν^z	0.73	3.4	4.3
Top quark mass constraint	0.69	3.6	4.5

J.3 Imaginary Solutions

An alternate treatment for imaginary solutions was also studied by taking the norm of the imaginary p_ν^z instead of using the real component only. In this study, multiple solutions were treated using the top quark mass constraint scheme. Figure J.4 shows the reconstructed W boson and top quark mass distributions using the norm scheme and Table J.2 compares it with the alternate scheme using the real component only.

The scheme using only the real component of the imaginary solution performs slightly better than the alternate and is thus used in this analysis in conjunction with the top quark mass constraint scheme for multiple solutions.

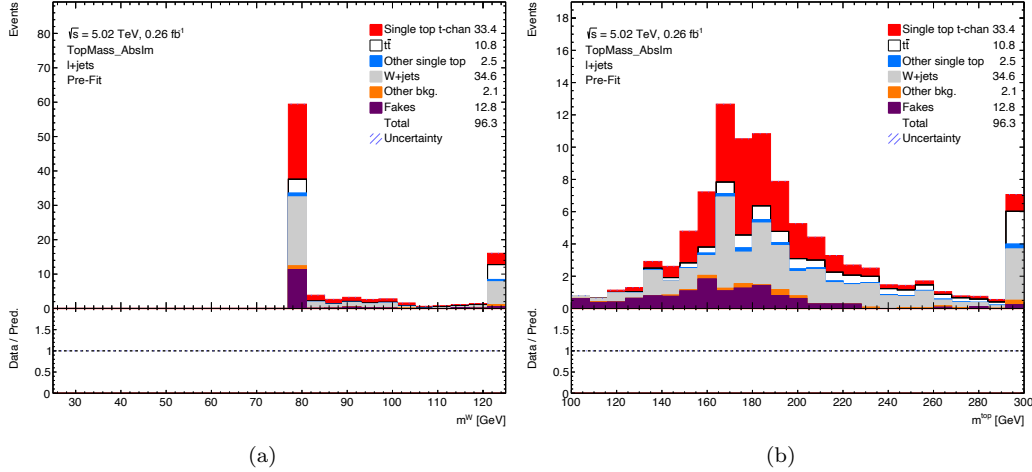


Figure J.4: The (a) reconstructed W boson mass and (b) reconstructed top quark mass distributions passing the selection and using the norm scheme for the W boson and top-quark reconstruction. Only the MC simulation of the signal (red histograms) and various backgrounds (represented by histograms of different colours) are shown. No uncertainties are shown in this plot.

Table J.2: A summary of the results for the two schemes used to treat imaginary solutions. Note that the top quark mass constraint scheme is used to treat multiple solutions for the results shown.

Scheme	$\frac{S}{B}$	$\frac{S}{\sqrt{S+B}}$	Significance from Asimov fit
Real component only	0.69	3.6	4.5
Norm of p_ν^z	0.71	3.5	4.4

Appendix K

Distributions of Kinematic Variables - t -channel Measurement

Figures [K.1](#), [K.2](#), and [K.3](#) show pre-fit distributions of various kinematic variables in the ℓ^+ +jets region while Figures [K.4](#), [K.5](#), and [K.6](#) show the same distributions but in the ℓ^- +jets region. These plots show that the two regions are well modelled by the MC simulation and data-driven misidentified lepton background.

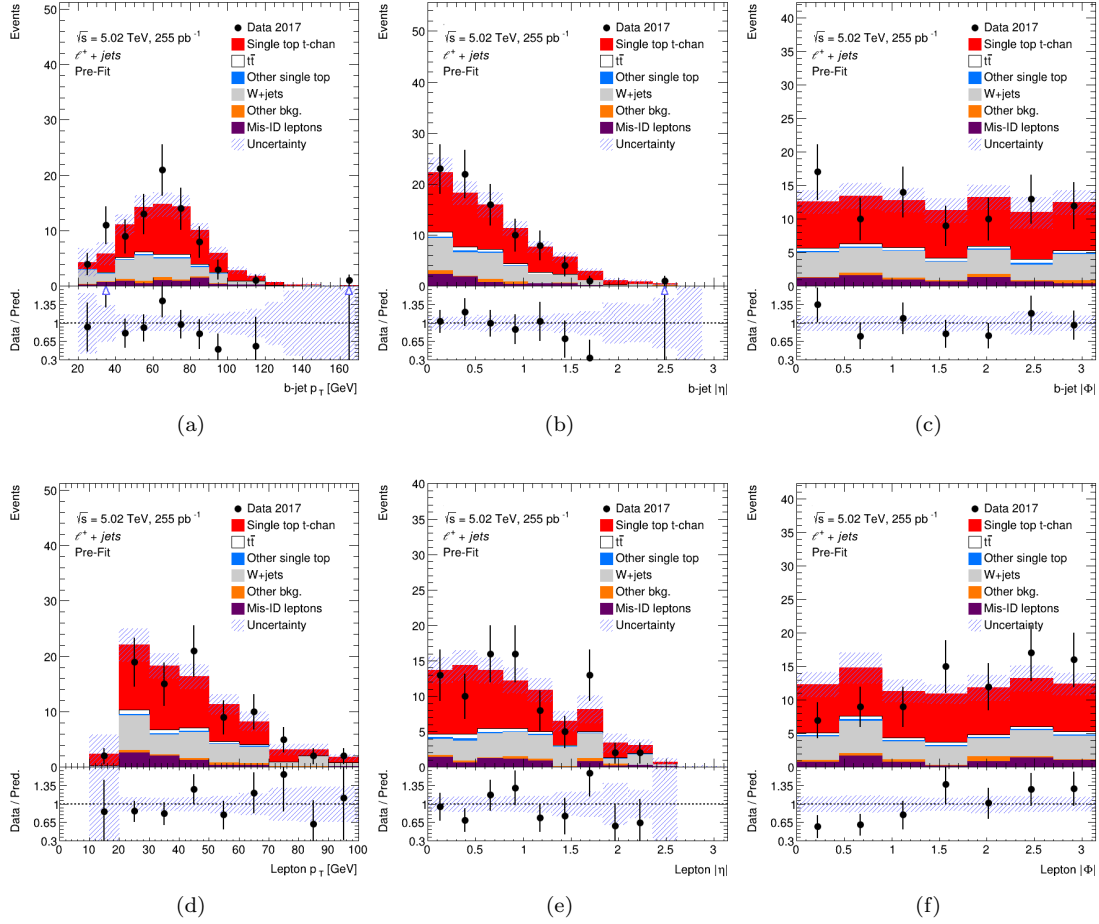


Figure K.1: The pre-fit (a) b -tagged jet p_T , (b) b -tagged jet $|\eta|$, (c) b -tagged jet $|\Phi|$, (d) lepton p_T , (e) lepton $|\eta|$, and (f) lepton $|\Phi|$ distributions for data (dots) in the $\ell^+ + \text{jets}$ region. The MC simulation of the signal (red histograms) and various backgrounds (represented by histograms of different colours) are also included. The error bars on the dots represent the statistical uncertainty on the data while the blue cross-hatched lines correspond to the total uncertainties on the prediction. The lower panels show the ratio of the data and predicted distributions, along with the uncertainty in the ratio.

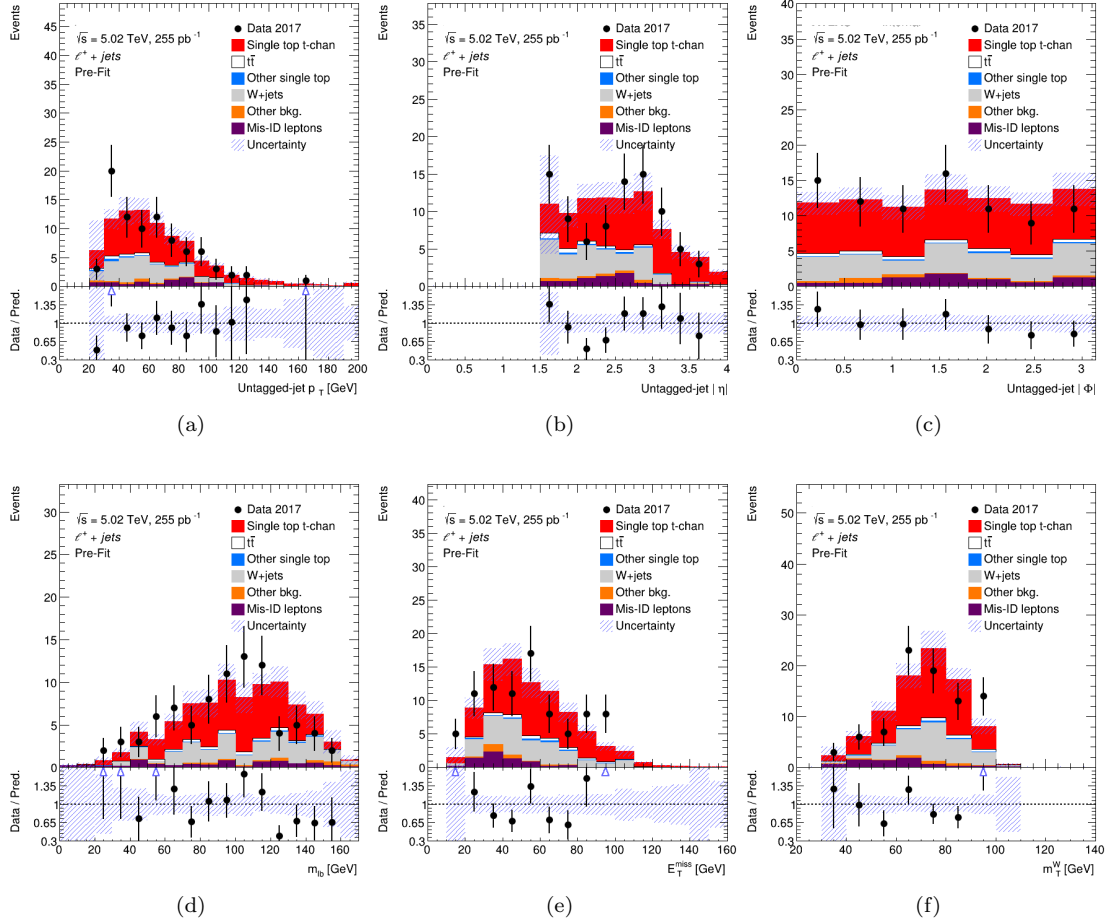


Figure K.2: The pre-fit (a) untagged jet p_T , (b) untagged jet $|\eta|$, (c) untagged jet $|\Phi|$, (d) invariant mass of the lepton and b -tagged jet pair, (e) E_T^{miss} , and (f) m_T^W distributions for data (dots) in the ℓ^+ +jets region. The MC simulation of the signal (red histograms) and various backgrounds (represented by histograms of different colours) are also included. The error bars on the dots represent the statistical uncertainty on the data while the blue cross-hatched lines correspond to the total uncertainties on the prediction. The lower panels show the ratio of the data and predicted distributions, along with the uncertainty in the ratio.

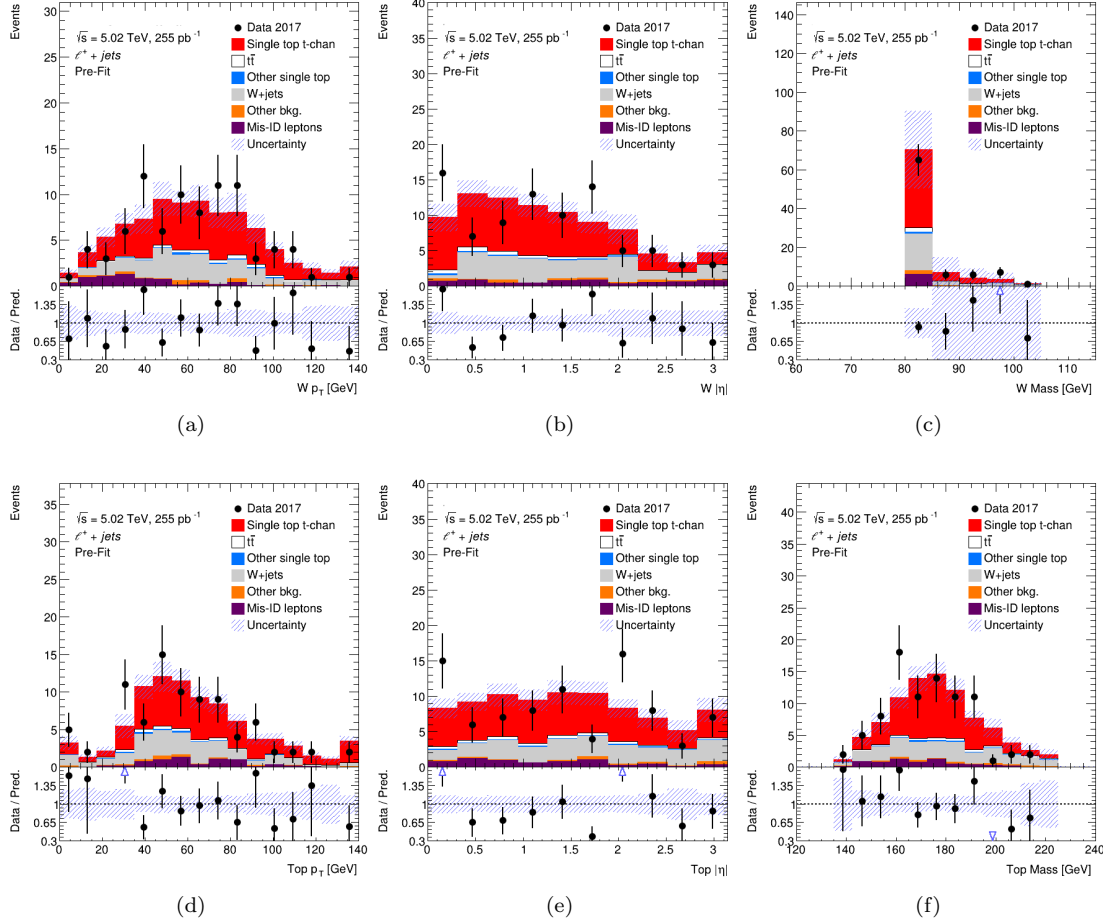


Figure K.3: The pre-fit reconstructed (a) W boson p_T , (b) W boson $|\eta|$, (c) W boson mass, (d) top quark p_T , (e) top quark $|\eta|$, and (f) top quark mass distributions for data (dots) in the $\ell^+ + \text{jets}$ region. The MC simulation of the signal (red histograms) and various backgrounds (represented by histograms of different colours) are also included. The error bars on the dots represent the statistical uncertainty on the data while the blue cross-hatched lines correspond to the total uncertainties on the prediction. The lower panels show the ratio of the data and predicted distributions, along with the uncertainty in the ratio.

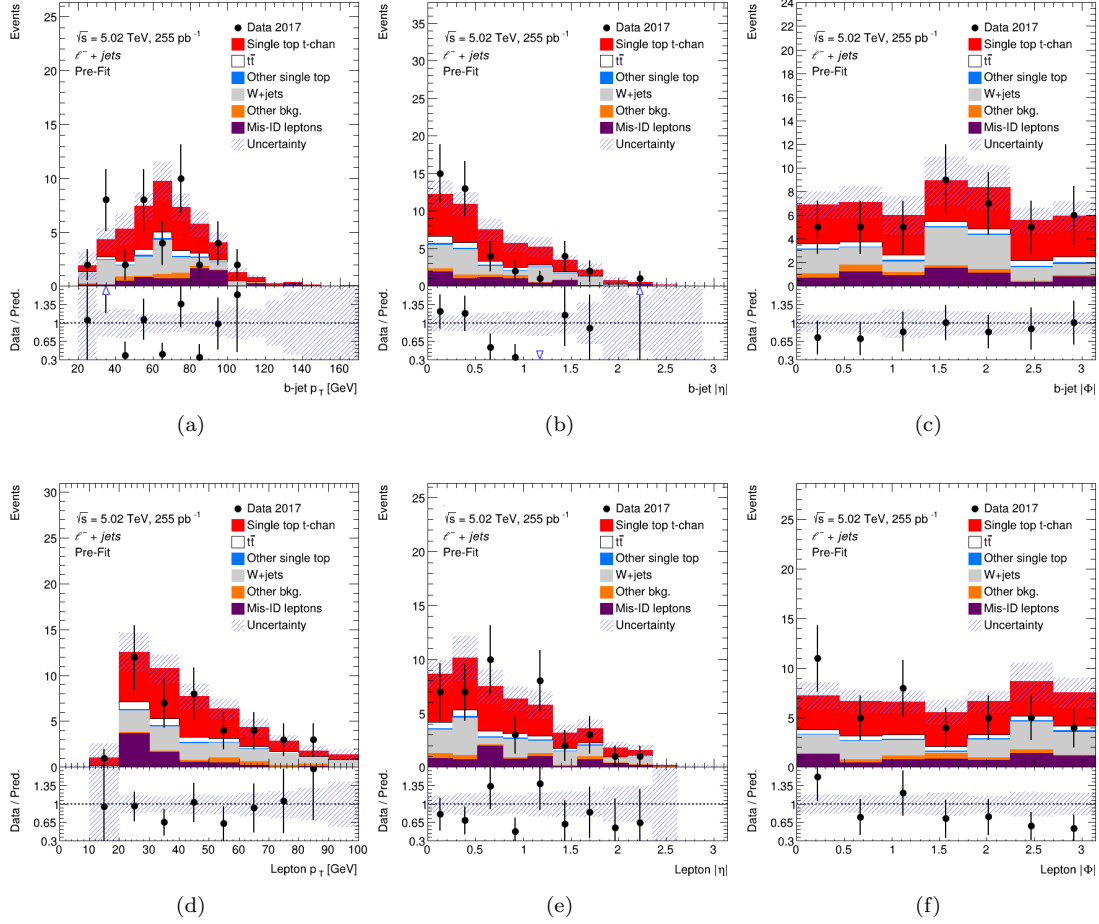


Figure K.4: The pre-fit (a) b -tagged jet p_T , (b) b -tagged jet $|\eta|$, (c) b -tagged jet $|\Phi|$, (d) lepton p_T , (e) lepton $|\eta|$, and (f) lepton $|\Phi|$ distributions for data (dots) in the ℓ^- +jets region. The MC simulation of the signal (red histograms) and various backgrounds (represented by histograms of different colours) are also included. The error bars on the dots represent the statistical uncertainty on the data while the blue cross-hatched lines correspond to the total uncertainties on the prediction. The lower panels show the ratio of the data and predicted distributions, along with the uncertainty in the ratio.

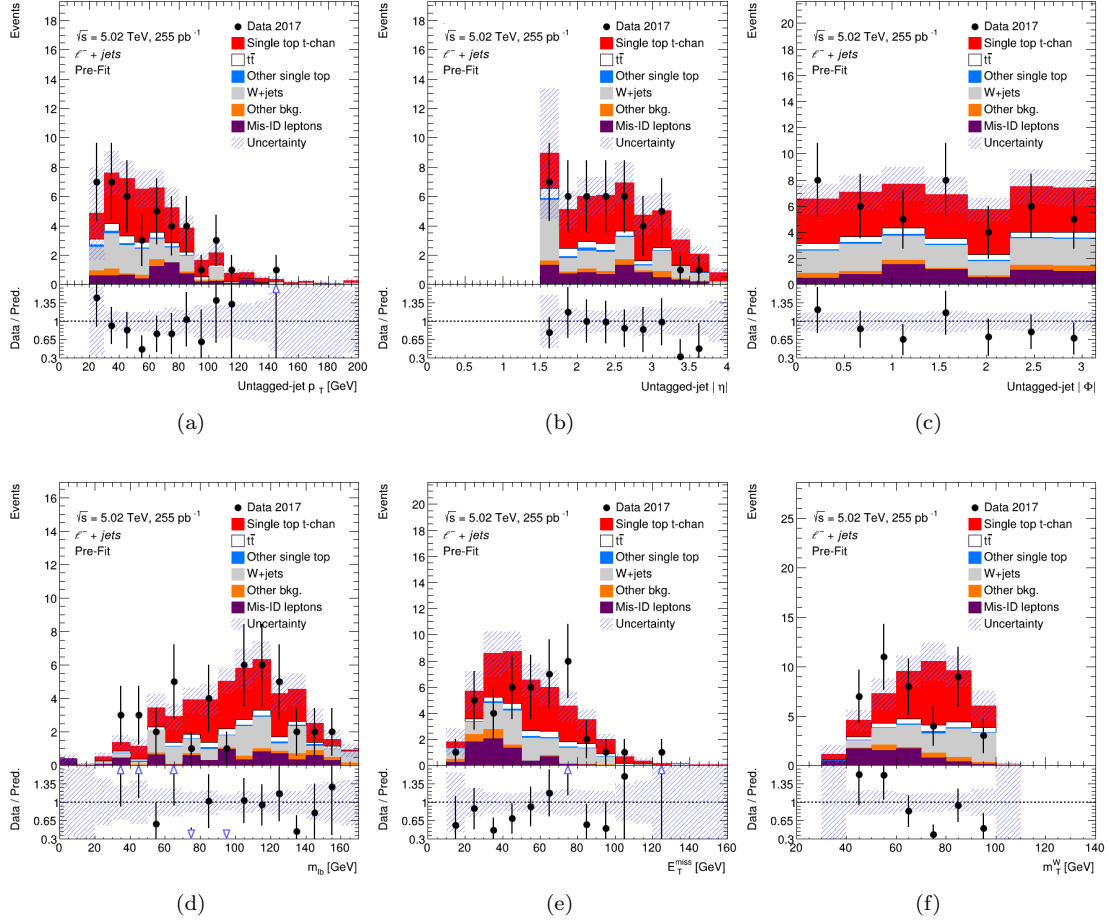


Figure K.5: The pre-fit (a) untagged jet p_T , (b) untagged jet $|\eta|$, (c) untagged jet $|\Phi|$, (d) invariant mass of the lepton and b -tagged jet pair, (e) E_T^{miss} , and (f) m_T^W distributions for data (dots) in the $\ell^- + \text{jets}$ region. The MC simulation of the signal (red histograms) and various backgrounds (represented by histograms of different colours) are also included. The error bars on the dots represent the statistical uncertainty on the data while the blue cross-hatched lines correspond to the total uncertainties on the prediction. The lower panels show the ratio of the data and predicted distributions, along with the uncertainty in the ratio.

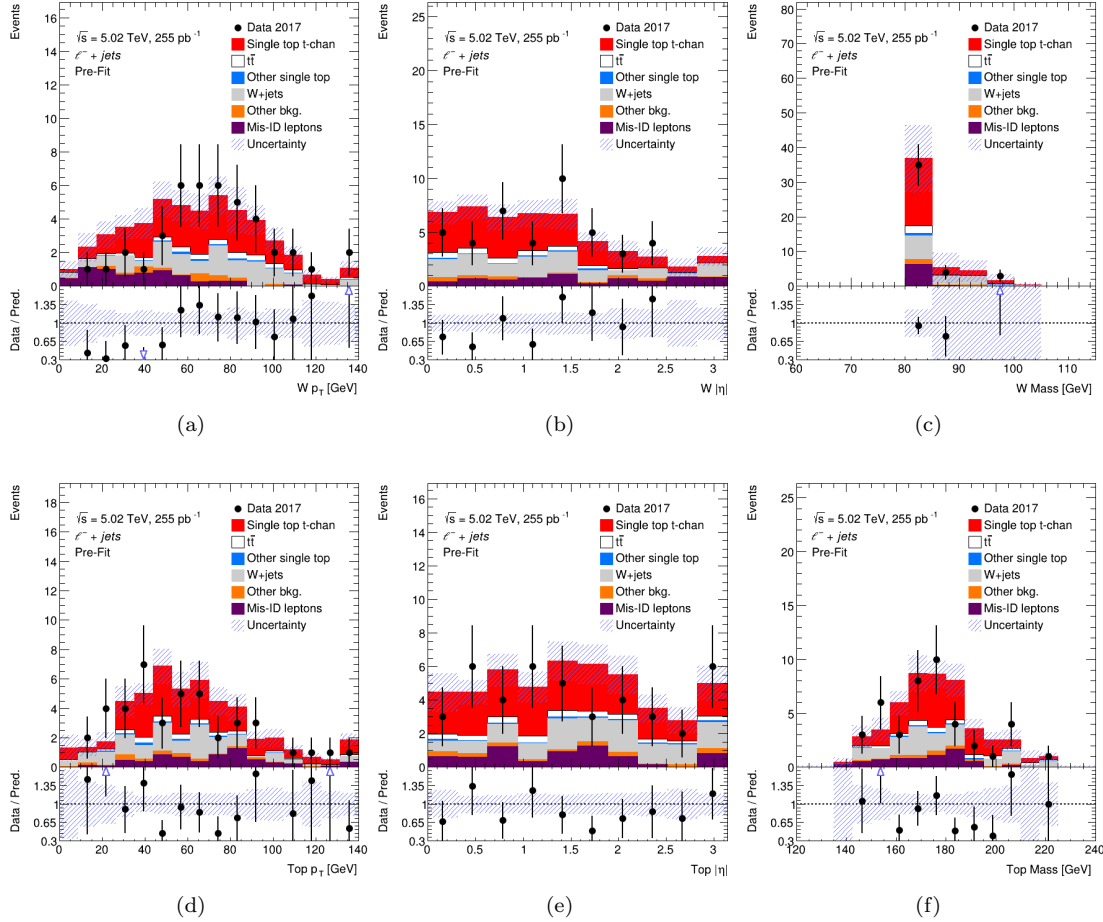


Figure K.6: The pre-fit reconstructed (a) W boson p_T , (b) W boson $|\eta|$, (c) W boson mass, (d) top quark p_T , (e) top quark $|\eta|$, and (f) top quark mass distributions for data (dots) in the $\ell^+ + \text{jets}$ region. The MC simulation of the signal (red histograms) and various backgrounds (represented by histograms of different colours) are also included. The error bars on the dots represent the statistical uncertainty on the data while the blue cross-hatched lines correspond to the total uncertainties on the prediction. The lower panels show the ratio of the data and predicted distributions, along with the uncertainty in the ratio.

Appendix L

Distributions of BDT Input Variables - t -channel Measurement

This Appendix provides plots showing the distribution and separation off the 9 input variables used to train the BDT.

Figures [L.1](#), [L.2](#), and [L.3](#) show a comparison between data and prediction for the nine BDT input variables and the expected shapes of the distributions in the ℓ +jets region that the BDT was trained in.

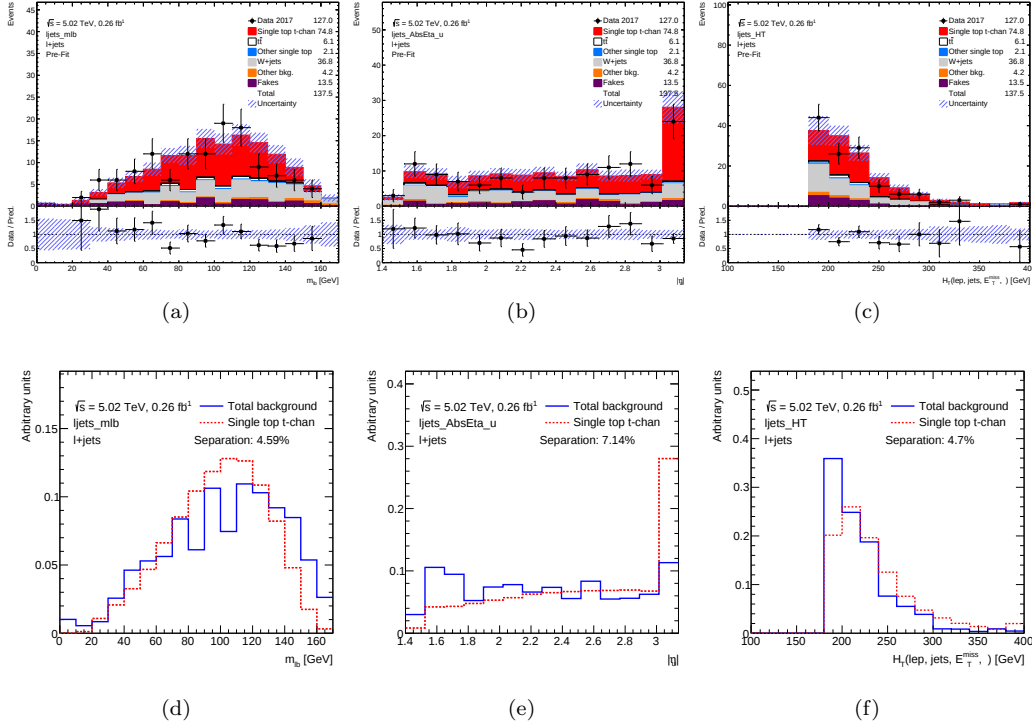


Figure L.1: The top row shows the pre-fit (a) mass of the b -tagged jet and lepton pair, (b) untagged jet $|\eta|$, and (c) H_T distributions for data (dots) in the ℓ +jets region. The MC simulation of the signal (red histograms) and various backgrounds (represented by histograms of different colours) are also included. The error bars on the dots represent the statistical uncertainty on the data while the blue cross-hatched lines correspond to the total uncertainties on the prediction. The lower panels show the ratio of the data and predicted distributions, along with the uncertainty in the ratio. The bottom row is a comparison between the shapes of the (d) mass of the b -tagged jet and lepton pair, (e) untagged jet $|\eta|$, and (f) H_T distributions for the single-top-quark signal (red) and total background (blue). The distributions in the bottom row are normalized to unit area in order to visualize the separation between signal and background.

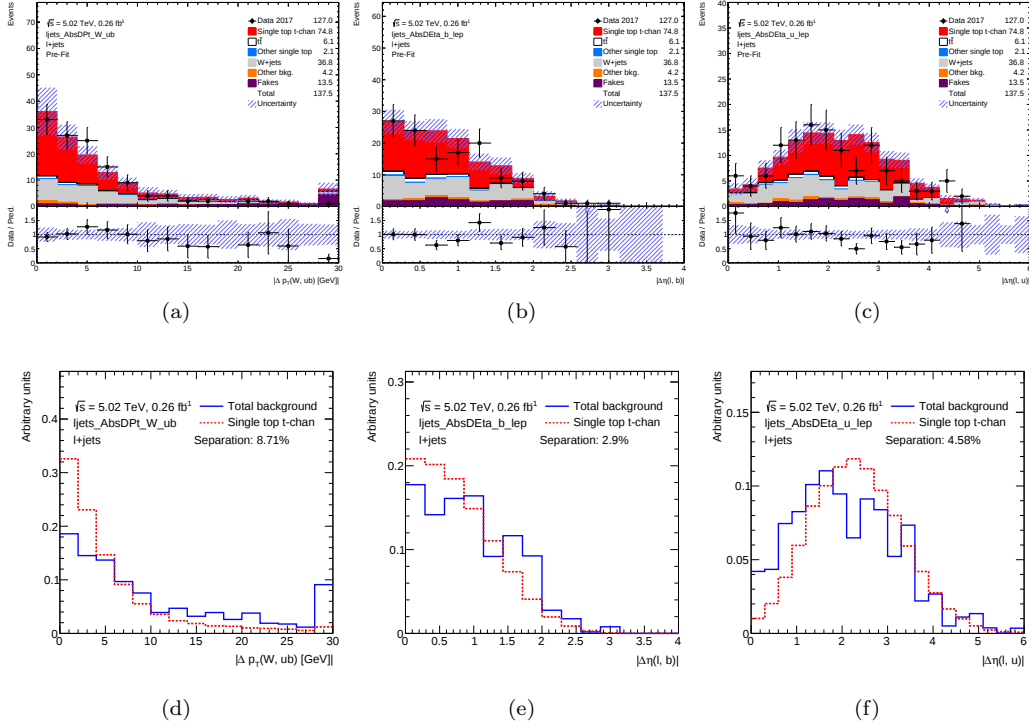


Figure L.2: The top row shows the pre-fit (a) absolute scalar difference in p_T between the reconstructed W boson and dijet pair, (b) absolute difference in η between the lepton and b -tagged jet, and (c) absolute difference in η between the lepton and untagged jet distributions for data (dots) in the ℓ +jets region. The MC simulation of the signal (red histograms) and various backgrounds (represented by histograms of different colours) are also included. The error bars on the dots represent the statistical uncertainty on the data while the blue cross-hatched lines correspond to the total uncertainties on the prediction. The lower panels show the ratio of the data and predicted distributions, along with the uncertainty in the ratio. The bottom row is a comparison between the shapes of the (d) absolute scalar difference in p_T between the reconstructed W boson and dijet pair, (e) absolute difference in η between the lepton and b -tagged jet, and (f) absolute difference in η between the lepton and untagged jet distributions for the single-top-quark signal (red) and total background (blue). The distributions in the bottom row are normalized to unit area in order to visualize the separation between signal and background.

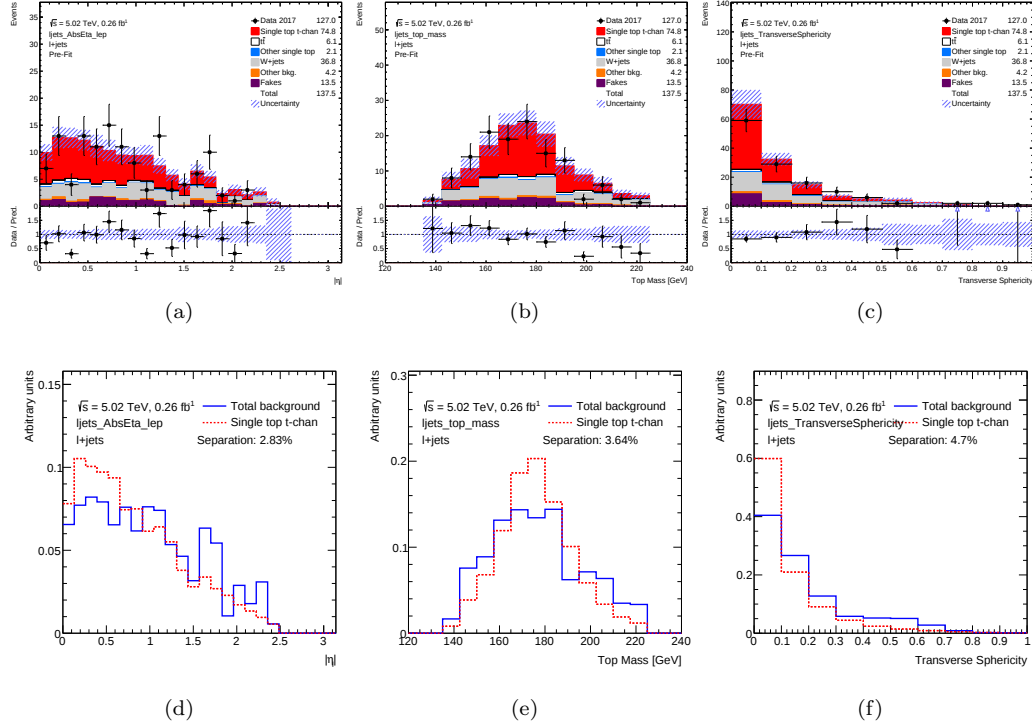


Figure L.3: The top row shows the pre-fit (a) lepton $|\eta|$, (b) reconstructed top quark mass, and (c) transverse sphericity distributions for data (dots) in the ℓ +jets region. The MC simulation of the signal (red histograms) and various backgrounds (represented by histograms of different colours) are also included. The error bars on the dots represent the statistical uncertainty on the data while the blue cross-hatched lines correspond to the total uncertainties on the prediction. The lower panels show the ratio of the data and predicted distributions, along with the uncertainty in the ratio. The bottom row is a comparison between the shapes of the (d) lepton $|\eta|$, (e) reconstructed top quark mass, and (f) transverse sphericity distributions for the single-top-quark signal (red) and total background (blue). The distributions in the bottom row are normalized to unit area in order to visualize the separation between signal and background.

Appendix M

Fit Sensitivity to Shape Effects in Misidentified Lepton Background

M.1 Sensitivity to a Shape Uncertainty

An uncertainty on the fake shape was estimated by taking the envelope of two alternate parametrizations (defined in App. I) used to calculate the fake efficiencies. The envelope is taken as a one-sided shape uncertainty that is smoothed and split into the e +jets and μ +jets channels. Figures M.1 and M.2 show the template representing the shape uncertainties for the e +jets and μ +jets NPs, respectively.

Table M.1 compares an Asimov fit to the BDT response distribution in the ℓ +jets channel (this is based on an older fitting scheme that was eventually superseded) with and without this additional shape uncertainty. From this study, one can conclude that this measurement is insensitive to variations in the shape of the misidentified lepton background.

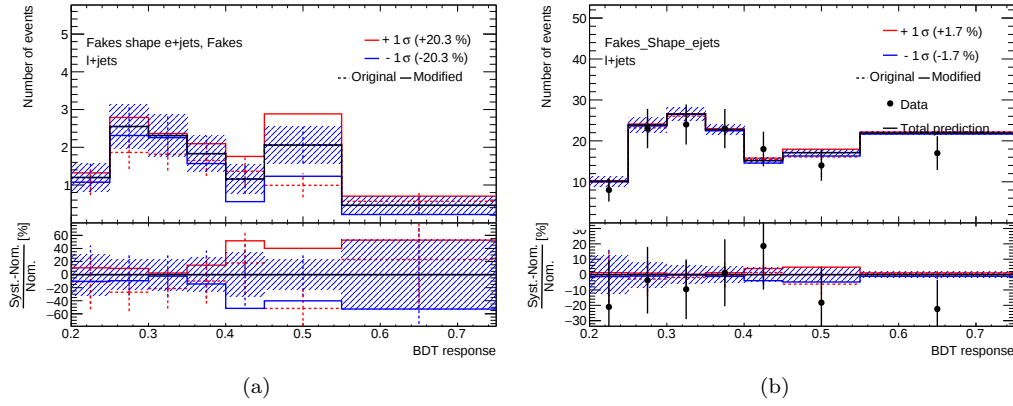


Figure M.1: (a) The template of the shape uncertainty on the misidentified lepton background in the e +jets channel shown with respect to the misidentified lepton background prediction in the e +jets channel. The solid black line represents the nominal variation while the red (blue) line represents the “up” (“down”) variation from the shape uncertainty. The dashed and solid coloured lines represent the original template and the template after smoothing and symmetrization, respectively. Note that the shape uncertainty is “one-sided”, thus the up and down variations are equal and opposite after symmetrization. The numbers on the legend correspond to the normalization difference between the variation and nominal samples but are not considered in the fit for this study. (b) shows the shape uncertainty on the misidentified lepton background in the e +jets channel with respect to the total prediction. The data (dots) is also overlaid. The error bars on the dots represent the statistical uncertainty on the data while the blue cross-hatched lines correspond to the statistical uncertainty in the respective prediction. The lower panels show the percentage deviation on the templates, along with the uncertainty on the deviation.

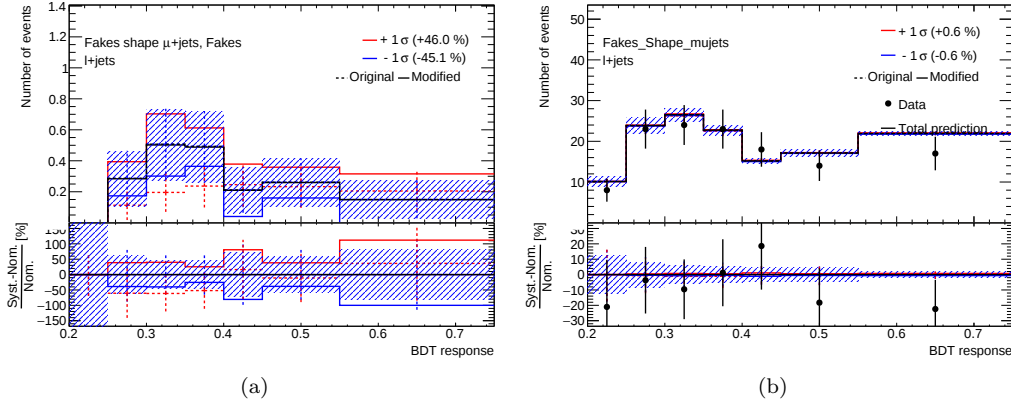


Figure M.2: (a) The template of the shape uncertainty on the misidentified lepton background in the μ +jets channel shown with respect to the misidentified lepton background prediction in the μ +jets channel. The solid black line represents the nominal variation while the red (blue) line represents the “up” (“down”) variation from the shape uncertainty. The dashed and solid coloured lines represent the original template and the template after smoothing and symmetrization, respectively. Note that the shape uncertainty is “one-sided”, thus the up and down variations are equal and opposite after symmetrization. The numbers on the legend correspond to the normalization difference between the variation and nominal samples but are not considered in the fit for this study. (b) shows the shape uncertainty on the misidentified lepton background in the μ +jets channel with respect to the total prediction. The data (dots) is also overlaid. The error bars on the dots represent the statistical uncertainty on the data while the blue cross-hatched lines correspond to the statistical uncertainty in the respective prediction. The lower panels show the percentage deviation on the templates, along with the uncertainty on the deviation.

Table M.1: Table summarizing the fit results with and without a fake shape uncertainty.

Fit	Fit result (μ)	Significance
Without a shape uncertainty	1.0 ± 0.24187	7.990
With a shape uncertainty	1.0 ± 0.24192	7.989

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