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*Search for new resonances and rare top decays to Higgs
bosons at the LHC*

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“Nothing in life is to be feared, it is only to be understood. Now is the time to understand more, so that we may fear less.”

Marie Curie

Search for new resonances and rare top decays to Higgs bosons at the LHC

Abstract

Many searches targeting the discovery of Beyond the Standard Model Physics (BSM) take place at the different Large Hadron Collider (LHC) experiments. This thesis describes in detail two of these analyses performed within the ATLAS experiment.

One analysis consists in a search for localised excesses in dijet mass distributions of low dijet mass events produced in association with a high transverse energy photon. The search uses 76.6–79.8 fb⁻¹ of LHC pp collisions collected by ATLAS at a centre-of-mass-energy of 13 TeV during 2015–2017 period. Two variants are presented: one which makes no jet flavour requirements and one which requires both jets to be tagged as b -jets. Since the observed mass distributions are consistent with multi-jet processes in the Standard Model (SM), the data are used to set upper limits on the production cross-section for a benchmark Z' model and, separately, on generic Gaussian-shaped contributions, extending the current ATLAS constraints on dijet resonances to the mass range between 225 and 1100 GeV.

The other one targets a search for a light charged Higgs boson in $t \rightarrow H^+b$ decays, with $H^+ \rightarrow c\bar{b}$. The analysis searches for top quark pair events in which one top quark decays to Wb , with the W boson decaying leptonically, and the other top quark decays to H^+b . The search is based on pp collisions at $\sqrt{s}=13$ TeV recorded between 2015 and 2018 with the ATLAS detector at the LHC and uses an integrated luminosity of 138.9 fb⁻¹. Data are analysed in the lepton-plus-jets final state, characterised by an isolated electron or muon and at least four jets. The search exploits the high multiplicity of b -quark jets characteristic of signal events, and employs a neural network discriminant that uses the kinematic differences between the signal and the background, which is dominated by $t\bar{t} \rightarrow WbWb$ decays. No significant excess of events above the background expectation is found, and expected 95% CL upper limits are derived for $t \rightarrow H^+b$ branching ratio as a function of the mass of the charged Higgs boson, ranging between 80 to 160 GeV.

Keywords: ATLAS, LHC, R -scan jets, BSM, resonance production, Z' , light charged Higgs

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Introduction

The work presented in this thesis was carried out between 2015 and 2019, within the ATLAS experiment [1] at the European Centre for Nuclear Physics Research (CERN) in Geneva, Switzerland. The institute is home to some of the most relevant high energy physics experiments in the world, and in particular to the Large Hadron Collider (LHC) [2]. The LHC is the largest hadron collider ever built, boasting a 27 km ring that can accelerate protons to collide at a centre-of-mass energy of up to 13 TeV.

Proton-proton collisions at this new energy frontier have the potential to create new, heavy particles that are not predicted by the Standard Model (SM). If a new particle couples to the SM it may be created by parton collisions at the LHC and can therefore subsequently decay into SM particles, leaving evidence of its existence. This potential evidence of Beyond Standard Model (BSM) physics may be found in searches of non-standard-model resonant signals decaying into SM particles or in rare decays of SM particles, among other processes. Therefore, many searches targeting the discovery of BSM evidence take place at the different LHC experiments. This thesis describes in detail two of these analyses performed within the ATLAS experiment.

On one side, searches for new particles decaying to pairs of jets have been a fundamental part of the physics programme at collider experiments. Since any strongly interacting new particle directly produced at a hadron collider via quarks and gluons must decay to them, dijet signatures offer a simple way to search for a wide array of possible new physics models. The increase in energy (and luminosity) allows searches to access higher mass ranges for possible new particles. However, this means that lower masses and smaller hypothesised couplings are rendered inaccessible by the trigger prescales required to control increasing instantaneous luminosities.

ATLAS presents a wide programme of complementary searches targeting this low-mass, low-coupling region in several ways. One of these approaches assumes the production of a high- p_T initial-state radiation (ISR) object, in this case a photon, against which the new particle recoils [3]. This ISR object can be used for triggering, allowing the resonance to be reconstructed from lower- p_T jets that would not pass an unprescaled single-jet trigger.

For a resonance of intermediate mass, too light to be accessible to the dijet analysis and too heavy to produce a strongly boosted decay, a final state is studied consisting of two small- R jets in addition to the ISR object. A resolved final state, consisting of two jets and one photon, is the subject of the first analysis presented in this thesis. It has been previously studied in several preliminary results but has never yet been published by ATLAS or CMS. For this analysis, a leptophobic axial-vector mediator Z' particle is used as a benchmark model [4]. For some BSM models, new particles are expected to preferentially decay to third-generation quarks. Sensitivity to such models can be dramatically improved by requiring that one or both of the jets from the resonance decay be tagged as originating from a b -quark.

The analysis presented uses data collected with the ATLAS detector during 2015–2017 period at a centre-of-mass energy of 13 TeV. This dataset corresponds to an integrated luminosity between 76.6–79.8 fb⁻¹, depending on the particular triggers used. The invariant mass distribution of a selected pair of jets (m_{jj}) in each event is compared to a smooth SM-only background prediction taken from a fit. A model-nonspecific search phase compares the data to the expected background over the mass range 169 GeV to 1200 GeV to determine whether any significant discrepancy is observed. In case the search phase does not show any significant excess, limits are then set on the production cross-section for a benchmark Z' model for signal masses in the range 250 GeV to 1100 GeV. Four channels are analysed in total. These consist of two different trigger selections, one optimised for higher m_{jj} (combined trigger) and the other allowing access to lower m_{jj} ranges (single-photon trigger), and two different jet selections: one which makes no jet flavour requirements and one which requires both jets to be tagged as b -jets. The results of this analysis are reported in [5].

On the other hand, the discovery on 2012 of a boson whose properties and mass are consistent with the Higgs boson predicted by the SM not only represented the last remaining feature to complete the SM theory but it also began a new era of searches of BSM physics that could be intimately associated with the Higgs boson. Since there are still many unresolved problems on the current SM theory (such as the nature of dark matter or the origin of neutrino masses, among others), there are several BSM hypotheses that have been introduced and tested to answer these questions, and many of them include more than one Higgs doublet. For example, the so-called two-Higgs doublet model (2HDM) [6], which results in five Higgs bosons: two charged ($H^\pm$) and three neutral (A, H, h).

The second analysis of this thesis presents a search for charged Higgs bosons ($H^\pm$). In particular for light ones (ranging from 80 to 160 GeV), where its mass is lighter than the top quark mass. Hence, H^+ can be produced in rare decays of the top quark $t \rightarrow H^+b$. This search focuses on the $H^+ \rightarrow c\bar{b}$ decay, which is one of the dominants in this regime and it can be interpreted in terms of the 2HDM flipped model [7–9], where it shows a higher branching ratio than the other decays for certain configurations. Results for this particular decay have not been published by ATLAS yet.

The analysis searches for top quark pair events in which one top quark decays to Wb , with the W boson decaying leptonically, and the other top quark decays to H^+ . The search is based on pp collisions at $\sqrt{s}=13$ TeV recorded between 2015 and 2018 with the ATLAS detector at the LHC and uses an integrated luminosity of 138.9 fb⁻¹. Data are analysed in the lepton-plus-jets final state, characterised by an isolated electron or muon and at least four jets. The search exploits the high multiplicity of b -quark jets, characteristic of signal events, and employs a neural network discriminant that uses the kinematic differences between the signal and the background, which is dominated by $t\bar{t} \rightarrow WbWb$ decays. In case no significant excess of events above the background expectation is found, expected 95% CL upper limits will be derived for $t \rightarrow H^+b$ branching ratio as a function of the mass of the charged Higgs boson, ranging between 80 to 160 GeV.

Unfortunately, by the time this thesis has been written the final results for this search were not available yet, since data was not unblinded at the moment. Nevertheless, the whole analysis strategy is already optimised and tested with promising results that are presented on this thesis.

As part of the graduate student activities, a large number of infrastructure developments were carried on within the jet performance group. Among the most important

ones, the introduction of a new method and the later derivation of an *in-situ* calibration for jets with radius parameter $R = 0.2$ and $R = 0.6$, known as R -scan jets, is presented as an example in this thesis.

The energetic pp collisions produced by the LHC yield final states that are predominantly characterised by jets, which constitute an essential piece of the physics programme carried out using the ATLAS detector, either via their presence in the signal processes being measured and searched for, or as a ubiquitous feature of various background processes and the pile-up due to simultaneous pp collisions.

The standard jet radius used by ATLAS with a full calibration is $R = 0.4$, however there are jets with smaller $R = 0.2$ and bigger $R = 0.6$ radii, and since there are many motivations to use them it is crucial to have an optimised calibration. For instance, the $R = 0.6$ jets represent a better choice for Standard Model precision measurements in general, since they leave out some effects that only affect the jet reconstruction in smaller radii jets. While the usage of $R = 0.2$ jets is motivated for example by those searches looking for a low mass particle at high energy in a boosted regime where the reconstruction on the decaying pair of jets from this particle could be better resolved with a smaller jet size reconstruction. On the other hand, derive a full calibration for the R -scan jets in the same way that it is done for the $R = 0.4$ ones would require many resources (computational power and person power too), so the collaboration ultimately decided to provide only a full calibration for the standard jet size. Other methods are implemented instead that make benefit of the already full calibrated $R = 0.4$ jets to calibrate the ones with smaller and bigger sizes.

This thesis is organised as follows. Chapter 1 begins with an introduction of the Standard Model of particle physics, a motivation for new physics, and a description of Monte Carlo simulations. Given that the Standard Model is a well known theory, it is not the aim of this chapter to be extensive, but to present a summary of the basic parts of the theory on which the work in this thesis relies. The LHC and the ATLAS detector are introduced in chapter 2, as well as a brief description on the reconstruction and identification of the physical objects. The *in-situ* calibration method for R -scan jets is presented in chapter 3 along with their latest results. The search for resolved dijet resonances produced in association with a photon is described in chapter 4, while the search for top-quark decays to a charged Higgs boson and a b -quark is detailed in chapter 5. Finally, the conclusions are given at the end.

Chapter 1

Theoretical introduction

1.1 The Standard Model

The Standard Model (SM) [10, 11] is the theoretical framework that describes more accurately all elementary particles known up to now and their interactions. It has been widely tested along the years and it has been very successful in describing experimental observations. In addition, all the predicted phenomena have found experimental confirmation, the last one being the observation of the Higgs boson at the Large Hadron Collider in July 2012 [12, 13].

The SM is a renormalisable quantum field theory based on the total invariance under the gauge group:

$$\mathrm{SU}(3)_C \otimes \mathrm{SU}(2)_L \otimes \mathrm{SU}(1)_Y \quad (1.1)$$

where $\mathrm{SU}(3)_C$ represents the symmetry group of the strong interaction and $\mathrm{SU}(2)_L \otimes \mathrm{SU}(1)_Y$ corresponds to the electroweak one. This theory describes the interactions between the constituents of matter, called *fermions*, through the exchange of force mediators, known as *bosons*. Bosons have integer spin and obey the Bose-Einstein statistics, whereas fermions have half-integer spin and follow the Fermi-Dirac statistics. Fermions can be separated into quarks and leptons, which are organized into three families or generations. The structure is repeated within each generation, but the masses of the particles vary from the lighter first generation to the heavier third one. Each quark and lepton has an additional anti-particle, carrying the same mass but opposite quantum numbers, thus doubling the number of fermions. A summary of the fermion family and their properties is provided in table 1.1.

Fermions are described as spin- $1/2$ Dirac fields, satisfying the lagrangian

$$\mathcal{L} = \bar{\psi}(i\gamma^\mu\partial_\mu - m)\psi \quad (1.2)$$

where ψ is the fermion field, γ^μ represent the Dirac matrices and m is the mass of the fermion. Given a certain symmetry group, imposing the lagrangian to be invariant under local transformations requires the introduction of gauge fields known as *boson fields*. The number of associated boson fields is equal to the number of generators of the symmetry group. Even though there are four fundamental interactions in Nature, the bosonic mediators of the SM can only describe three (electromagnetic, weak and strong)

Generation	Name	Mass	Electric charge
Quarks			
1^{st}	Up (u)	2.2 MeV	$2/3$
	Down (d)	4.7 MeV	$-1/3$
2^{nd}	Charm (c)	1.28 GeV	$2/3$
	Strange (s)	96 MeV	$-1/3$
3^{rd}	Top (t)	173.1 GeV	$2/3$
	Bottom (b)	4.18 GeV	$-1/3$
Leptons			
1^{st}	Electron (e^-)	0.511 MeV	-1
	Electron neutrino (ν_e)	< 2 eV	0
2^{nd}	Muon (μ^-)	105.7 MeV	-1
	Muon neutrino (ν_μ)	< 0.19 MeV	0
3^{rd}	Tau (τ^-)	1776.9 MeV	-1
	Tau neutrinos (ν_τ)	< 18.2 MeV	0

Table 1.1: Fermionic sector of the Standard Model. Values are taken from the Particle Data Group (PDG) [14].

out of the four. Gravitational interactions cannot be interpreted in terms of the SM, which is one of the main motivations to look for physics beyond the SM (BSM). A summary of the boson classification and its properties is presented in table 1.2.

Mediator	Mass [GeV]	Interaction	Electric charge	Spin
Gluon $\times 8$ (g)	0	strong	0	1
Photon (γ)	0	electromagnetic	0	1
Z	91.19	weak (neutral)	0	1
$W^\pm$	80.39	weak (charged)	± 1	1
Higgs (H)	125.09	-	0	0

Table 1.2: Bosonic sector of the Standard Model. Values are taken from the Particle Data Group (PDG) [14].

The interactions are pictured in terms of exchanges of elementary particles and the couplings between them, mathematically characterised in the lagrangian by quadratic and higher order terms. The probability of a certain process is obtained by considering all relevant Feynman diagrams. These diagrams connect the incoming and outgoing particles via the allowed vertices (couplings) and propagators (force mediating particles). The quarks interact between them via the strong interaction and with other fermions both electromagnetically and via the weak interaction. On the lepton side, since the neutrino does not carry electric charge, its dynamics are driven by the weak force only. The electron, muon and tau leptons interact both electromagnetically and weakly.

The couplings allowed by the SM, and the kind of interaction they describe, are de-

tailed in table 1.3.

Electromagnetic	$\gamma q \bar{q}$ $\gamma \ell \bar{\ell}$ $\ell = (e, \mu, \tau)$
Electroweak	$W q \bar{q}'$ $W \ell \bar{\nu}$ $Z q \bar{q}$ $Z \ell \bar{\ell}$ $W^+ W^- \gamma$ $W^+ W^- Z$ $W^+ W^- \gamma \gamma$ $W^+ W^- Z Z$ $W^+ W^- Z \gamma$ $W^+ W^- W^+ W^-$
Strong	$g q \bar{q}$ $g g g$ $g g g g$
Higgs interactions	$H \ell \bar{\ell}$ $H q \bar{q}$ $H W^+ W^-$ $H Z Z$ $H H Z Z$ $H H W^+ W^-$ $H H H$ $H H H H$

Table 1.3: Couplings allowed by the Standard Model, and the kind of interaction they describe [14, 15].

The SM lagrangian can be divided into two parts, accounting separately for each type of interaction, one describing electroweak interactions and the other, the strong ones. An additional term called the Higgs sector needs to be added to account for masses.

$$\mathcal{L}_{SM} = \mathcal{L}_{EW} + \mathcal{L}_{QCD} + \mathcal{L}_H \quad (1.3)$$

A complete discussion of the SM is broadly available in the literature [16, 17], a brief description is given in the next sections.

1.1.1 Electroweak theory

The electroweak theory unifies the forces in the last two groups of equation 1.1 [10, 11, 18], and describes the weak and electromagnetic interactions. The theory was developed by Feynman, Schwinger and Tomonaga throughout the 1940s [19] among others. The gauge group corresponding to weak interactions is $SU(2)_L$, and the state is described by the isospin (T). The generators of the group are the weak isospin operators $\hat{T} = \hat{\sigma}_i/2$, ($i = 1, 2, 3$), where σ_i are the three Pauli matrices. The subscript L comes from the fact that the weak interaction only affects left handed particles (right-handed anti-particles). Thus, when the fermion field is projected onto right and left components, the left-handed fermions transform as doublets, while the right-handed fermions as singlets:

$$f_L^i = \begin{pmatrix} \nu_L^i \\ l_L^i \end{pmatrix}, \begin{pmatrix} u_L^i \\ d_L^i \end{pmatrix} \quad f_R^i = l_R^i, u_R^i, d_R^i$$

where i is the family (generation) index. The hypercharge, Y , is the property conserved through the second part of the term, $U(1)_Y$. The electric charge is related to the combination of T_3 and Y through the Gell-Mann Nishijima formula

$$\hat{Q} = \hat{T}^3 + \hat{Y}/2 \quad (1.4)$$

In order to respect local invariance under both symmetry groups, the covariant derivative is introduced in the lagrangian, in equation 1.2

$$D_\mu = \partial_\mu - ig \vec{T} \vec{W}_\mu - ig' \frac{Y}{2} B_\mu \quad (1.5)$$

where g and g' are the coupling constants of the weak and hypercharge groups respectively, and W_μ^a and B_μ are the four corresponding gauge bosons. Self interaction should also be taken into account, which is why terms corresponding to interactions within the W_μ and B_μ fields are added as well. The electroweak lagrangian can then be written as the sum of the fermion and the gauge lagrangian:

$$\mathcal{L}_{EW} = \mathcal{L}_f + \mathcal{L}_{gauge} = \sum_{f=l,q} \bar{f} i \gamma^\mu D_\mu f - \frac{1}{4} W_{\mu\nu}^i W_i^{\mu\nu} - \frac{1}{4} B_{\mu\nu} B^{\mu\nu} \quad (1.6)$$

where $W_{\mu\nu}^i$ and $B_{\mu\nu}$ are the field tensors of the $SU(2)_L$ and $U(1)_Y$ groups respectively.

The introduction of mass terms for either the fermion or gauge fields breaks the local $SU(2)_L$ gauge invariance of the lagrangian. This is not in agreement with experimental measurements of their masses, which were indicated in tables 1.1 and 1.2. A mechanism was therefore introduced in order to generate non-zero masses while preserving the consistency of the theory at high energies. This is the Higgs-Englert-Brout mechanism, in which a new spinless boson - the Higgs boson - is defined, and it is described in the next section.

1.1.2 The Higgs mechanism

This mechanism was proposed as a solution to the fact that gauge fields, as presented in equation 1.6, are massless. It postulates an elementary spin zero Higgs boson, whose coupling to other particles determines their masses. It consists of a scalar field with four real components, arranged into a complex scalar $SU(2)_L$ isospin doublet, $\phi = \begin{pmatrix} \phi^+ \\ \phi^0 \end{pmatrix}$. The field is included in the lagrangian through its covariant derivative and a potential, where the covariant derivative D_μ is as defined in equation 1.5 and the potential, as well as the lagrangian, are shown below.

$$\mathcal{L}_H = |D_\mu \phi|^2 - V(\phi) \quad V(\phi) = \mu^2 \phi^\dagger \phi + \lambda (\phi^\dagger \phi)^2 \quad (1.7)$$

The potential $V(\phi)$ depends on two parameters, μ and λ , and if their values are such that $\mu^2 < 0$ and $\lambda > 0$ the minimum of the ϕ field potential is degenerated. In other words, the fundamental vacuum state is no longer $SU(2)_L \otimes U(1)_Y$ invariant, and acquires a non-zero vacuum expectation value (VEV). The Goldstone theorem [20, 21] states that a massless scalar (called Goldstone boson) appears when a continuous symmetry is spontaneously broken. These bosons can then be absorbed by a gauge field as a longitudinal polarization component and therefore, the gauge field acquires mass. In this case the gauge fields are those corresponding to the $W^\pm$ and Z^0 bosons, the photon being massless, taking three out of the four scalar field components. The remaining scalar field is the one with zero electric charge, and its value can be expanded around the minimum to obtain

$$\phi_0(x) = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ v + H(x) \end{pmatrix} \quad (1.8)$$

where $H(x)$ represents ground state fluctuations around the vacuum expectation value and corresponds to the massive electrically-neutral Higgs boson predicted in 1964 [22–25]. The same Higgs isospin doublet is necessary for the generation of fermion masses. A term of the form $y_i \bar{\psi}_i \psi_j \phi$ is added to the lagrangian to account for interactions between the Higgs field and the fermionic field, where y_i is the coupling constant of Yukawa. Combining the resulting lagrangian terms and the scalar field expansion presented in 1.8, the additional terms for the fermion masses are obtained.

1.1.3 Quantum Chromo Dynamics

Quantum Chromo Dynamics (QCD) is the theory that describes strong interactions in the SM carried out by quarks and gluons, collectively known as partons. It was developed as a way to describe the behaviour of the quarks being held together by the strong force, carried by gluons. It describes the state of a quark with a quantum number called *colour*, which can take three possible values, and corresponds to the $SU(3)_C$ group in equation 1.1 which is the starting global symmetry. The global gauge symmetry is promoted to a local one by introducing the covariant derivative:

$$D_\mu = \partial_\mu - i4\pi\alpha_s T_a G_\mu^a \quad (1.9)$$

where α_s is the strong coupling constant, T_a are the $SU(3)_C$ generators (with $a=1\dots 8$) and G_μ^a are the gluon fields. After introducing this term and a kinematic term for the gluon fields, the QCD lagrangian is given by:

$$\mathcal{L}_{QCD} = \bar{q}(i\gamma^\mu D_\mu)q - \frac{1}{4}G_{\mu\nu}^a G_a^{\mu\nu} \quad (1.10)$$

where γ^μ are the Dirac matrices and q is a three-component vector corresponding to the different colour states of a quark type. Gluons transform under the adjoint representation, while quarks are in the fundamental representation of the $SU(3)_C$ group. The interactions between quarks and gluons are enclosed in the definition of the covariant derivative in equation 1.9: an interaction between a quark and a gluon will rotate the quark's colour in $SU(3)_C$ space. The field tensor $G_{\mu\nu}^a$ is given by:

$$G_{\mu\nu}^a = \partial_\mu G_\nu^a - \partial_\nu G_\mu^a - 4\pi\alpha_s f_{abc} G_{\mu\nu}^{b\ c} \quad (1.11)$$

where f_{abc} are the structure constants of the $SU(3)_C$ group. The third term of the tensor describes the gluon self-interaction and is responsible for the non-abelian nature of QCD. The value of the strong coupling constant α_s varies with the square of the scale of the interaction, Q^2 . In the high energy regime its value is sufficiently small so that it can be calculated using perturbation theory, giving the QCD theory, good mathematical properties and predictive power. Its value vanishes for infinitely large energies, so that in this limit quarks can propagate freely, a property known as *asymptotic freedom* [26, 27]. In the opposite direction, the value of α_s increases for lower energy, to the point of diverging. Figure 1.1 shows the running of α_s at various scales, illustrating the good consistency between the measurements. This results in the *confinement* [28] of quarks and gluons, which cannot appear as free particles. This means that when partons charged with colour start to separate from one another, the potential energy increases to the point that it is energetically convenient to create a quark-antiquark pair with opposite charge from the first one from the vacuum. As a consequence, coloured partons produced in high-energy interactions will give place to a shower of hadrons (colour-neutral composite particles), forming a jet. The importance of jet measurements rely in their direct relation to the scattering of quarks and gluons. QCD interactions are dominant at the LHC because the colliding particles carry colour charge, and α_s is much larger than the electroweak coupling constants. Jets are, therefore, one of the most produced objects at the LHC.

1.1.4 Perturbative Quantum Chromodynamics

The experimental consequence of asymptotic freedom is that the hard interactions of quarks and gluons at the energy scale probed by hadron colliders can be described by

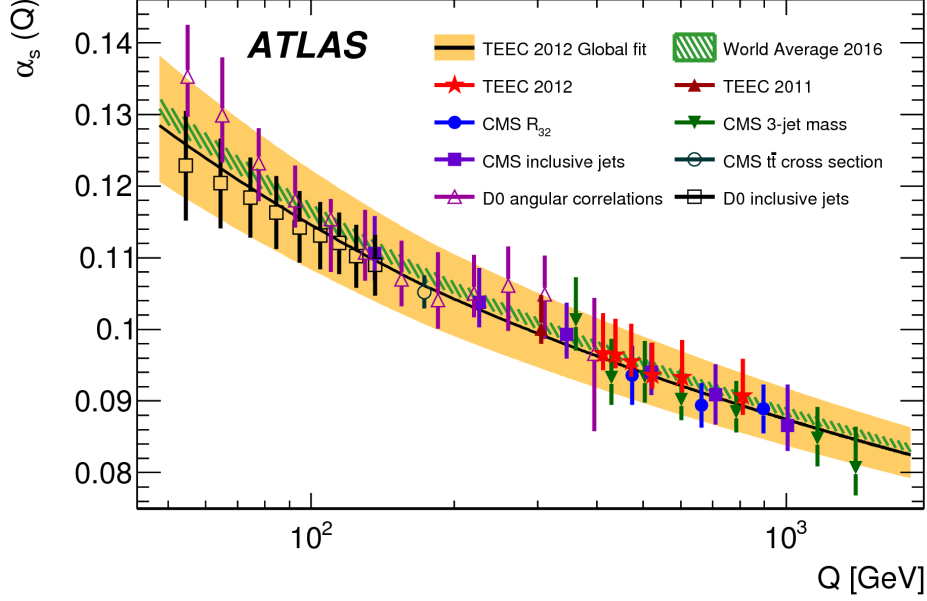


Figure 1.1: The QCD coupling determined in different experiments, together with the (green) band from the world average. Image from ref.[29].

perturbative QCD (pQCD), although their presence in the final state can only be inferred indirectly, as they appear confined in colourless hadrons. Each order of the perturbative expansion corresponds to an additional power in the coupling constant. This power is related to the number of vertices in the matrix element QCD Feynman diagrams¹, with $\sqrt{\alpha_s}$ per vertex, with the exception of the 4-gluon vertex which contributes with α_s . Each increasing order in α_s of the perturbative expansion simply corresponds to a set of diagrams with the correct combination of vertices. By drawing all possible Feynman diagrams for a given order of perturbation theory, all the terms in the calculation can be read off. In this context, leading-order diagrams are also known as “tree-level” diagrams (with no internal loops). Since the value of α_s varies with energy, it must be evaluated at the energy scale of the interaction. In particular, at the electroweak scale, $\alpha_s(M_Z) \sim 0.117$, the perturbative expansion converges relatively fast, allowing all except the lower order terms to be ignored. The complexity of the process determines the order to which the calculation can be performed.

Using this formalism, the two parton hard interaction cross-sections can be computed to some fixed order in perturbation theory. However, hadron colliders such as the LHC do not produce simple parton-parton interactions, but instead collisions of hadrons that consist of multiple partons. The factorisation theorem [30, 31] allows the perturbative calculations for parton interactions to be extended to proton-proton collisions as well as to separate the short-distance component of the scattering process described by pQCD from the non-perturbative long-distance component. This theorem states that the total cross-section for two hadrons can be obtained by weighting and combining the cross sections for two particular partons. This weighting is done using $f_i(x, Q^2)$, the parton distribution functions (PDFs), which describe the parton density for a parton of species i in a hadron, with a fraction x of the hadron energy-momentum when the hadron is

¹Feynman diagrams are illustrative representations of the mathematical expressions describing the behaviour of sub-atomic particles, named after its inventor, Richard Feynman.

probed at a resolution scale Q^2 . The cross-section for a hard scattering process $pp \rightarrow X$, initiated by two hadrons with four-momenta P_1 and P_2 can be written as:

$$\sigma_{pp \rightarrow X} = \sum_{i,j} \int_0^1 dx_1 dx_2 f_i(x_1, \mu_F^2) f_j(x_2, \mu_F^2) \hat{\sigma}_{ij}(p_1, p_2, \alpha_s(\mu_R^2), Q^2/\mu_R^2, Q^2/\mu_F^2). \quad (1.12)$$

Here, x_1 and x_2 are the momentum fractions carried by the interacting partons, and $p_1 = x_1 P_1$ and $p_2 = x_2 P_2$ are the interacting parton momenta. The partonic cross-section $\hat{\sigma}_{ij}$, corresponding to the interaction of partons i and j , is calculated at a fixed order in α_s , which is evaluated at some renormalisation scale, μ_R , and factorisation scale, μ_F . The total cross-section is obtained by summing over all possible parton flavours and integrating over all possible momentum fractions. The parton distribution functions, f_i and f_j , are evaluated at a factorisation scale, μ_F , which can be thought of as the scale that separates short-distance, perturbative physics, from long-distance, non-perturbative physics (i.e., separates hard and soft processes). Figure 1.2 shows the parton distribution function evaluated at two different factorisation scales for all possible partons.

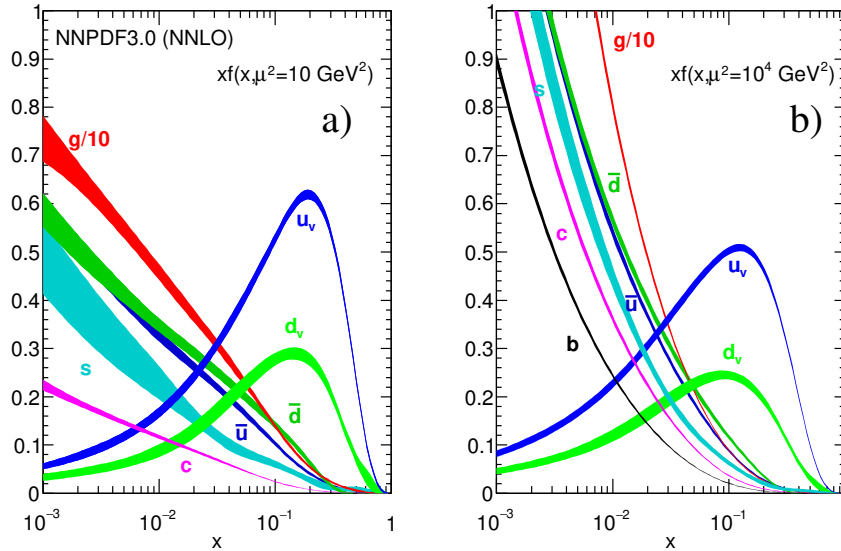


Figure 1.2: The bands are x times the parton distribution functions $f_i(x, Q^2)$ (where $i = u_v = u - \bar{u}, d_v = d - \bar{d}, \bar{s} \simeq \bar{s}, c \simeq \bar{c}, b \simeq \bar{b}, g$) obtained in an NNLO NNPDF3.0 global analysis [32] at scales $\mu_F^2 = 10 \text{ GeV}^2$ (left) and $\mu_F^2 = 10^4 \text{ GeV}^2$ (right), with $\alpha_s(M_Z^2) = 0.118$. Images from ref.[14].

If the perturbative expansion were carried to all orders, the cross-section $\sigma_{pp \rightarrow X}$ in equation 1.12 would be independent of μ_F and μ_R . In actual finite order calculations this is not true. They are usually both taken to be equal, $\mu_F = \mu_R = \mu$, chosen at the typical scale Q^2 of the process, in order to minimise the contribution of (uncalculated) higher order terms which appear as logarithmic terms of the form $\log(Q^2/\mu_R^2)$ and $\log(Q^2/\mu_F^2)$.

The dependence of the prediction on μ_F and μ_R is assigned as a theoretical uncertainty. The fact that the cross-section of a process should be independent of the factorisation scale μ_F led to the DGLAP equations, published separately in the 1970s by Yuri Dokshitzer, Vladimir Gribov and Lev Lipatov, and Guido Altarelli and Giorgio Parisi [33]. These equations determine the evolution of the PDFs with Q^2 .²

²The DGLAP evolution equations describe the change with Q^2 of the quark densities due to gluon radiation and gluon splitting, and of the gluon density due to radiation from quarks and gluons.

On the other hand, the dependence on x must be obtained by fitting possible cross-section predictions to data from hard scattering experiments. The understanding of the PDFs plays a key role for interpreting the data at hadron colliders in terms of the SM predictions and possible deviations. Dedicated groups perform the parametrisation of PDFs using data from different experiments and processes.

1.1.5 Particle physics in hadron colliders

The variety of physics processes occurring in a hadron-hadron collision is highlighted next in an inwards-outwards flow (i.e., from short-distance to long-distance processes).

Initially two hadrons are coming in on a collision course, where each hadron can be thought as a group of essentially collinear partons quantitatively characterised by the parton distributions (see section 1.1.4). In a collision scenario with accelerated particles carrying electromagnetic and colour charges, bremsstrahlung can occur, e.g. as gluon radiation such as $q \rightarrow qg$. A collision between two partons, one from each side, takes place producing the hard process of interest, that can be calculated by a perturbative approach to some order in α_s , which corresponds to the number of outgoing partons. Emissions that are started off from the two incoming colliding partons are called “initial-state radiation” (ISR). After the collision, outgoing partons can also radiate. This emission is referred to as “final-state radiation” (FSR). With the parton shower development, the colour field strength increases as partons move away and they can break up by the production of quark-antiquark pairs. Thus, quarks and antiquarks may combine to produce a primary hadron. The creation of hadrons as a consequence of the confinement phenomenon is referred to as *hadronisation* (see section 1.3.3). Each of the incoming hadrons is made up of a multitude of additional partons, which may also interact within the same hadron-hadron collision. These semi-hard secondary collisions are referred to as “multiple parton interactions” (MPI).³ Each of these further collisions also may be associated with its radiation. The additional products of the collision that are not explicitly related to the hard process (radiation, hadron remnants, products of multiple parton interactions, etc.), are generally grouped altogether and called *underlying event* (UE).

Overall, the complex picture of a hadron-hadron collision introduced in this section is illustrated in figure 1.3.

The processes that take place during a hadron-hadron collision cannot be completely calculated through pQCD. Currently, there are different Monte Carlo (MC) simulations available, involving various suitable approximations, that have been developed to address some of the phenomena mentioned above (see [35, 36] and references therein). The key features of the MC simulations required for the understanding of the analyses presented in this thesis are described in section 1.3.

1.2 Beyond Standard Model

The SM provides a strong theoretical foundation to our understanding of high energy physics and agrees remarkably well with experimental results. However, theoretical discrepancies point to the possibility of new physics Beyond the Standard Model (BSM). An example is the hierarchy problem [37–39], described simply as a theoretical inconsistency

³The multiple parton interactions are a completely separate effect from the multiple proton interactions that may occur in each bunch collision event in a hadron collider.

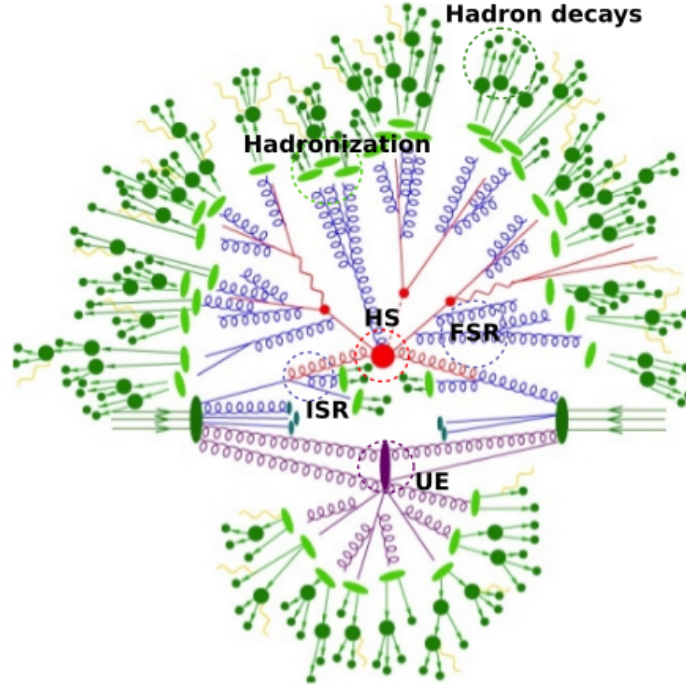


Figure 1.3: Illustration of the stages of a hadron-hadron collision: the hard interaction (HS), the initial- and final-state radiation (ISR and FSR, respectively), the hadronisation, the subsequent hadron decays, and the underlying event. Image from ref.[34].

between the relative strengths of the gravitational and electroweak forces. The differences can only be accounted for through very fine-tuned cancellations of force couplings against quantum corrections, an overly arbitrary and unlikely scenario. Experimental evidence for BSM physics is also piling up. Analysis of galactic rotation curves [40] and gravitational lensing [41] point to discrepancies between the mass of galaxies as calculated through gravitational predictions and through extrapolations of the aggregate stellar luminosity. This discrepancy leads to the existence of a hypothetical type of matter distinct from ordinary matter known as dark matter. Many cosmological observations, including the measurement of the cosmic microwave background [42], indicates a universal composition of 5% matter, 27% dark matter, and 68% dark energy, another unknown form of energy.

Proton-proton collisions at a new energy frontier of 13 TeV have the potential to create new, heavy particles that are not predicted by the SM. If a new particle couples to the SM it may be created by parton collisions at the LHC and can therefore subsequently decay into SM particles, leaving evidence of its existence. This potential evidence of BSM physics may be found in precision measurements of cross-sections as deviations from the SM, or in searches of non-standard-model resonant signals decaying into SM particles.

1.3 Monte Carlo simulations

Having QCD predictions is crucial in precision measurements as well as in searches for new physics. The “fixed-order predictions” include the first terms in the QCD perturbative expansion for a given cross-section. As more terms are involved in the expansion, an improvement in the accuracy of the prediction is expected. The complexity of the pQCD calculations increases significantly with the number of outgoing partons. Furthermore,

pQCD calculations do not provide the full hadronic level event description. An alternative approach is provided by the so-called Monte Carlo programs.

1.3.1 Hard interaction and parton shower

In order to describe a $2 \rightarrow n$ process from the lagrangian of the theory (where n represents a given number of partons in the final state), a set of Feynman diagrams has to be laid down and evaluated following precise rules, so that matrix elements (ME) can be calculated in powers of the strong coupling constant α_s . The factorial increase of Feynman diagrams with the number of outgoing partons makes it hard to have calculations at high order. Nevertheless, a complex $2 \rightarrow n$ process can be factorised into a simple core process, e.g. $2 \rightarrow 2$, convoluted with parton splitting probabilities to mimic a higher order process. Simulation programs implementing this approach are for instance PYTHIA [43] and Herwig [44, 45]. These use leading-order (LO) perturbative calculations of matrix elements of $2 \rightarrow 2$ processes and implement higher-order QCD processes approximately via the so-called initial- and final-state “parton showers” (PS) [36, 46] to produce the equivalent of multi-parton final states.

In a hard process with virtuality Q^2 , the incoming (outgoing) partons are expected to radiate a succession of harder (softer) gluons while approaching (retreating from) the collision. The emission ratio for a branching such as $q \rightarrow qg$ diverges when the gluon either becomes collinear with the quark or when the gluon energy vanishes. Furthermore, the non-Abelian character of QCD⁴ leads to $g \rightarrow gg$ branchings with similar divergences. The third main branching $g \rightarrow q\bar{q}$ does not have the soft divergence. For next-to-leading-order (NLO) perturbative QCD MC programs, like SHERPA [34] and POWHEG [47], the parton shower needs to be matched to the ME⁵ calculation⁶ to avoid double counting of radiation generally modelled by a sequence of emissions that, starting from the scale where confinement becomes important, increase the virtuality in each emission until it matches the Q^2 of the hard process. Similarly, the final-state radiation is constituted by a sequence of emissions that decrease the virtuality of the partons until a lower cut-off is reached ($Q_0^2 \equiv \Lambda_{\text{QCD}}^2 \lesssim 1 \text{ GeV}^2$). Thus, the whole phase space is expected to be covered with a smooth transition from ME to PS. Below Q_0^2 , no further branchings are simulated. Perturbation theory ceases to be meaningful, and confinement effects and hadronisation phenomena take over. Different MC programs control the coherence of successive emissions by ordering them in terms of their transverse momenta ($p_\perp$) or angle with respect to the parton direction. In particular, PYTHIA and Herwig use shower models that are $p_\perp$ - and angular-ordered, respectively.

1.3.2 Underlying event

In addition to the hard interaction that is generated by the Monte Carlo simulation, it is also necessary to account for the interactions between the incoming proton remnants

⁴The transformations of the symmetry group do not commute in the case of the Quantum Chromodynamics and weak groups.

⁵The interfacing of matrix element calculations to PS is generally done using a matching procedure (MLM [48] or CKKW [49, 50]), that essentially relies on a slicing of the phase space where some region is constrained to be generated by the parton shower, whereas the rest is covered by the ME calculation (i.e., where the PS approximation has limitations).

⁶POWHEG is interfaced with other programs, PYTHIA or Herwig, to provide the parton shower and the hadronisation model (see section 1.3.3).

(MPIs). This is usually modelled through multiple extra $2 \rightarrow 2$ scattering, occurring at a scale of a few GeV. The modelling of the underlying event is crucial in order to give an accurate reproduction of the energy flow that accompanies hard scatterings in hadron colliders. The UE can include additional hard interactions and soft processes which can not be calculated perturbatively. These are modelled with adjustable parameters which are tuned to experimental data.

1.3.3 Hadronisation

As the evolution reaches $Q_0^2 \equiv \Lambda_{\text{QCD}}$, the parton shower phase is truncated since the coupling forces become significant and confinement takes place. This phenomenon cannot still be described from first principles, and therefore, it involves some modelling to transform all the outgoing coloured partons into colourless hadrons of a typical 1 GeV mass scale. The dynamics of this evolution is generally absorbed in fragmentation functions that represent the probability of a parton to fragment into a certain hadron of the final state. Many of these primary hadrons are unstable and decay further at various timescales. Those that are sufficiently long-lived have their decays visible in the detector, or they are stable. There are several models of the hadronisation process that attempt to connect the results of the parton shower and the final particle spectrum observed. These models can be complemented and tuned using experimental observations. The hadronisation is commonly described by either the Lund string fragmentation model [51] (as implemented in PYTHIA), or the cluster fragmentation model [52] (as implemented in nd SHERPA⁷). Essentially, the Lund string fragmentation model assumes a linear confinement, where the energy stored in the colour field between quarks and antiquarks is assumed to increase linearly with the separation of colour charges. Thus, it depicts the colour force by means of a linearly rising potential as charges separate. The potential energy stored increases as partons move away, so it may break up by the production of new quark-antiquark pairs that screen the endpoint colours. Then, quarks and antiquarks may combine to produce hadrons. The cluster fragmentation model is based on the colour preconfinement property of the branching processes, which assumes that the separation of the colour charges forming a singlet are inhibited. After the perturbative parton branching process, the remaining gluons are splitted into light $q\bar{q}$ pairs, and then neighbouring quarks and antiquarks can be combined into colour singlets (colourless “clusters”), with masses distributions peaking at low values and asymptotically independent of the hard subprocess scale.

1.3.4 Tunes

Due to the non-perturbative, and therefore incalculable, nature of much of the soft physics processes, like the shower approximations, hadronisation and underlying event, MC generators inevitably contain a number of free parameters. These different parameters are usually tuned with data from colliders. A specific set of chosen parameters for a MC generator is referred to as a *tune*.

Two ATLAS PYTHIA tunes are used for event simulations in this thesis: the A14 tune [53] for the hard interaction and the AU2 tune [54] for pile-up collisions. The A14 tune is based on the MONASH tune [55] of the PYTHIA authors which uses e^+e^- collision data for the hadronisation parameters, and minimum bias pp collision data at LHC to constrain parameters sensitive to initial state radiation and the underlying event. The A14 tune

⁷SHERPA can use its own hadronisation model or be interfaced to PYTHIA.

uses in addition a large variety of ATLAS data sensitive to multiple parton interactions and ISR/FSR, and includes jets built from tracks and variables sensitive to the internal jet structure. The AU2 tune targets the PYTHIA parameters sensitive to the modelling of minimum bias pp collisions and is based on tracks and calorimeter clusters information.

1.3.5 Detector simulation

In order to use events⁸ produced by Monte Carlo generators to model particle collisions that one might observe with the detector, the output of these generators is passed through a detector simulation [56]. ATLAS uses the GEANT 4 [57] toolkit. GEANT 4 is an extensive particle simulation package that governs all aspects of the propagation of particles through detectors, based on a description of the geometry of the detector components and the magnetic field. The physics processes include, among others, ionisation, Bremsstrahlung, photon conversions, multiple scattering, scintillation, absorption and transition radiation. The last step involves the digitalisation, which simulates the detector outputs in the same format as the actual raw data.

The detector is described in terms of almost 30 million volumes with properties, which in case of the ATLAS detector (described in section 2.2) are constructed based on two databases: the geometry database and the conditions database. The former contains all basic constants, e.g. dimensions, positions and material properties of each volume. The latter is updated according to the circumstances at a given time and contains for instance dead channels, temperatures and misalignments. As a result, several layouts of the detector are available. Test beam data taken with components of the ATLAS detector before completion have aided the validation and further improvement of the detector simulation. Due to the detailed and complicated geometry of ATLAS and the diversity and complexity of the physics processes involved, the consumed computing time per event is large ($\mathcal{O}(1 \text{ hour})$).

⁸An event refers to the results just after a particle collision, occurring in a very short time span, at a well-localised region of space. Here, the meaning of an event is different from the one used in the theory of relativity, in which an “event” is a spacetime coordinate.

Chapter 2

The ATLAS experiment

“If I have seen further it is by
standing on the shoulders of Giants.”

Isaac Newton

2.1 The Large Hadron Collider

The Large Hadron Collider (LHC) [2] at the European Organization for Nuclear Research (CERN) is the most advanced and powerful particle collider ever built. It is located 100 metres underground below the border between France and Switzerland and installed in the 27-kilometre circular tunnel that housed the Large Electron Positron (LEP) collider until the year 2000. The LHC is a precision instrument capable of colliding energetic beams of protons (or heavier nuclei) at energies ranging between 45 GeV and 13 TeV. The precision and high beam energy make the LHC an extraordinary tool to explore the tera-electronvolt (TeV) scale, an energy range never before achieved in controlled collider experiments for elementary particle physics, particularly promising for searches of new physics. It has also been crucial for the discovery of the Higgs boson and a stunning amount of new and high-precision measurements.

2.1.1 Machine design

The LHC has been originally designed to produce head-on collisions between beams of protons at a centre-of-mass energy ($\sqrt{s}$) of 14 TeV. An unexpected technical incident took place on September 2008 [58] delaying the LHC’s physics programme and forcing to operate below the design specifications at $\sqrt{s}=7$ TeV during the first years (2010-2011) and at $\sqrt{s}=8$ TeV during 2012. The period of data-taking from 2010 to 2012 is commonly known as “Run 1”. During 2013 and 2014, the LHC entered for the first time of its life, a period named “Long Shutdown” (LS1). Even though there were no collisions during LS1, large-scale work was going on under way to modernise the infrastructure and prepare the machine to operate at higher energy. In 2015, the LHC started its second run of data-taking, known as “Run 2”, operating at $\sqrt{s}=13$ TeV [59]. This period finished at the end of 2018, leading to the second “Long Shutdown” (LS2) that will end at the beginning of 2021 with the start of “Run 3”, yielding the same centre-of-mass energy achieved in

Run 2 but increasing the luminosity (see sec.2.1.2) four times with respect to the previous data-taking period.

The LHC ring is the last shackle in a series of intermediate accelerators, some of which have been operating for decades, that successively increase the energy of the protons. They are first extracted from a simple bottle of hydrogen gas, which is stripped from its electrons with an electric field, and directed into Linac2. This first step is a linear accelerator, and the resulting 50 MeV beam is injected into the Proton Synchrotron Booster (PSB), which accelerates the protons to 1.4 GeV. Then, the Proton Synchrotron (PS) further increases the energy to 25 GeV, and finally the Super Proton Synchrotron (SPS) produces the beam which will be injected into the two LHC beam pipes at 450 GeV. Up to this stage, all protons flow in the same direction, but the injection to the LHC ring occurs in two points resulting in two contra-rotating beams.

The LHC contains two adjacent, high-vacuum beam pipes (maintained to an impressive pressure of 10^{-13} atm) running in parallel throughout all the ring, except for some discontinuities in the vicinity of the interaction points where the beams cross. The bending of the proton beam into a nearly circular trajectory is primarily driven by 1232 dipole superconducting magnets designed to operate at 11.08 kA, generating a magnetic field of 8.3 T necessary for 6.5 TeV proton beams. These magnets are cooled down to 1.9 K (colder than the 2.7 K of outer space) by liquid-helium vessels for proper operation at the superconducting state. A large series of smaller quadrupole, sextupole, octupole, and decapole magnets provide beam shaping to counteract Coulomb repulsion of the proton aggregate by squeezing the beam in its transverse plane. Beam acceleration within the LHC occurs in eight radiofrequency (RF) resonant cavities per beam where the electromagnetic field oscillates at a frequency that is a multiple of the protons revolution frequency (f_{rev}). Charged particles passing through the cavity are accelerated or decelerated by the electromagnetic force until becoming synchronised to the oscillating field in the cavity. The net effect is that protons tend to be grouped in tight bunches of tens of centimetres long each. Each bunch contains approximately 1.15×10^{11} protons, that ensure high instantaneous luminosity at the collision points and hence maximise the number of collisions. Not all stationary regions of the RF potential (known as “buckets”) are occupied, only every 10th bucket is treated as a possible bunch slot. There are 3564 possible bunch slots.¹ During Run 2, the bunches were separated by a time of 25 ns. As a consequence of the SPS and LHC injection strategy, the bunches are organised in “bunch-trains”. The number of bunches per bunch-train and the separation (empty bunches) between bunch-trains is different for each data-taking period and tend to vary during data-taking. In addition to organise protons longitudinally along the beam, once a stable time structure has been achieved the frequency of the cavities is slowly increased to transfer power to push the protons forward along the accelerator. This process is called synchrotron acceleration. Each cavity delivers 2 MV (an accelerating field of 5 MV/m) at 400 MHz, and is kept at 4.5 K. Plateau energy is reached in around 15 minutes. Both beams traveling in opposite directions are squeezed and focused at four intersection points where the detectors are placed: the multipurpose ATLAS [1] and CMS [60] experiments, and two other dedicated detectors ALICE [61] and LHCb [62] for heavy ion and b -physics experiments respectively. The picture shown in figure 2.1 presents the accelerators previously mentioned, as well as other accelerators that are connected to the LHC complex and the many experiments which rely on the complex for data-taking. In particular, the four main LHC experiments

¹The exact number of possible bunch slots is obtained when considering the exact LHC perimeter, 26.659km, and 24.95 ns as bunch time separation, usually approximated to 25ns.

mentioned above.

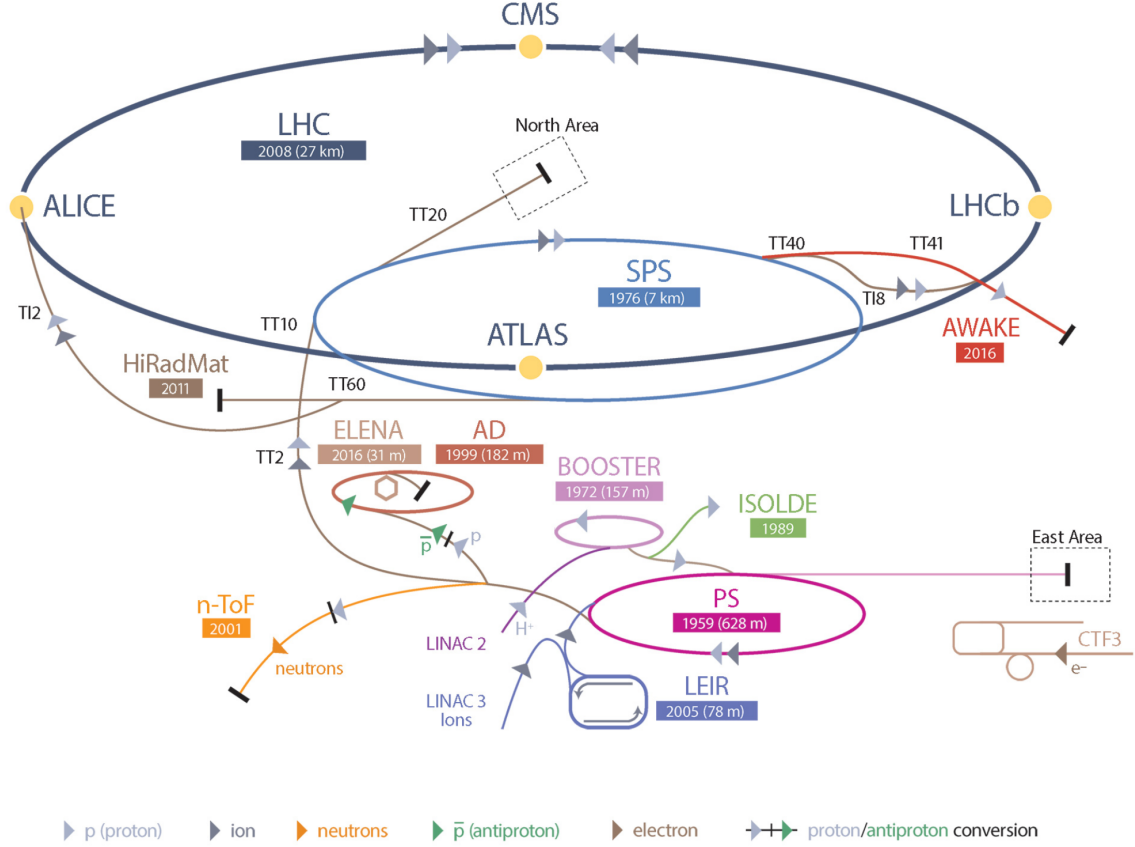


Figure 2.1: Schema of the CERN accelerator complex, showing the LHC together with its pre-acceleration stages, as well as other independent projects. The first year of operation and the length of each accelerator is indicated under its name, and the type of particle is indicated by the colour. Several experiments are indicated as well, in particular the four main experiments at the LHC. Image taken from ref.[63].

2.1.2 Machine operation during Run 2

The rate of production of a certain process i is directly related to the cross-section $\sigma_{pp \rightarrow i}$ and the LHC capability to put the protons into close contact, as encoded by the instantaneous luminosity L_0 . Formally the rate is expressed by

$$\mathcal{R}_i = L_0 \sigma_{pp \rightarrow i} \quad (2.1)$$

where the cross-section is a purely physical magnitude (calculable from scattering amplitudes), whereas the luminosity depends exclusively on the beams optics. It can be expressed by

$$L_0 = n_c f_{rev} \frac{N_1 N_2}{4\pi \sigma_x^* \sigma_y^*},$$

where n_c is the number of colliding bunch pairs, N_b is the number of protons per bunch in the beam b , and $\sigma_{x,y}^*$ are the transverse sizes of the beam at the interaction point. Clearly the luminosity -and by inheritance the production rate- increases as bunches have

more protons, more bunches crossings occur (either because there are more filled bunches in the pipe or the crossings are more frequent) or if the beams are more collimated at the interaction points reducing the transverse spread of protons. As a consequence, the observation of unlikely scattering processes with small cross-sections requires to maximise the delivered instantaneous luminosity, which is in turn limited by the machine performance and protection thresholds. The timeline of peak luminosity as measured on-line during the 2018 data taking period is shown in figure 2.2a. The time integrated luminosity $L_0^{int} = \int L_0 dt$ along Run 2 is shown in figure 2.2b.

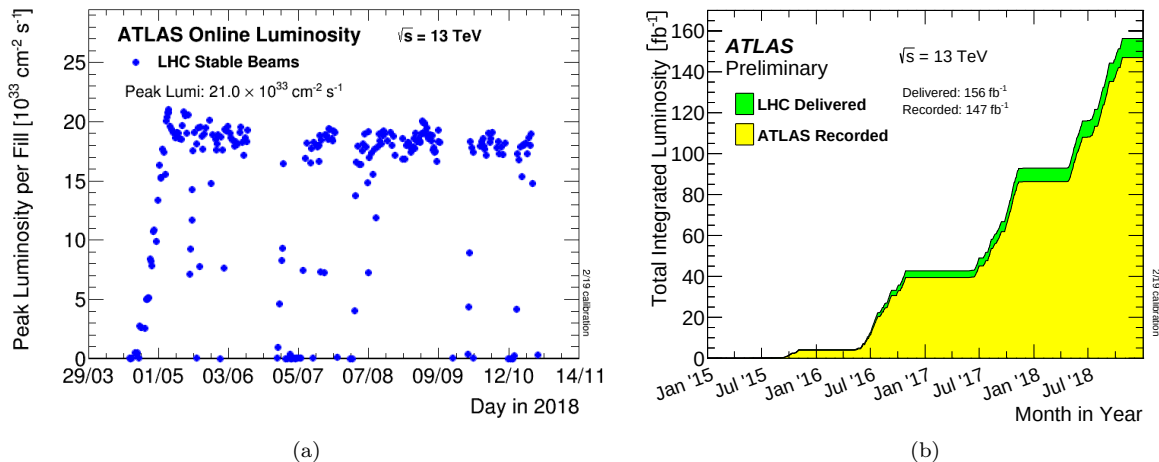


Figure 2.2: (a) The peak of instantaneous luminosity delivered to ATLAS for each LHC fill as a function of time during stable beams for pp collisions at $\sqrt{s} = 13 \text{ TeV}$ for 2018 data-taking period, and (b) the cumulative luminosity versus time delivered to (green) and recorded by ATLAS (yellow) during the whole period of stable beams for pp collisions at $\sqrt{s} = 13 \text{ TeV}$. Images taken from ref.[64].

A pp collision is in essence a stochastic process. As such the high luminosity not only enhances the probability of a single pp scattering but also increases the likelihood for multiple pp collisions per bunch crossing. The average expected number of inelastic collisions per bunch crossing is referred to as $\langle \mu \rangle$. This variable follows a Poisson distribution whose mean is dependent on L_0 by virtue of equation 2.1. Beam optics and bunch parameters at the interaction points can change across different periods of data-taking resulting in clear changes of the luminosity of the machine. Therefore, the underlying Poisson distribution can be shifted towards higher or lower values of $\langle \mu \rangle$ as shown in figure 2.3 for Run 2.

In general, in each bunch crossing there is only one hard-scatter process that usually triggers the event (see section 4.2.2), while the remaining inelastic interactions contribute to soft additional deposition of energy in the detector that blur the resolution of the hard process of interest. This phenomenon is called *pile-up* and it can occur in two forms. The first one coming from the multiple pp collisions happening in the same bunch crossing and known as “in-time” pile-up. In-time pile-up conditions can be reasonably estimated by the number of primary vertices NPV, as measured using the tracking system in ATLAS (section 2.2.3). The second form is a consequence of the short time separation between subsequent bunches (25 ns in Run 2). Due to the long time taken to produce and read-out the electronic signal in some sub-detectors, pp scatterings from a given bunch crossing can affect the signal shape of future bunch crossings. This case is called “out-of-time” pile-up.

The Run 2 pp programme started effectively on June 3rd 2015 when the LHC shift crew declared “stable beams” as two 6.5 TeV proton beams were brought into collision at the LHC’s four interaction points. The pp data-taking continued until November 3rd. The

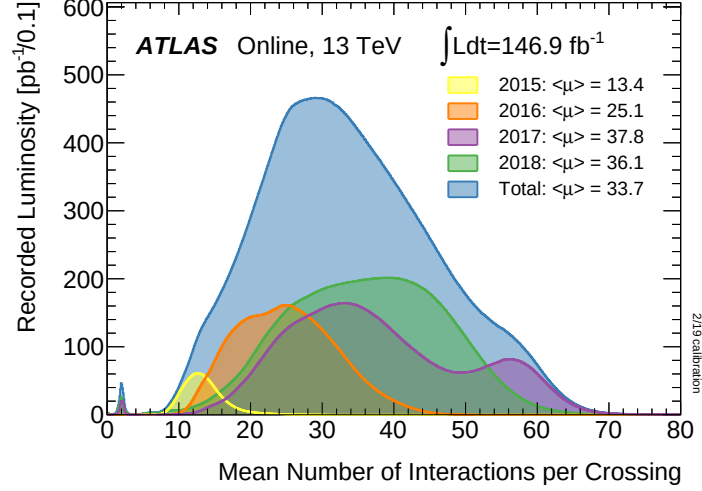


Figure 2.3: Luminosity-weighted distribution of the mean number of interactions per crossing for the 2015 to 2018 pp collision data-taking period at $\sqrt{s}=13$ TeV. The mean number of interactions per crossing corresponds to the mean of the Poisson distribution on the number of interactions per crossing calculated for each bunch. The different LHC configuration conditions over the years result in overlapping poissonian distributions with different means. More details on this can be found in ref.[64].

2016 data-taking period occurred from 22 April to 26 October, while the 2017 period took place from 29 April to 4 December; and the 2018 one from 28 April to 3 December. The instantaneous luminosity peaks reached for each year of Run 2 data taking are summarised in table 2.1. All numbers are close to the design value of $1034 \text{ cm}^{-2}\text{s}^{-1}$. Also the average number of pp collisions per bunch crossing ($\langle\mu\rangle$) are shown in the table.

Period	Peak of instantaneous luminosity [$\text{cm}^{-2}\text{s}^{-1}$]	$\langle\mu\rangle$
2015	5×10^{33}	13.4
2016	13.8×10^{33}	25.1
2017	20.9×10^{33}	37.8
2018	21×10^{33}	36.1

Table 2.1: Instantaneous luminosity peaked for each data-taking period during Run 2 and it respective average number of pp collisions per bunch crossing. More details can be found in ref.[64].

The average efficiency throughout the whole Run 2 ATLAS data-taking period was of 95.6%, corresponding to a delivered integrated luminosity of 153 fb^{-1} and a recorded integrated luminosity of 146 fb^{-1} . Runs with specialized physics goals are not included. Dedicated luminosity calibration activities during LHC fills used 0.6% of recorded data in 2018 and are included in the inefficiency. Trigger specific data quality problems (0.4% inefficiency at Level-1) are included in the overall inefficiency also.

The search for localised excesses in events with low dijet mass distributions produced in association with a photon presented in this thesis is based on data collected from 2015 to 2017 data-taking period. Only data collected during stable beam periods in which all sub-detectors were fully operational are used. A brief description of the ATLAS detector and its sub-systems is given in the next section.

2.2 The ATLAS detector

ATLAS (A Toroidal LHC ApparatuS) is one of the multi-purpose detectors at the LHC. It spans over 44 m in length and 25 m in height and it weighs 7000 t. It is located in one of the intersection points at the LHC and is composed of many sub-systems as illustrated in figure 2.4. The detector presents a forward-backward symmetric cylindrical geometry with nearly 4π coverage in solid angle, and consists of three primary detection systems layered radially upon each other:

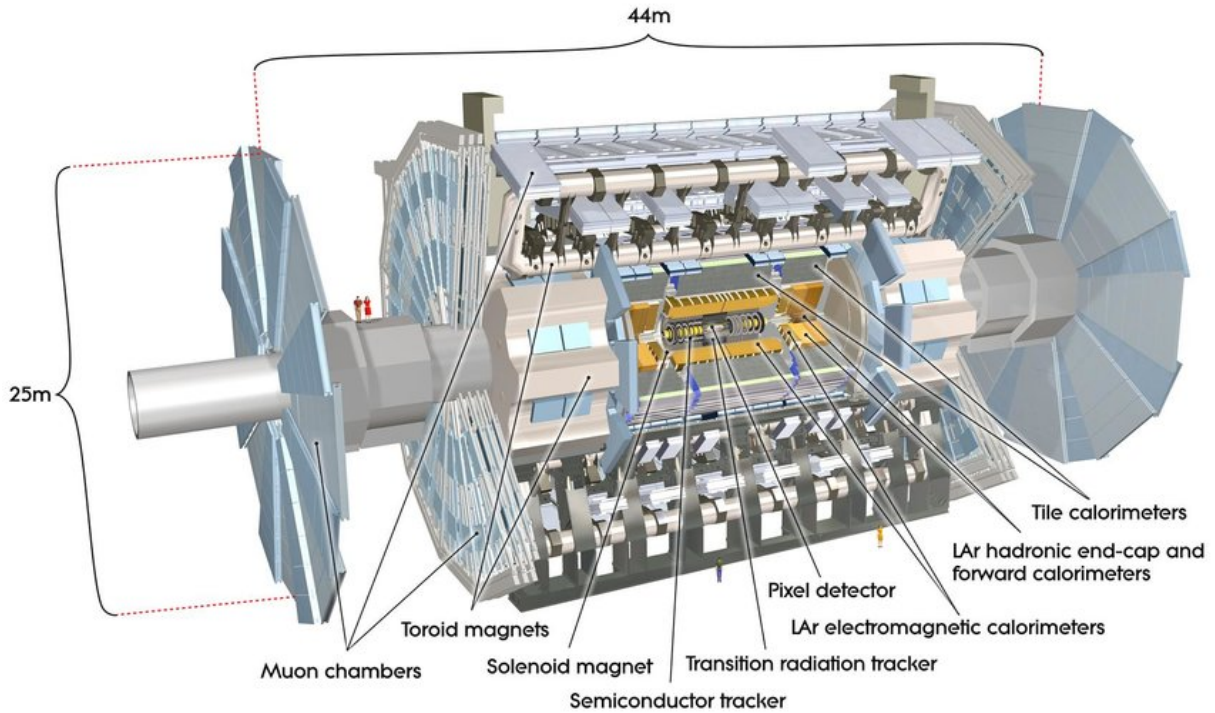


Figure 2.4: Computer generated sketch of the ATLAS detector. The different subdetectors and magnet systems are labelled, and two persons are presented for scale purposes.

Central inner tracker which is used to measure the position and momentum of charged particles and is embedded in a powerful magnetic field. Since vertex identification requires high resolution track reconstruction, the tracking system is inserted as close as possible to the interaction point in order to minimise the large extrapolations (see section 2.2.3).

Calorimeter system that determines the energy of both neutral and electrically charged particles. It has a large volume and is made of materials that guarantee a large number of radiation and interaction lengths. Ideally, particles are completely absorbed within the calorimeter(s) volume and their energy is measured as the sum of the energy deposited by the showered products of the original particles (see section 2.2.4).

Muon spectrometer located within a large toroidal magnetic field, it allows to measure the position and momentum of muons (see section 2.2.5).

A common factor to all sub-systems forming ATLAS is that they have to resolve physics signals and correctly identify different fundamental particles emerging from the collision spot at enormous rates, and be radiation resistant to survive the harsh environment [65]. Each sub-system is uniquely designed to detect the energy signature of passing leptons, photons, and hadrons.

Another difficulty, consequence of the huge amount of collisions per second, is the computing power and network speeds needed to transfer the information collected at the detector, convert the measured electric pulses into physical entities (reconstructed physical objects) and store the information. The following sections are intended to provide a brief overview of each of the ATLAS sub-systems and of its trigger and acquisition system. A complete description of the experiment can be found in the technical design report[1].

2.2.1 Coordinate system

The coordinate system used in ATLAS is a right-handed Cartesian system centred at the nominal interaction point (IP), the geometric centre of the detector. The z -axis lies along the beam line, while the transverse x - y plane is defined with x pointing towards the centre of the LHC ring and y points upwards. The direction of positive z (counter-clockwise in the LHC ring when viewed from above) is denoted as side-A of the detector and side-C is the one with negative z . The azimuthal angle ϕ is measured around the beam axis, and the polar angle θ is obtained from the beam axis. Since the momentum of the colliding partons along the z -axis is unknown, it is useful to define the transverse component of variables of interest, like energy and momentum, defined as the projection on the x - y plane, which are boost-invariant along the z -axis:

$$E_T = E \sin \theta \qquad p_T = p \sin \theta$$

Accordingly, another commonly used variable is the rapidity (y), because it is boost invariant along the z -axis. It is an angular variable dependent on θ as

$$y = \frac{1}{2} \ln \left(\frac{E + p_z}{E - p_z} \right) \quad (2.2)$$

and is defined in terms of energy (E) and momentum projection along the z -axis (p_z). Even more common than the rapidity, it is the use of the pseudorapidity

$$\eta = -\ln \tan(\theta/2) \quad (2.3)$$

which is equal to the rapidity for massless particles, but in a general case it is only a function of a geometrical variable which is really practical to immediately match the position of a particle with a given sub-detector in the same η range.

The distance between two points (either calorimeter cells, or reconstructed objects) in the rapidity-azimuthal angle space is defined as

$$\Delta R(1, 2) = \sqrt{(\eta_1 - \eta_2)^2 + (\phi_1 - \phi_2)^2} \quad (2.4)$$

2.2.2 Magnet system

The measurement of charged particles momenta is based on their deflection in a magnetic field. The magnet system displayed in the sketch of figure 2.5 represents a particular

characteristic of the ATLAS experiment, largely defining its size and layout. This system is 22 m in diameter and 26 m in length, and it is composed of four large superconducting magnets: a central solenoid and three open-air toroids, designed to provide a field mostly orthogonal to the particle trajectory. The central solenoid surrounds the Inner Detector and provides a magnetic field parallel to the beam axis bending charged particles in the ϕ direction. At the IP the value of the magnetic field is 2 T and it remains constant in the radial direction. As the distance from the IP increases in the z direction, the field strength decreases as a result of the finite size of the solenoid. The toroid system produces the field needed by the muon spectrometer to deflect particles in the η direction: two end-cap toroids at the two extremes of the detector and a barrel toroid centrally located around the calorimeters. Each toroid is composed of eight independent coils equally distributed in the azimuthal plane. The barrel toroid generates a magnetic field of 3.9 T while the end-cap produces a field of 4.1 T.

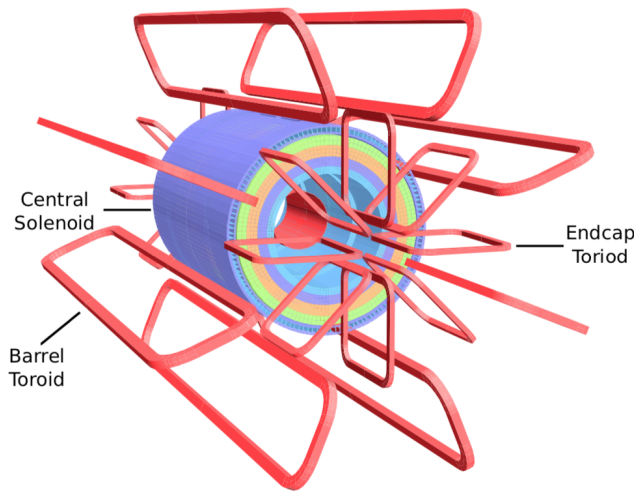


Figure 2.5: Simple sketch for the geometry of ATLAS magnet system. Image taken from ref.[1].

2.2.3 Inner detector

The Inner Detector (ID) [66], the closest sub-detector to the IP, is a complex high precision tracking system aimed at reconstructing the tracks of charged particles. Tracks are also used, among other things, for vertex reconstruction and identification (see section 2.3.1). Combined with a solenoidal magnetic field of 2 T aligned with the beam line, tracks are used to measure the direction and momentum for particles having nominally $p_T > 500$ MeV. It has full ϕ coverage and reaches up to $|\eta| < 2.5$. It is divided in three different concentric subdetectors, as can be seen in the sketch in figures 2.6a and 2.6b. The detector design required fast response electronics, good radiation resistance and reducing to a minimum the amount of material to be placed in front of the calorimeters to avoid degrading the energy measurement.

The ID components are described next from the most inner one to the most external one.

Silicon pixel detector. The part of the detector closest to the IP is the silicon

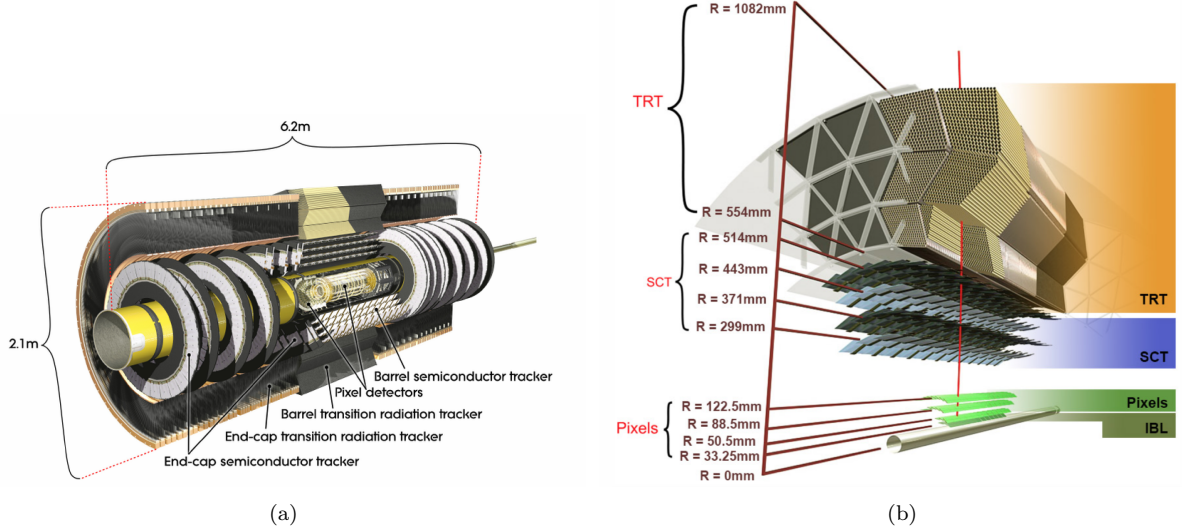


Figure 2.6: Cut-away view of the ATLAS inner detector. Image from ref.[1].

pixel, composed of four concentric barrel layers of $50 \mu\text{m}$ by $400 \mu\text{m}$ semiconducting pixels. Three additional disks at each end-cap are settled at distances of 495, 580, and 650 mm from the IP along the beam direction. A new pixel layer (insertable b -layer, or IBL) was inserted only 50.5 mm away from the collision point during LS1 [67], and it allows for the reconstruction of secondary vertices associated with the production of long-lived particles. This information is very useful to identify jets originating from the fragmentation of b -quarks. It contains a total of approximately 92 million pixels.

Semi-conductor tracker (SCT). The following layer implements long, narrow silicon strips making the coverage of a larger area more economical in terms of the number of channels. The physical principle is the same as for the pixel detector; ionizing particles traversing the semiconductor produce electron-hole pairs whose currents are read out by the front-end chips, providing a binary response: a “hit” is registered only if the pulse height in a channel exceeds a preset threshold. There are 4088 SCT modules, each composed of two single-sided 64mm silicon strip sensors attached to one another with a 40-mrad angular pitch to provide two-dimensional hit localisation. The SCT operates in the same environment conditions as the pixel detector at approximately -10°C to reduce the leakage current. The SCT is divided into four concentric barrel layers ($|\eta| < 1.1$) and nine end-cap disks ($1.1 < |\eta| < 2.5$) at each side. The disks are placed at a distance between 934 and 2720 mm from the interaction point along the beam direction. This system provides a total of approximately 6.3 million channels.

Transition radiation tracker (TRT). It surrounds the silicon detectors providing measurements of charged particles up to $|\eta| = 2.0$. It consists of proportional 4 mm diameter drift gaseous tubes (straws) arranged longitudinally in up to 73 layers in the barrel ($|\eta| < 1.0$) and 160 radial straw planes in each end-cap ($1.0 < |\eta| < 2.0$). The barrel straws span over 1440 mm in length and are further arranged into three cylindrical groups divided in 32ϕ sectors. There are 52544 axially oriented tubes in the barrel. End-cap TRTs have 122880 straws, each of 370 mm long. In total, there are approximately 350000 readout channels. Drift tubes are filled with a Xenon- CO_2 - O_2 gas mixture that is ionized upon the passage of charged particles. Ions within the gas drift to the straw wall (acting as

a cathode) and towards a tungsten (gold-coated) wire running inside the tube (that acts as an anode) due to a large electric potential of -1530 V applied between the wall and the wire. Under normal operating conditions, the maximum electron collection time is ~ 48 ns. In addition, the barrel drift tubes are embedded in a matrix of polypropylene fibers that aid in electron identification via transition X-rays produced when charged particles cross inhomogeneous materials. In the end caps, the transition radiation is generated by foil interleaved between the straws.

2.2.4 Calorimeters

The ATLAS calorimeter is the central piece of the detector, spanning full ϕ -symmetry and a pseudorapidity range of $|\eta| < 4.9$. Broad coverage allows an adequate reconstruction of the energy of the event, and in particular helps to accurately determine the missing energy in physics processes where weakly interacting particles are expected, such as neutrinos. The calorimetry system is composed by two different subdetectors: an electromagnetic and a hadronic calorimeter. Both divided into a central barrel with finer granularity and two symmetric, more coarse end-caps, as shown in figure 2.7. They are segmented into towers in η and ϕ which point towards the centre of the detector. Both are *sampling* calorimeters, meaning that intercalated layers of absorber and active materials are used to induce particle showers, absorbing most of its energy and producing a signal proportional to the deposited energy [68]. They are also *non-compensating* calorimeters, which means that hadrons, that interact strongly with the nuclei in the active material, will have a lower response than particles of the same energy that have a predominantly electromagnetic interaction [14].

Minimising the resolution of the energy response is essential to providing an accurate measurement of particle energy. The fractional calorimeter resolution as a function of energy is described as:

$$\frac{\sigma_E}{E} = \frac{N}{E} \oplus \frac{S}{\sqrt{E}} \oplus C$$

where N is a measurement of the noise, dominant at low energies, arising from background and electronics, S parametrises the stochastic uncertainty due to the random sampling of the active and passive materials, and C is a constant term, dominant at higher energies arising from non-uniformities in the detector. These terms are added in quadrature to derive the fractional resolution.

Construction details for each calorimeter system are described next.

Electromagnetic Calorimeter (ECAL). It is the innermost type of calorimeter. The central barrel covers the range up to $|\eta| < 1.475$, and the end-caps extend it to $1.375 < |\eta| < 3.2$. It uses liquid argon (LAr) as active material, and therefore must be contained within cryostats kept at 89 K using liquid nitrogen. LAr was chosen for its intrinsic linear behaviour, high ionization yield, stability and radiation hardness. The absorber material is lead both in the central barrel (EMB) and end-caps (EMEC). The absorber plates are shaped into accordions and oriented in the radial direction allowing for a full symmetric coverage without cracks in the azimuthal direction, as shown in the sketch in figure 2.8a. The ECAL is segmented into three layers and spans a total thickness of 22 to 33 radiation lengths (X_0), increasing with η . The span in the end-caps is 24-38 X_0 . This allows to fully contain electrons of energies up to a few TeV. The first layer,

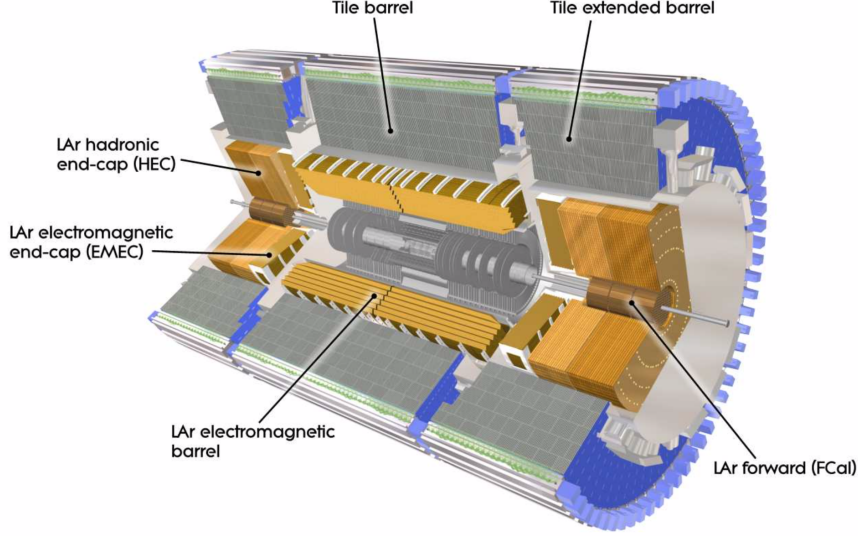


Figure 2.7: Computer simulated view of the ATLAS calorimeter system. Image from ref.[1]

with a thickness of $4.3 X_0$, is finely divided into segments of $\Delta\eta \times \Delta\phi = 0.003 \times 0.01$ in order to measure precisely the direction in pseudorapidity of the particles. The strip layer is of particular importance for photon and electron identification and, combined with the information from the second layer, can be used to obtain precise information on the photon's production vertex. The second layer is $16 X_0$ thick, it represents most of the thickness of the calorimeter and absorbs about 80% of the energy in electromagnetic showers. It is divided into towers, each of size $\Delta\eta \times \Delta\phi = 0.25 \times 0.25$ forming a 3×7 matrix. The third layer is just $2X_0$ thick, and has coarser granularity, as the towers measure $\Delta\eta \times \Delta\phi = 0.05 \times 0.0245$. It is mainly used to estimate the amount of energy lost beyond the ECAL. In the central region an additional pre-sampler layer is present. The information from this layer can be used to estimate the energy lost by the electron or photon in the passive material of the solenoid (and cryostat) that surrounds the ECAL. More details can be found in the technical design report [69].

Hadronic Calorimeter The hadronic calorimeter surrounds ECAL, and comprises three different types of calorimeters according to the different radiation conditions and resolution requirements. The Tile Calorimeter (TileCal) can be found in the central area. It consists of a central barrel section (LB) covering the $|\eta| < 1.0$ region and two extended barrels (EB) covering $0.8 < |\eta| < 1.7$, which use a polystyrene scintillator tile as the active material and steel plates as the absorber medium. Each structure is divided into 64 wedges of $\Delta\phi \sim 0.1$ for full azimuthal coverage, that go from 2 m from the IP to 4 m, measuring 2 m in the radial direction. A wedge is in itself divided into different sized cells, going from 0.1×0.1 to 0.2×0.2 as the distance to the IP increases. The sketch in figure 2.8b shows the structure of one of these TileCal modules. The photomultiplier tubes (PMTs) used to collect the signal can also be appreciated on the top of the module, in the electronics rack. The signal is collected by wavelength-shifting (WLS) fibres that run on each side of every scintillator tile, and are then grouped so that each cell is read by two PMTs; the PMT is then linked to one read-out channel.

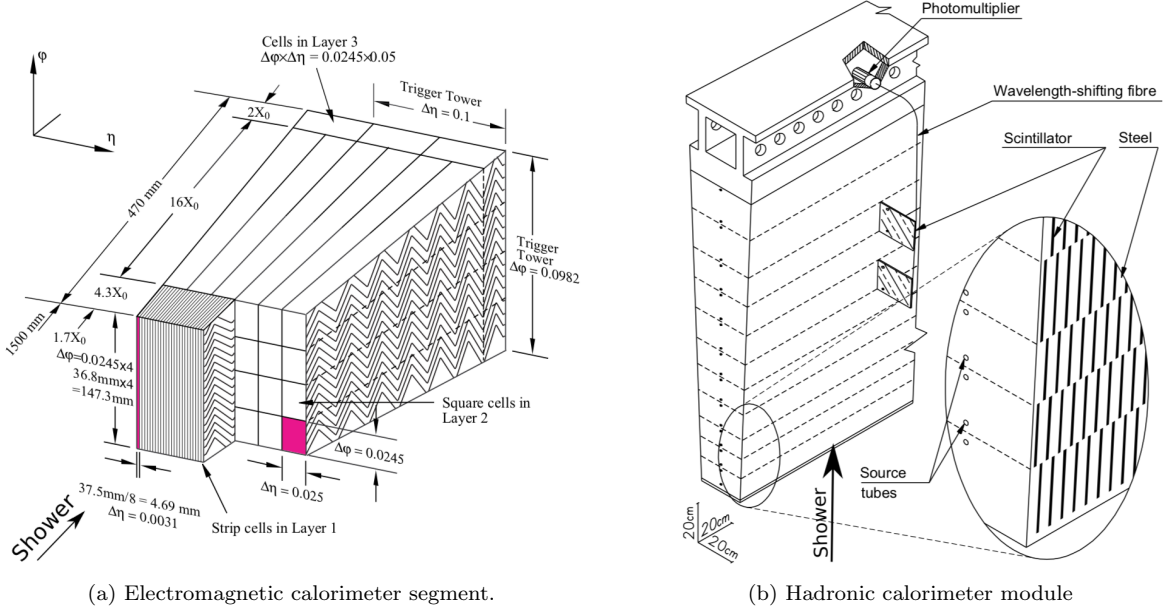


Figure 2.8: Sketches that detail the design of (a) a part of the barrel electromagnetic calorimeter and (b) a module of the tile calorimeter.

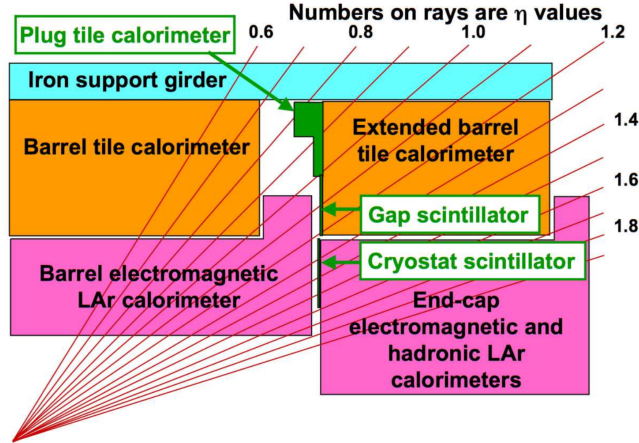


Figure 2.9: Schematic of the transition regions between the barrel and end-cap calorimeters, where additional scintillator elements are installed to provide corrections for energy lost in the inactive material.

The region between the LB and the EBs has a gap through which cooling and power supply services pass, and therefore is less instrumented. Some special detectors are located there in order to estimate the energy loss in this region. The gap scintillators cover the region of $1.0 < |\eta| < 1.2$, while the crack scintillators are installed on the front of the LAr end-cap and cover $1.2 < |\eta| < 1.6$.

There are two remaining hadronic calorimeters, both aimed at covering higher rapidity regions: the Hadronic End-Cap (HEC) and the Forward Calorimeter (FCal). They both use LAr as the active medium, like ECAL, but the absorber is copper in HEC and copper-tungsten in FCal. The material choice is due to the high radiation exposure in the region. HEC covers the range of $1.5 < |\eta| < 3.2$, with a granularity that increases with η . For

$|\eta| < 2.5$ its first two layers are divided into $\Delta\eta \times \Delta\phi = 0.1 \times 0.1$ cells, while the third one is 0.2×0.1 . For $2.5 < |\eta| < 3.2$ all the layers have the latter cell size. The Forward Calorimeter covers the most forward region ($3.1 < |\eta| < 4.9$), giving the ATLAS calorimeter its high hermeticity which allows to minimise the energy loss.

2.2.5 Muon spectrometer

The muon spectrometer (MS) is the most outer layer of the ATLAS subdetectors [70]. It is conformed by precision chambers that, combined with the magnetic field generated by the toroids, provide an accurate measurement of the muon momentum for the $|\eta| < 2.7$ region. It has been built using four different types of detector chambers, which are distributed differently in the barrel and end-cap regions, as can be seen in figure 2.10: the barrel consists of three cylindrical layers around the beam axis, one within each other and one on the inside of the toroid magnet; in the end-caps the chambers are arranged perpendicular to the beam, into discs. Different technologies were chosen following the resolution and timing requirements for precise measurements and triggering, as well as the large variation in particle flux with rapidity. Thus, the four types of chambers can be divided into precision chambers and trigger chambers.

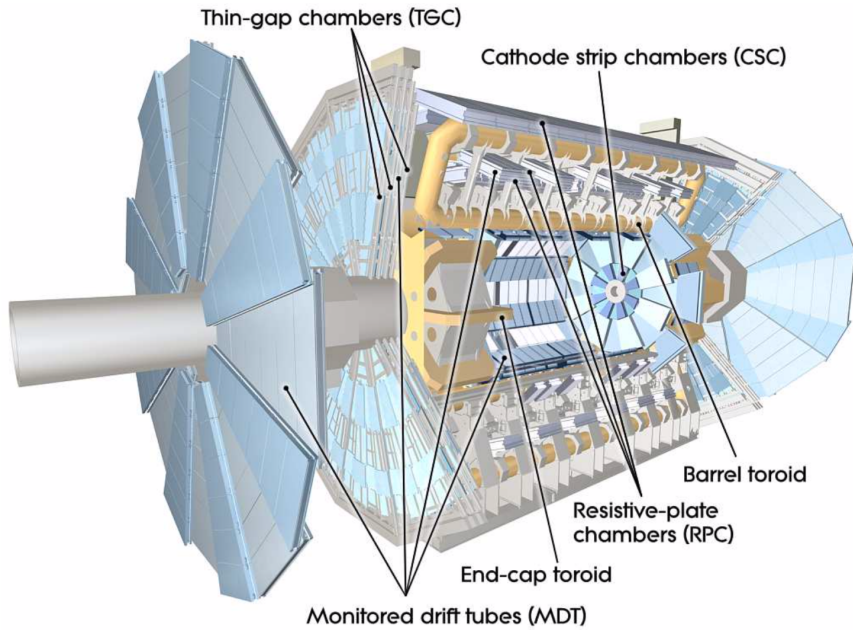


Figure 2.10: Computer generated sketch showing the different components of muon spectrometer. Image taken from ref.[1].

Precision Chambers One of the precision-type chambers are the monitored drift-tube chambers (MDT). Each chamber contains 6 to 8 drift tubes filled with a mixture of argon and carbon dioxide, while the wire within them is made of tungsten and rhenium that generates a radial electric field. A muon passing through a tube will ionize the gas, and the resulting electrons will drift towards the wire due to the potential applied. The spatial resolution achieved is $80 \mu\text{m}$ for each tube, $40 \mu\text{m}$ for a complete chamber, and $30 \mu\text{m}$ when the three layers of MDTs are taken into account. This allows for very good

track reconstruction and low number of fake tracks. These chambers are used to cover the largest area of $|\eta| < 2.7$ (2.0 in the inner layer). But around the area of $|\eta| < 2.0$, in the end-caps, the counting rate exceeds the MDTs operation limit of 150 Hz cm^2 , which is why the first layer is conformed of cathode strip chambers (CSC). Their operation limit is 1000 Hz cm^2 . They are multi-wire proportional chambers, with wires oriented in the radial direction within 2.5 mm of one another, and use the same gas mixture as the MDTs. The spatial resolution of the four layers of CSCs is $40 \mu\text{m}$ in the bending plane and 5 mm in the non-bending one. The maximum drift time for signal collection is 40 ns compared to the 700 ns of the MDTs, which gives the possibility to achieve higher acquisition rates.

Trigger Chambers A faster design is needed in the triggering chambers. The Resistive Plate Chambers (RPCs) follow a different concept, consisting of two resistive bakelite plates and a gas mixture in the middle. The electron avalanches are collected by two sets of orthogonal strips that provide position and time resolutions of 1 cm and 1 ns. The small time resolution allows for individual bunch-crossing discrimination, and these chambers provide the ϕ coordinate for the muon tracks since the MDTs can only measure the position in η . Similarly to the CPCs, the Thin Gap Chambers (TGC) are multi-wire chambers, but the wire-to-cathode distance was made smaller than the wire-to-wire distance to achieve smaller drift times. They cover the region of $1.05 < |\eta| < 2.7$ (2.4 for triggering) in the end-cap wheels. Their timing resolution is comparable to the RPCs, and they provide the position with a resolution between 2-7 mm for both coordinates.

2.2.6 Trigger and data acquisition

The pp interaction rate at the LHC is 40 MHz (proton bunches collide every 25 ns). Since the information coming from the ~ 100 million readout channels from all sub-systems constitute 1.6 MB of data per event, if no filtering is applied, this corresponds to a total recording rate near 60 TB/s. At this rate and due to limitations in processing power and storage in the data acquisition system², a continuous extraction of collision data is not feasible. In addition, the vast majority of processes of interest have smaller cross-sections than the inclusive collisions, dominated by low energy interactions, and therefore there is no practical reason to save the information of events which do not provide interesting physics. In addition, the cross-section is massively dominated by QCD interactions such as multijet production, whereas processes like Higgs boson production only contribute few *parts per trillion* to the total cross-section. This can be appreciated in figure 2.11, which shows cross-section predictions for different physics processes, obtained for $p\bar{p}$ and pp collisions.

Hence, a sophisticated system is needed for selecting and reconstructing events online efficiently (maximising the rejection of unwanted events while minimising the rejection of interesting events). The ATLAS Trigger and Data Acquisition (TDAQ) [74] system is a highly optimised network of hardware and software providing a solution to this problem. This trigger system is an essential component of the experiment as it is responsible to make (fast) the decision to whether or not select given bunch-crossing for later study. In Run 2, the TDAQ system consists of a hardware-based first-level trigger (L1) and a software-based high-level trigger (HLT) with a total rate of approximately 1.6 GB/s. The original design of the TDAQ system, utilised in Run 1, consisted on a three level

²The event data recording rate, based on technology and resource limitations, is of the order of 1 kHz [71].

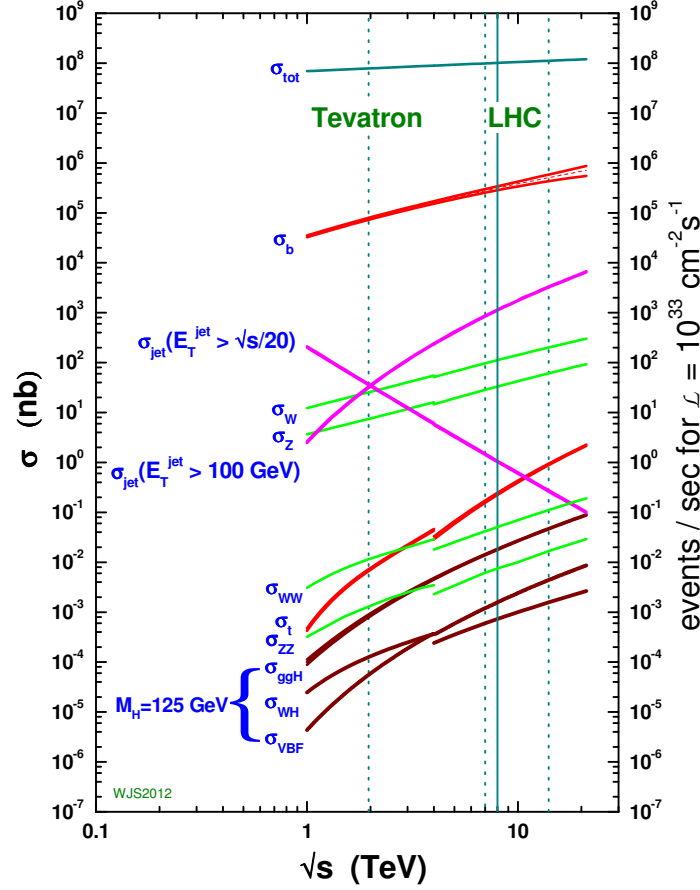


Figure 2.11: Cross sections from proton collisions as a function of centre-of-mass energy. The discontinuity between Tevatron [72] and LHC energies reflects the switch from $p\bar{p}$ to pp collisions. Image from ref. [73].

triggering system with a final recording rate of 960 MB/s, where the HLT consisted of separate Level-2 (L2) and Event Filter (EF) triggers. In Run 2, nearly all components received an upgrade, to maintain acceptably low p_T thresholds while dealing with increasingly challenging demands: increased centre-of-mass energy from 8 TeV to 13 TeV, increased pile-up, decreased bunch spacing interval from 50 ns to 25 ns, and increased instantaneous luminosity [71, 75]. In addition, L2 and EF triggers were merged into a single homogeneous system, the HLT, simplifying development and reducing the CPU and network consumption [76]. A comprehensive description of the Run 1 Trigger and Data Acquisition system of the ATLAS experiment can be found in ref.[77], while the performance of the Run 2 TDAQ system is detailed in ref.[71].

The L1 trigger consists of fast, custom-made electronics that can perform event selections using complex quantities such as missing transverse energy. It is capable of reducing the data rate from 40 MHz down to 100 kHz; however, it is built for speed rather than precision measurements.

The L1 trigger receives coarse measurements from the calorimeters and muon systems. Sums of calorimeter energy deposits from 7000 trigger towers are collected by the “L1Calo” trigger, while RPC and TGC track information is collected by the “L1Muon” trigger. Event data is buffered on detector-specific front-end electronics while the L1 trigger decision is being formed. Muon triggers at L1 are based on a coincidence of hits

among several layers of the trigger muon chambers. Electrons and photons are triggered on energy deposits in the EM calorimeter. Jet candidates are constructed at L1 from coarse calorimeter towers made of trigger-elements using a sliding window algorithm [78]. A trigger-element is defined as a sum of cells in a 0.2×0.2 ($\eta - \phi$) region, and a sliding window algorithm examines the total E_T against a trigger threshold value in a 4×4 region. Various criteria are used to decide which events pass the L1 trigger and the HLT, such as the p_T and η of reconstructed objects or the calculated missing E_T of an event (E_T^{miss}). For each set of criteria, unique trigger exists.

A “trigger menu” consisting of 512 “trigger items”, logical combinations of trigger inputs from L1Calo and L1Muon, is processed by the Central Trigger Processor (CTP) [79, 80] which produces a trigger decision within $2.5 \mu\text{s}$. The items in the trigger menu can be “prescaled” so that a predetermined fraction of events passing the trigger are randomly ignored, thereby reducing the overall rate. Triggers that are more stringent in their selection are unprescaled, and are able to save all passing events. The CTP is also responsible for limiting the time between L1 accepts (simple dead time) and a leaky bucket algorithm to limit the number of L1 accepts in a given number of bunch crossings (complex dead time) [81]. A detector may issue a “busy” signal to the CTP in order to signal that its buffers are full, preventing further L1 accepts until the busy signal is cleared. After the L1 trigger acceptance, the events are buffered in the ReadOut System (ROS) and processed by the HLT. The L1 trigger sends the η and ϕ coordinates which caused the L1 trigger to fire, the so-called “region of interest” (RoI), to the HLT.

The second level of the triggering system is the software-based HLT, which reduces the 100 kHz L1 rate to a final ~ 1 kHz event output rate, with an average latency (decision time) of 200 ms. The HLT has access to fine-granularity calorimeter information, precision measurements from the muon spectrometer, and tracking information from the ID, which are not available at L1. The HLT uses reconstruction algorithms and calibrations similar to those used offline. As needed, the HLT reconstruction can either be executed within RoIs (approximately 2% of the total event data) identified at L1 or for the full detector. In both cases the data is retrieved on demand from the readout system. Several (~ 2500) triggers are provided in a trigger menu, based on the number of objects, their transverse momentum, missing transverse energy, and certain identification and isolation criteria. As in Run 1, in order to reduce the processing time, most HLT triggers use a two-stage approach with a fast first-pass reconstruction to reject the majority of events and a slower precision reconstruction for the remaining events. However, with the merging of the previously separate L2 and EF triggers, there is no longer a fixed bandwidth or rate limitation between the two steps.

If an event is accepted, the data is stored to perform full offline event reconstruction (see section 4.2.1). The luminosity of the proton beams decreases steadily as collisions progress, causing data collection conditions to vary as a function of time. Data is therefore collected in time intervals of one minute, referred to as lumi-blocks. Each one is assigned an integrated luminosity depending upon detector and beam conditions over that lumi-block. They are also useful for isolating problematic data which may have been taken while a sub-detector was inoperative or malfunctioning, allowing their easy rejection during data analysis. ATLAS provides lists of lumi-blocks of “good” data for each data taking period known as Good Run Lists (GRL). Most events passing the HLT are written to the “main” physics stream, while a few events which require a larger processing time are saved to a “debug” stream for future reprocessing.

2.3 Object reconstruction & identification

The technical complexity of the accelerator and of the detector are necessary to study (and discover) fundamental particles and their interactions. But what actually happens at the femtoscopic level can only be inferred by studying the kinematics and nature of the particles that leave the collision. They, however, are not always directly observed or measured. For instance, a reconstructed object that we may identify with an *electron* (or more properly a *reconstructed electron candidate*) is actually a measurement of a shower of particles that hit the detector and has some likelihood of being initiated by an electron decay. To overcome this, ATLAS counts with a sophisticated reconstruction software that uses a wide variety of different algorithms to identify individual particles and jets from tracks and energy depositions recorded by the detector. As these algorithms greatly influence the efficiency and performance of the reconstruction process, they are under constant development.

The following section gives a short overview on how experimental observables are reconstructed from the information provided by the ATLAS sub-systems into objects that can be identified with physical particles.

2.3.1 Track and vertex reconstruction

Tracks are reconstructed using information of the inner detector (see section 2.2.3). The ID tracking algorithms cover two stages, the main track reconstruction, and the second stage of pattern recognition to find primary vertices.

Track reconstruction. It refers to the process of identifying individual charged particles coming from the interaction and measuring their traces in the inner detector. Such charged particles can be measured up to $|\eta| = 2.5$, which corresponds to the η coverage of the tracking system. It is possible to calculate the momenta of the charged particles with the curvature radius and the known magnetic field. This procedure is sub-divided in four stages (more details can be found in ref.[82]):

1. The initial step of the ID reconstruction consists of the cluster and drift circle creation and the transformation of clusters into 3D space points (seeds). Clusters are formed by finding connected cells in the pixel and strip detectors. A neural network is then used to identify and resolve merged clusters from close-by particles in dense environments. Also timing information from the TRT is converted into drift-circles.
2. Track seeds are identified from a combination of pixel and strip layer hits, requiring a total of three hits. They are processed by applying a set of thresholds as well as a combinatorial Kalman filter to form a combined particle track.
3. Ambiguities are resolved using a scoring function that applies positive scores for unique measurements and good fit quality, while penalising missing measurements where they would be expected (also called holes) or shared measurements with other track candidates.
4. Tracks within the TRT coverage that survive the ambiguity solver are extended and combined with the TRT tracking information. This step significantly increases the momentum resolution exploiting the longer lever arm for field integration.

The found measurements are then used in a track fit to estimate the track parameters. And combined with data about the magnetic field strength, they are used to measure the momentum of the particle associated to the track.

Vertex reconstruction. A “primary vertex” (PV) is known as the location where two protons collide. Primary vertices are reconstructed by matching up intersecting tracks, which proceeds in three main steps: seeding, track assignment, and fitting. A brief outline of the procedure is as follows:

- All reconstructed tracks satisfying certain criteria are extrapolated to the beam axis. The impact parameter (z_0), defined as the longitudinal distance at the point of closest approach, is computed for every track with respect to the nominal beam spot. This information is used to generate seeds, for which an iterative likelihood maximisation method is used.
- Tracks compatible with a seed are grouped together for fitting.
- An adaptive vertex fitting algorithm [83] is used to estimate the position and uncertainty of the vertex.
- Incompatible tracks not used in a previous vertex fit are used to repeat the procedure starting from the creation of a new seed.

The vertex with the largest $\sum p_T^2$ for all associated tracks is labeled as the hard-scatter vertex. All other reconstructed vertices are considered to be pile-up. The identification of vertices becomes more challenging as the average number of interactions per bunch crossing (pile-up) increases, and thus new algorithms are being developed to increase the resilience of ATLAS vertexing [84].

2.3.2 Electron reconstruction

Electrons are reconstructed by matching reconstructed tracks in the ID to clusters of EM calorimeter energy deposits, whose shower profile is consistent with an EM shower [85]. To build the EM cluster, a sliding window algorithm is used [78]. The window is a fixed-size grid of cells, $N_\eta \times N_\phi = 3 \times 5$, in the middle layer of the LAr calorimeter where approximately 80% of the energy of an EM shower is deposited. For each cell, the energy is summed across all the longitudinal layers, forming a tower. If the transverse energy of the towers in the window is above 2.5 GeV and is a local maximum, a seed cluster is formed.

Pattern recognition and track fitting algorithms are then used to match ID tracks to seed clusters. Track seeds from the ID with $p_T > 1$ GeV are tested against pion and electron pattern recognition algorithms, and are required to reside in a cluster seed. A track fit is performed twice to extrapolate the ID track to the calorimeter, using the track momentum or the cluster momentum, and is required to be near the cluster. If either succeeds, a final optimised track reconstruction is performed using a Gaussian Sum Fitter (GSF) [86].

An electron candidate is formed if there is at least one ID track matched to the seed cluster. The EM cluster is then rebuilt by summing energy in a grid of 3×7 (5×5) cells in each layer of the barrel (end-cap) region, starting in the middle layer. After corrections (mostly for radiative losses) are applied, the four-momentum of the electron candidate is

calculated using the energy measurement of the EM cluster and the η and ϕ measurements from the track.

Background objects like hadronic jets, non-prompt electrons from photon conversions, and semi-leptonic decays of hadrons with heavy quarks can “fake” an electron signature and be reconstructed at this stage as an electron candidate [87]. A multivariate analysis technique (MVA) [88] takes into account several cluster and track variables to create a likelihood identification for each candidate as either signal or background. Different working points with different levels of electron efficiency and background rejection are provided from the performance groups. These are “Loose”, “Medium”, and “Tight”, which correspond respectively to approximately 95%, 90% and 80% identification efficiency for an electron with $E_T > 40$ GeV. The identification efficiencies for all working points in $Z \rightarrow ee$ events are shown in figure 2.12.

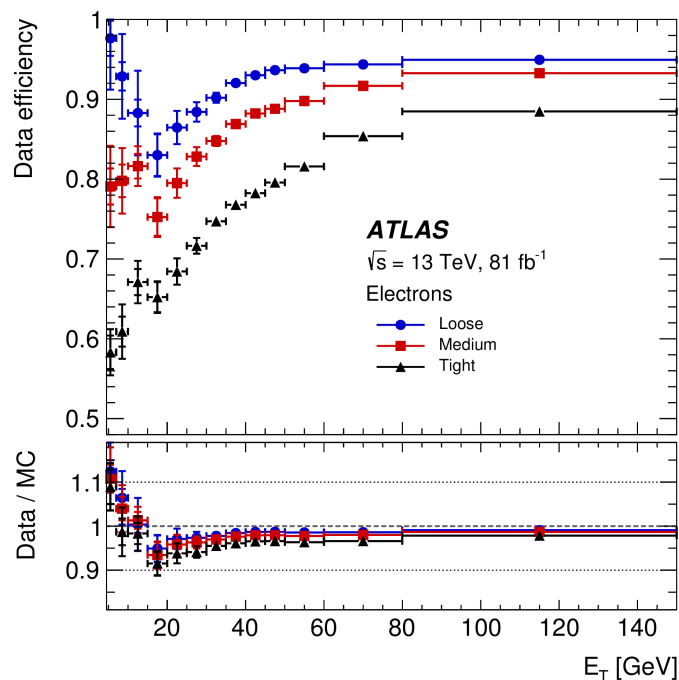


Figure 2.12: The electron identification efficiency in $Z \rightarrow ee$ events in data (2015-2017) as a function of E_T the Loose, Medium and Tight operating points. The efficiencies are obtained by applying data-to-simulation efficiency ratios measured in $J/\psi \rightarrow ee$ and $Z \rightarrow ee$ events to $Z \rightarrow ee$ simulation. Image from ref.[89].

Further suppression of background electrons is provided by applying isolation requirements [85], where both tracking and calorimeter information is used. This allows to select, as much as possible, prompt electrons, removing those coming from hadron decays and contained within jets. Working points using calorimeter and/or track based isolation are provided for either a specific efficiency with variable cuts or fixed cut values. The calorimeter isolation uses the sum of the transverse energy (E_T) in a cone of $\Delta R < 0.2$ around the electron centre ($E_T^{\text{cone}0.2}$), subtracting the 5×7 cell window contribution from the electron. For the track isolation, the sum of the transverse momenta for quality tracks in a variable cone of size $\Delta R < \min(0.2, 10 \text{ GeV}/E_T)$ centred around and excluding the electron track, $p_T^{\text{varcone}0.2}$, is used.

2.3.3 Photon reconstruction

At photon energies above 1 GeV, the interaction of the photons with the tracker is completely dominated by e^+e^- pair production, also known as “photon conversion”. All other interactions between the photons and the tracker material, such as Compton or Rayleigh scattering, have cross-sections which are orders of magnitude below and can then be ignored.

Photon candidates are reconstructed from clusters of energy deposited in the EM calorimeter [90, 91]. Those matching a reconstructed conversion vertex or a track, consistent with originating from a photon conversion, are classified as “converted photons”. Candidates without a matching track or reconstructed conversion vertex in the ID are “unconverted photons”. Those matched to a track consistent with a track originating from an electron from the hard-scatter vertex are kept as electrons.

Like for the electron case, also photon identification criteria are based on shower shapes in the calorimeter system as well as discriminating variables (DVs). A loose selection is derived using only the information from the hadronic calorimeter and the lateral shower shape in the second layer of the electromagnetic calorimeter, which contains most of the photon energy. The final tight selection applies tighter criteria to these variables, based on the shower shape in the finely segmented first calorimeter layer to ensure the compatibility of the measured shower profile with that originating from a single photon impacting the calorimeter. In all cases, the requirements on the DVs are tuned separately for unconverted and converted photons, in several pseudorapidity regions. To further reject the background from jets misidentified as photons, the photon candidates are required to be isolated using both calorimeter and tracking detector information.

The efficiency of both unconverted and converted photons is shown in figure 2.13 for data and MC simulations under different pile-up conditions. For the photon efficiency measurements, a data sample enriched in $Z \rightarrow l\bar{l}\gamma$ events is exploited.

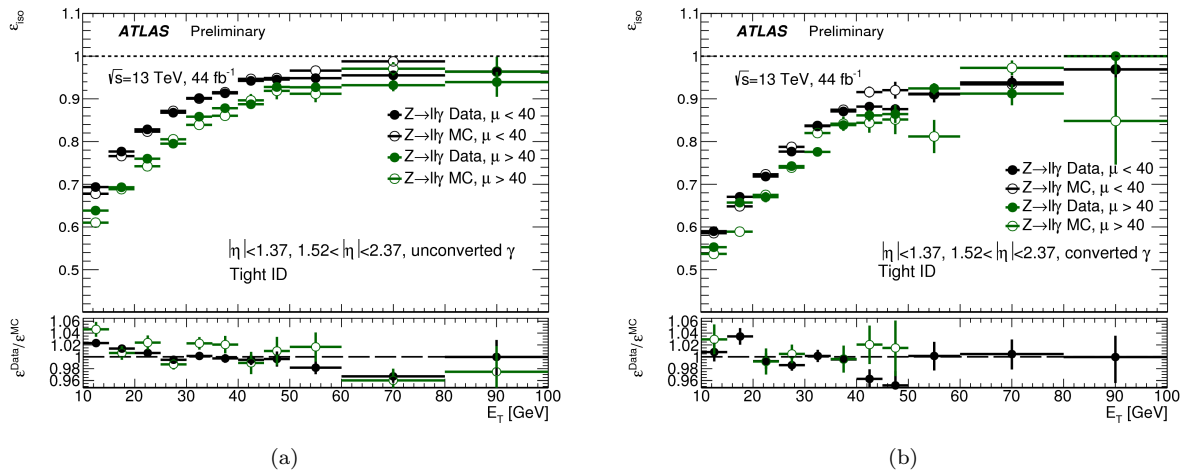


Figure 2.13: Efficiency of the tight identification requirement for unconverted (a) and converted (b) photons from radiative Z decays as a function of the transverse energy E_T , averaged over pseudorapidity. The efficiencies have been measured in 44.3 fb^{-1} of data recorded by the ATLAS experiment in 2017 at $\sqrt{s}=13 \text{ TeV}$ for the range of number of interactions per bunch crossing (μ) of $\mu < 40$, and are compared to the 2017 data in the range of $\mu > 40$. Image taken from ref.[92].

No significant differences are observed between data-driven measurements and simulations mainly because this last one does not model the distribution of the photon shower

accurately. Corrections are applied to the simulated values, which are optimised separately for unconverted and converted photons, and as a function of the pseudorapidity. The small differences in the efficiency between the simulation and the data are taken into account by computing data-to-MC efficiency ratios, also referred to as scale factors. The energy scale and resolution of the photon candidates after the MC-based calibration are further adjusted based on a correction derived using $Z \rightarrow e^+e^-$ events from data and MC simulation.

2.3.4 Muon reconstruction

Muon reconstruction in ATLAS is performed based on the information collected from the ID and the MS [93]. Until they reach the MS, muons cross typically 100 radiation lengths, mostly instrumented by the EM and hadronic calorimeters. They deposit an amount of energy in the calorimeter system of about 3-4 GeV [94].

In the ID, muons are reconstructed like any other charged particle. A Hough transform [95] is used to search for hits aligned on a trajectory in the bending plane of the detector. Muon track candidates are then built by fitting together hits from segments in different layers. The segments are selected using criteria based on hit multiplicity and fit quality and are matched using their relative positions and angles. The information on energy deposit in the calorimeter system is also used and corrections are applied to take into account the energy loss in the material.

Four different types of muons are defined in ATLAS, depending on which sub-detectors are used for the reconstruction. They are listed below:

- **Combined (CB) muons:** track reconstruction is performed independently in the ID and MS, and a combined track is formed with a global fit that uses the hits from both sub-detectors. Muons are firstly reconstructed in the MS, where the track density is much smaller, and then extrapolated inward and matched to an ID track. They are the most commonly used muons in physics analyses since they have the highest purity and the best kinematic resolution.
- **Segment-tagged (ST) muons:** a muon is classified as ST if a track in the ID, once extrapolated to the MS, is associated with at least one local track segment in the MDT or CSC chambers. ST muons are used when muons cross only one layer of MS chambers, either because of their low p_T or because they pass through regions with reduced MS acceptance.
- **Calorimeter-tagged (CT) muons:** a track in the ID is identified as a muon if it can be matched to an energy deposit in the calorimeter compatible with a minimum ionising particle. This kind of muons have the lowest purity with respect to all the other muon types but they allow to recover the acceptance in regions where MS is partially instrumented, close to $\eta = 0$.
- **Extrapolated (ME) muons:** the muon trajectory is reconstructed based only on the MS track and a loose requirement on compatibility with originating from the IP. ME muons are mainly used to extend the acceptance for muon reconstruction into the region $2.5 < |\eta| < 2.7$, which is not covered by the ID.

In the same way as for electrons, muon candidates are defined as “Loose”, “Medium”, and “Tight”, with increasing purity, according to the quality of the reconstruction and identification.

The ATLAS muon reconstruction efficiency is very high (close to 100%). It can be seen as a function of η in figure 2.14 for all three candidates.

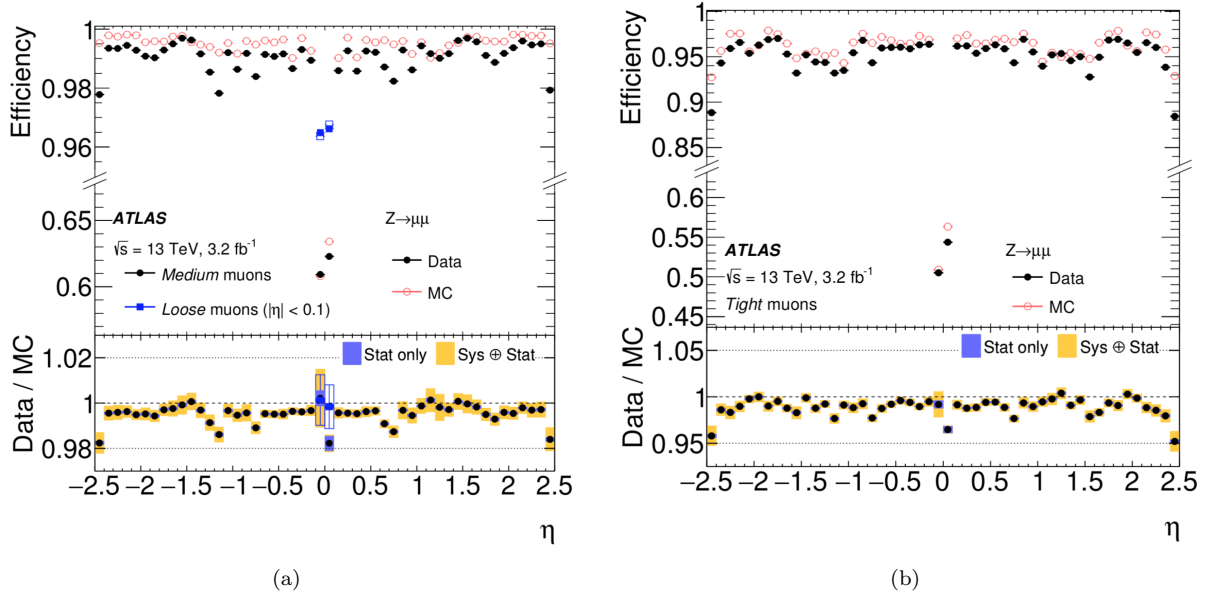


Figure 2.14: (a) and (b) show the muon reconstruction efficiency as a function of η measured in $Z \rightarrow \mu\mu$ events for muons with $p_T > 10$ GeV for respectively the Medium and Tight muon selections. Panel (a) also shows the efficiency of the Loose selection in the region $|\eta| < 0.1$ where the Loose and Medium selections differ significantly. The error bars on the efficiencies indicate the statistical uncertainty. Panels at the bottom show the ratio of the measured to predicted efficiencies, with statistical and systematic uncertainties. Images from ref.[93].

Concerning the isolation requirements, similar considerations as for electrons are made for muons: track-based and calorimeter-based isolation measurements are used to create working points with either efficiency based variable cuts or fixed cuts. The track-based muon isolation, $p_T^{\text{varcone}0.3}$, uses a slightly larger cone ($\Delta R < 0.3$) with respect to the electron case.

2.3.5 Jets

Jets are the experimental realisation of the partonic showering and subsequent hadronisation of particles carrying colour charge. This section summaries the algorithms and inputs that are used to reconstruct jets.

2.3.5.1 Jet algorithms

There is not a unique definition of a jet. The jet definition may be adapted for a specific application (i.e. particular signatures) or experimental condition (high/low luminosity, high/low centre-of-mass energy, etc.) in order to reconstruct more closely the hard scattering process. Different jet reconstruction algorithms were built to fulfill each definition. This flexibility is an accepted practice in many analyses, as long as the same definition is consistently used when comparing data to theoretical calculations or Monte Carlo simulations. However, there are some criteria that jet algorithms must satisfy to ensure stable definitions. They are the following:

- Infrared and collinear (IRC) “safe” (see below).

- Minimal sensitivity to hadronisation, underlying event and pile-up.
- Applicability in both experimental analyses and theoretical calculations.
- Reliability of (finite) results at all orders in perturbation theory.

Commonly, ATLAS uses jet definitions from the family of sequential recombination algorithms [96–98]. These were specifically designed to be insensitive to the presence of soft (infrared) and collinear gluon emission, and are thus usable for calculations done to any order in perturbation theory. Recombination algorithms try to reverse the pattern of QCD parton showers and multi-gluon radiations characterised by softer emissions as the shower evolves [99]. For this, the algorithm defines a distance d_{ij} between entities (particles or energy deposits in the calorimeter) and between entity i and the beam d_{iB} :

$$d_{ij} = \min \left(p_{T_i}^{2p}, p_{T_j}^{2p} \right) \frac{\Delta R_{ij}^2}{R^2} \quad (2.5)$$

$$d_{iB} = p_{T_i}^{2p}$$

where ΔR_{ij}^2 is defined in equation 2.4, p_{T_i} is the transverse momentum of entity i , and parameters p and R regulate the evolution of the clustering. The algorithm identifies the smallest of the distances and if it is a d_{ij} then combines entities i and j , while if it is d_{iB} defines entity i as a jet and removes it from the list of entities. The new four-moment (p^μ) of the combined pair is defined as $p_{i+j}^\mu = p_i^\mu + p_j^\mu$. Then, distances for the set of remaining entities are calculated and the procedure is repeated until no entities are left.

Two examples of sequential recombination algorithms are the k_t algorithm [96], where $p = 1$, and the Cambridge-Aachen (C/A) algorithm [97, 98], with $p = 0$. In the k_t algorithm the soft particles are merged first, which introduces a strong sensitivity to small fluctuations of the energy density of the parton shower. The C/A algorithm relies only on angular ordering of emissions in order to reconstruct the shower by omitting the transverse momentum from d_{ij} , which again results in a strong dependence to the experimental conditions. A case of particular interest corresponds to $p = -1$, referred to as the “anti- k_t ” jet-clustering algorithm [100]. In this, the soft particles will tend to cluster with hard ones long before they cluster among themselves, effectively reducing the sensitivity to fluctuations of the parton shower or energy contributions from underlying event. If a hard particle has no hard neighbours within a distance $2R$, then it will simply accumulate all the soft particles within a circle of radius R , resulting in a perfectly circular cone-shape jet in the $(y - \phi)$ plane. More complex boundaries can occur for busy environments composed of many close-by showers.

The other free parameter in equation 2.5 is the radius R that sets a characteristic scale in the $(y - \phi)$ space, and generally speaking defines the area of the jet (πR^2) for highly energetic and isolated jets. There is no strict recommendation for the choice of R , but it is commonly advised to use values between 0.4 and 1.2, where effects of hadronisation and the influence of the underlying event are minimised [101] (see also figure 38 of ref.[102]). As the radius increases less energy is “splashed out” of the jet, a phenomena known as out-of-cone energy, but the influence of underlying event also increases as the area of the jet grows.

The most common values for anti- k_t jets in ATLAS are $R = 0.4, 1.0$ [103–105]. The so-called large- R jets ($R = 1.0$) are used (among other things) to identify boosted hadronically decaying vector bosons. Jets from two-body decays of boosted vector bosons have

a substructure typically absent from decays of gluons and light quarks [104]. To elucidate the substructure differences, grooming techniques [106–108] remove soft contributions to the jet. In particular, ATLAS commonly uses a grooming technique called trimmig [104, 108]. Jet trimming further aims to improve the jet mass resolution by removing contamination from initial state radiation, multiple parton interactions, and pile-up interactions.

There are also smaller and bigger anti- k_t jets of $R = 0.2, 0.6$ used by ATLAS. They are particularly important for studying the sub-structure of large- R jets and could be more sensitive than the regular ones for certain analyses. Their calibration slightly differs from the one of the anti- k_t $R = 0.4, 1.0$. A more detail discussion about it can be found in section 3.

2.3.5.2 Topological clusters

Some of the possible inputs for the jet reconstruction algorithm are the calorimeter cells, measured at the electromagnetic energy (EM) scale, or the set of towers of cells running longitudinally along the calorimeter (like the ones used in electron reconstruction). However, none of those inputs reproduce the actual shape of the particle cascade and are more susceptible to electronic noise and other sources of fluctuations such as pile-up. For that reason, the input objects to the jet algorithm are three-dimensional topological clusters, better known as topoclusters [109], built from individual calorimeter cells.

The topocluster formation follows cell signal-significance patterns generated by electromagnetic and hadronic showers, where the clustering algorithm implicitly performs a topological noise suppression by removing cells with insignificant signals which are not in close proximity to cells with significant signals. This is possible due to the high granularity of the calorimeter system. As the calorimeters are subject to a significant amount of background noise, the mean noise level is constantly measured and subtracted from measurements.

Topological clusters are formed through an iterative procedure [109] which identifies the most significant energy deposits, the seed cells, and then clusters neighboring cells into a single topocluster. Seed cells are first identified as the calorimeter cells with an energy significantly above a predefined noise threshold of $|E_{\text{cell}}| > 4\sigma_{\text{noise}}$. The seed cell forms a protocluster and neighbouring cells are iteratively added to it if they have an energy $|E_{\text{cell}}| > 2\sigma_{\text{noise}}$. Once the iterative process ends and a stable protocluster is formed, all cells adjacent to the protocluster are added, independent of the magnitude of their signal. Through this method a topocluster is formed by a core of cells with significant energy surrounded by an envelope of cells containing any residual or leaked energy.

The jet-finding algorithms treat the topoclusters as massless four-vectors of magnitude $E = \sum E_{\text{cell}}$ which point from the centre of the detector to the energy-weighted barycentre of the topocluster. The resulting topological cell clusters have shape and location information, which are used to improve the energy resolution. A local cell signal weighting (LCW) [109, 110] method can be applied to each topocluster, bringing clusters from the EM to the LCW scale, including corrections for dead material, out-of-cluster losses for pions and calorimeter response for hadronic clusters (identified using their topology and energy density).

2.3.5.3 Particle flow algorithm

An alternative approach is taken in the particle flow algorithm, in which measurements from both the tracker and the calorimeter are combined to form the signals, which ideally

represent individual particles. The energy deposited in the calorimeter by all the charged particles is removed. Jet reconstruction is then performed on an ensemble of “particle flow objects” consisting of the remaining calorimeter energy and tracks which are matched to the hard interaction. The benefits of reconstructing jets with the particle flow algorithm (detailed in ref.[111]) are:

- For low-energy charged particles, the momentum resolution of the tracker is significantly better than the energy resolution of the calorimeter.
- The acceptance of the detector is extended to softer particles, as tracks are reconstructed for charged particles with a minimum transverse momentum $p_T > 400$ MeV, whose energy deposits often do not pass the noise thresholds required to seed topoclusters [111].
- The angular resolution of a single charged particle, reconstructed using the tracker is much better than that of the calorimeter.
- Low- p_T charged particles originating within a hadronic jet are swept out of the jet cone by the magnetic field by the time they reach the calorimeter. By using the track’s azimuthal coordinate at the perigee, these particles are clustered into the jet.
- When a track is reconstructed, one can ascertain whether it is associated with a vertex. Therefore, in the presence of multiple in-time pile-up interactions, the effect of additional particles on the hard-scatter interaction signal can be mitigated by rejecting signals originating from pile-up vertices, which is very important while moving to higher luminosity values.

However, particle flow introduces a complication. For any particle whose track measurement ought to be used, it is necessary to correctly identify and subtract its signal in the calorimeter to avoid double-counting. In the particle flow algorithm, a Boolean decision is made as to whether to use the tracker or calorimeter measurement. The ability to accurately subtract all of a single particle energy, without removing energy deposited by other particles, forms the key performance criterion upon which the algorithm is optimised.

2.3.6 *b*-jet tagging

The identification of jets containing *b*-hadrons (*b*-jets) against the large jet background containing only *c*-jets or neither *b*- or *c*-jets (light-flavour jets) is of major importance in many areas of the physics programme of ATLAS.

Various algorithms are used to identify *b*-jets [112], referred to as *b*-tagging algorithms. These algorithms exploit the long lifetime, high mass and high decay multiplicity of *b*-hadrons as well as the properties of the *b*-quark fragmentation. Given a lifetime of the order of 1.5 ps, measurable *b*-hadrons have a significant mean flight length in the detector before decaying, generally leading to at least one vertex displaced from the hard-scatter collision point.

The whole identification process is based on a two-stage approach. Firstly, low-level algorithms reconstruct the characteristic features of the *b*-jets via two complementary approaches, one that uses the individual properties of the tracks associated with a hadronic jet, and a second which combines the tracks to explicitly reconstruct displaced vertices.

These algorithms, first introduced during Run 1, have been improved and retuned for Run 2. These algorithms are:

IP2D and IP3D. There are two complementary impact parameter-based algorithms, IP2D and IP3D [113]. The IP2D tagger makes use of the signed transverse impact parameter significance of tracks to construct a discriminating variable, whereas IP3D uses both the track signed transverse and the longitudinal impact parameter³ significance in a two-dimensional template to account for their correlation. Probability density functions (pdf) of these significances of tracks associated with the different jet flavours are derived from MC simulation. These pdfs are used to calculate ratios of the b -jet, c -jet and light-flavour jet probabilities and all this information is used in log-likelihood ratio discriminants. These likelihood discriminants for both the IP2D and IP3D algorithms are used as inputs to the high-level taggers.

Secondary vertex finding algorithm (SV1). The SV1 algorithm [114] reconstructs a single displaced secondary vertex in a jet. The reconstruction starts from identifying the possible two-track vertices built with all tracks associated with the jet, while rejecting tracks that are compatible with the decay of long-lived particles, photon conversions or hadronic interactions with the detector material. The SV1 algorithm runs iteratively on all tracks contributing to the cleaned two-track vertices, trying to fit one secondary vertex. In each iteration, the track-to-vertex association is evaluated using a χ^2 test. The track with the largest χ^2 is removed and the vertex fit is repeated until an acceptable vertex χ^2 and a vertex invariant mass less than 6 GeV are obtained. With this approach, the decay products from b - and c -hadrons are assigned to a single common secondary vertex.

Topological multi-vertex finding algorithm. This algorithm, commonly known as JetFitter [115], exploits the topological structure of weak b - and c -hadron decays inside the jet and tries to reconstruct the full b -hadron decay chain. A modified Kalman filter [116] is used to find a common line on which the primary, bottom and charm vertices lie, approximating the b -hadron flight path as well as the vertex positions. With this approach, it is possible to resolve the b - and c -hadron vertices even when a single track is attached to them.

Secondly, in order to maximise the b -tagging performance, the results of the low-level b -tagging algorithms are combined in high-level algorithms consisting of multivariate classifiers. The performance of a b -tagging algorithm is characterised by the probability of tagging a b -jet (b -jet tagging efficiency) and the probability of mistakenly identifying a c -jet or a light-flavour jet as a b -jet. There are mainly two high-level algorithms:

MV2. The MV2 algorithm [113] consists of a boosted decision tree (BDT) algorithm that combines the outputs of the low-level tagging algorithms. The BDT is trained using the ROOT Toolkit for Multivariate Data Analysis (TMVA) [117] on the hybrid $t\bar{t} + Z'$ sample. The kinematic properties of the jets (p_T and $|\eta|$) are included in the training in order to take advantage of the correlations with the other input variables. However, to avoid differences in the kinematic distributions being used to discriminate

³Longitudinal $IP_z = z_0 \sin(\theta)$ and transverse $IP_{r\phi} = d_0$ impact parameters. Signed significance is defined as $sgn(IP) \times IP/\sigma(IP)$.

between the different jet flavours, the b -jets and c -jets are reweighted in p_T and $|\eta|$ to match the spectrum of the light-flavour jets. No kinematic reweighting is applied at the evaluation stage of the multivariate classifier. The BDT training hyperparameters of the MV2 tagging have been optimised to provide the best separation power between the signal and the background.

DL1. The second high-level b -tagging algorithm, DL1 [113], is based on a deep feed-forward neural network (NN) trained using Keras [118] backend and the Adam optimiser [119]. The DL1 NN has a multidimensional output corresponding to the probabilities for a jet to be a b -jet, a c -jet or a light-flavour jet. The topology of the output consists of a mixture of fully connected hidden and Maxout layers [120]. The input variables to DL1 consist of those used for the MV2 algorithm with the addition of some of the JetFitter c -tagging variables. The latter relate to the dedicated properties of the secondary and tertiary vertices (distance to the primary vertex, invariant mass and number of tracks, energy, energy fraction, and rapidity of the tracks associated with the secondary and tertiary vertices). A jet p_T and $|\eta|$ reweighting similar to the one used for MV2 is performed. The DL1 algorithm parameters are optimised in order to maximise the b -tagging performance. Batch normalisation [121] is added by default since it is found to improve the performance.

Training with multiple output nodes offers additional flexibility when constructing the final output discriminant by combining the b -jet, c -jet and light-flavour jet probabilities. Since all flavours are treated equally during training, the trained network can be used for both b -jet and c -jet tagging. In addition, the use of a multi-class network architecture provides the DL1 algorithm with a smaller memory footprint than BDT-based algorithms. The final DL1 b -tagging discriminant is defined as:

$$D_{\text{DL1}} = \ln \left(\frac{p_b}{f_c \cdot p_c + (1 - f_c) \cdot p_{\text{light}}} \right)$$

where p_b , p_c , p_{light} and f_c represent respectively the b -jet, c -jet and light-flavour jet probabilities, and the effective c -jet fraction in the background training sample. Using this approach, the c -jet fraction in the background can be chosen a posteriori in order to optimise the performance of the algorithm.

The evaluation of the performance of the algorithms is carried out using b -jet tagging single-cut operating points (OPs). These are based on a fixed selection requirement on the b -tagging algorithm discriminant distribution ensuring a specific b -jet tagging efficiency (ε_b) for the b -jets present in the baseline $t\bar{t}$ simulated sample. The MV2 and the DL1 discriminant distributions are also divided into five ‘pseudo-continuous’ bins, $(0^k)_{k=1\dots 5}$, delimited by the selections used to define the b -jet tagging single-cut OPs for 85%, 77%, 70% and 60% efficiency. The value of the pdf in each bin is called the b -jet tagging probability and labelled P_b in the following. The b -jet tagging efficiency of the $\varepsilon_b = X\%$ single-cut OP can then be defined as the sum of the b -jet tagging probabilities in the range $[X\%, 0\%]$. The light-flavour jet and c -jet rejections as a function of the b -jet tagging efficiency are shown in figure 2.15 for the various low- and high-level b -tagging algorithms.

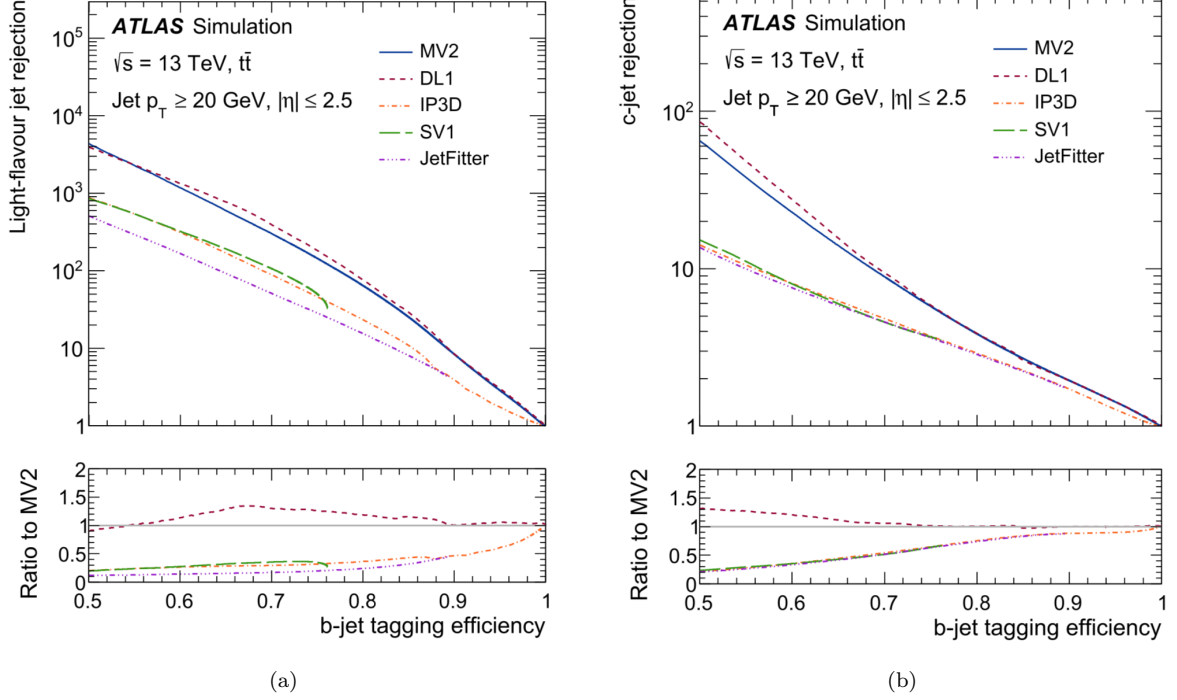


Figure 2.15: The (a) light-flavour jet and (b) c -jet rejections versus the b -jet tagging efficiency for the IP3D, SV1, JetFitter, MV2 and DL1 b -tagging algorithms evaluated on the baseline $t\bar{t}$ events. Image taken from ref.[122].

2.3.7 Missing transverse momentum

Observables described so far in this section are defined to measure the signatures of hadrons and fundamental particles. All electrically charged and/or strongly interacting particles are detected by some or a combination of the ATLAS sub-systems. The only exception are electrically neutral colour singlets like Standard Model neutrinos or some theoretical light particles that by weakly interacting can transverse the whole volume of the detector without notice. Missing transverse momentum (E_T^{miss}) is used to infer the existence of these otherwise invisible particles. Its reconstruction uses selected calibrated reconstructed objects to measure the missing transverse momentum in an event [123]. The $E_{x(y)}^{\text{miss}}$ components are calculated as:

$$E_{x(y)}^{\text{miss}} = E_{x(y)}^{\text{miss},e} + E_{x(y)}^{\text{miss},\gamma} + E_{x(y)}^{\text{miss},\tau} + E_{x(y)}^{\text{miss},\text{jets}} + E_{x(y)}^{\text{miss},\mu} + E_{x(y)}^{\text{miss},\text{soft}}$$

where each object term is given by the negative vectorial sum of the momenta of the respective calibrated objects. Calorimeter signals are associated with these reconstructed objects in the following order: electrons (e), photons (γ), hadronically decaying τ -leptons, jets, and muons (μ). The soft term is reconstructed from detector signal objects not associated with any object. Since Run 2 data (and so far), the soft-term was constructed from a track-based soft-term [123, 124]. Information about neutral particles is lost when only using tracks, but the neutral contribution cancels on average because charge-to-neutral fluctuations are symmetric in azimuth. The main motivation for the track-based term is the robustness to pile-up. At Run 2 conditions, the insensitivity to pile-up is the dominant effect and the E_T^{miss} with a track-based soft-term has a $\sim 10\%$ better resolution than the calorimeter-based soft-term used during Run 1.

From the components $E_{x(y)}^{\text{miss}}$, the azimuthal angle ϕ^{miss} and the magnitude of E_T^{miss} are

also calculated in the following way:

$$E_T^{\text{miss}} = \sqrt{(E_x^{\text{miss}})^2 + (E_y^{\text{miss}})^2} \quad \phi^{\text{miss}} = \arctan(E_y^{\text{miss}}/E_x^{\text{miss}})$$

Chapter 3

In-situ Calibration for R -scan jets

The energetic pp collisions produced by the LHC yield final states that are predominantly characterised by jets, or collimated sprays of charged and neutral hadrons. Jets constitute an essential piece of the physics programme carried out using the ATLAS detector, either via their presence in the signal processes being measured and searched for, or as a ubiquitous feature of various background processes and the pile-up due to simultaneous pp collisions. As described in section 2.3.5, their reconstruction and identification involves a complex process where different algorithms and inputs are used. Once these objects have been identified, measurements of their energy scale and resolution, as well as their associated systematic uncertainties, are therefore essential both for precision measurements of the Standard Model and sensitive searches for new physics beyond. Jets in data and simulation are calibrated following the procedure described in detail in [105].

The standard jet radius used by ATLAS with this full calibration is $R = 0.4$, however there are jets with smaller $R = 0.2$ and bigger $R = 0.6$ radii. Dragged mainly by theoretical requirements, the $R = 0.6$ jets represent a better choice for Standard Model precision measurements in general, since they leave out some effects that only affect the jet reconstruction in smaller radii jets, such as the out-of-cone radiation effects for instance. While the usage of $R = 0.2$ jets is motivated for example by those searches looking for a low mass particle at high energy in a boosted regime where the reconstruction on the decaying pair of jets from this particle could be better resolved with a smaller jet size reconstruction.

On the other hand, derive a full calibration for the $R = 0.2$ and $R = 0.6$ jets in the same way that it is done for the $R = 0.4$ ones would result in a resource intensive process, so the collaboration ultimately decided to provide only a full calibration for the standard jet size. Other methods are implemented instead that make benefit of the already full calibrated $R = 0.4$ jets to calibrate the ones with smaller and bigger sizes.

This chapter describes the methods used to calibrate the four-momenta of jets reconstructed with the anti- k_t algorithm [100] with radius parameter $R = 0.2$ and $R = 0.6$, also known as “ R -scan” jets. The name “ R -scan” alludes to the idea of having a “scan” in radius parameter between $R = 0.2$ and $R = 0.6$, not including $R = 0.4$, which is already supported by ATLAS in Run 2.

The inputs to the jet algorithm are three-dimensional topoclusters (see section 2.3.5.2) built from individual calorimeter cells. The topoclusters are corrected to point to the hard-scatter primary vertex rather than the centre of the detector, while keeping the topocluster energy constant. A local cell signal weighting [109, 110] method is applied to each topocluster, including corrections for dead material, out-of-cluster losses for pions

and calorimeter response for hadronic clusters (identified using their topology and energy density).

The calibrations presented in the following sections are derived in Monte Carlo (MC) simulation (section 3.1.1) and in pp collisions (section 3.1.2) collected by the ATLAS detector at a centre-of-mass energy of $\sqrt{s}=13$ TeV during the 2015 and 2016 data-taking periods of Run 2 at the LHC, as well as their respective uncertainties. Only some representative distributions are shown in the following section, for further details and plots the reader is kindly invited to consult the original internal note [125].

3.1 Introduction to the jet energy scale calibration

The jet energy scale (JES) calibrations restore the jet energy scale to that of jets reconstructed at the particle-level energy scale. All steps of the calibration correct the full four-momentum unless otherwise stated, scaling the jet p_T , energy, and mass. The JES calibration can be divided in two stages:

1. In the first calibration stage, MC-based corrections adjust the reconstructed jet four-momentum to that corresponding to jets built from the simulated stable particles. These calibrations apply the same “standard” procedure detailed in [105] to R -scan jets, with modifications that will be discussed in detail in the following section 3.1.1. This stage of the calibrations consists of five distinct steps.
2. In the second stage of the calibration, a new *in-situ* technique, known as “direct matching method”, is applied to measure the difference in jet response between data and MC simulation. In this approach, R -scan jets are compared to fully calibrated anti- $k_t R = 0.4$ [105] jets reconstructed from topoclusters at the electromagnetic scale. This stage is further discussed in section 3.1.2.

The individual steps of the calibration procedure are summarised in figure 3.1 and briefly detailed in the following sections.

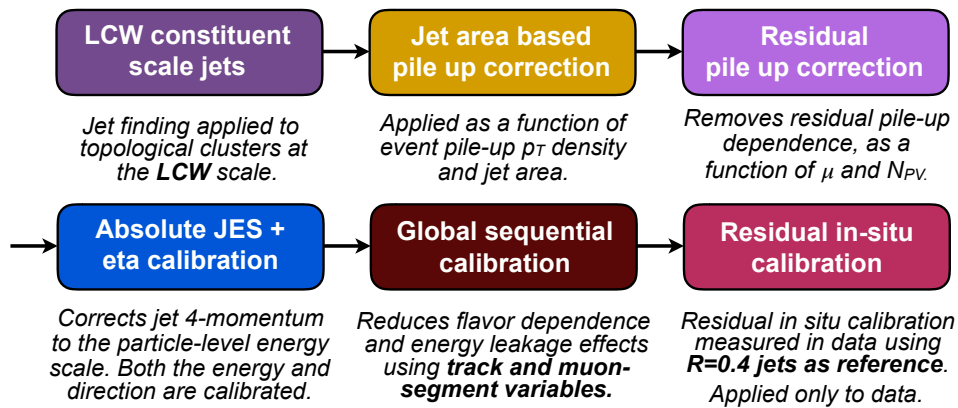


Figure 3.1: An overview of the R -scan calibration scheme. Differences relative to the standard calibration scheme [105] for $R = 0.4$ jets reconstructed from EM-scale topoclusters are highlighted in bold font. In particular, there is no dedicated origin correction step in new software releases, the global sequential calibration does not take into account calorimeter-based observables as they are already considered in the LCW-corrections for the clusters. Finally, the in-situ correction is derived using standard $R = 0.4$ jets reconstructed from EM-scale topoclusters as a reference.

3.1.1 MC based calibrations

The MC-based jet energy scale corrections are applied in three stages following the procedure described in [105] for jets at EM-scale, but with some differences for R -scan jets which are highlighted in fig. 3.1.

All MC-based corrections are therefore derived by comparing reconstructed jets to particle jets, both reconstructed with the same radius parameter, in simulated inclusive jet events [126]. Particle jets, also known as “truth” jets, are built at the event generator level from stable particles.

3.1.1.1 Pile-up correction

Jets are corrected for the contributions from additional proton-proton interactions within the same (in-time) or nearby (out-of-time) bunch crossings. First, a correction based on the jet area (A) and the average transverse energy density (ρ) of the event is applied [127], $\Delta p_T = -\rho \times A$. The jet area is a measure of the susceptibility of the jet to pile-up and is determined jet by jet. The average energy density serves as a measure of the pile-up activity and is calculated event by event as the median energy density of jets reconstructed with the k_t algorithm with a radius parameter value of $R = 0.4$. After this correction, there remains some dependence of the average jet p_T on pile-up activity. An additional correction is therefore derived by comparing reconstructed jets to matched particle jets in simulated inclusive jet events [126]. The correction is parameterised as a function of the number of reconstructed primary vertices in the event (N_{PV}) and of the mean number of interactions per bunch crossing (μ) such that both the out-of-time and in-time effects are taken into account. The residual p_T dependencies on both, parameterised by α and β respectively, are observed to be fairly linear and independent of one another for all R . Linear fits are used to derive the initial α and β coefficients separately in bins of p_T^{truth} and $|\eta|$. Since both α and β coefficients show a logarithmic dependence on p_T^{truth} , logarithmic fits are performed in the range $20 < p_T^{\text{truth}} < 200$ GeV for each bin of $|\eta|$ and the fitted value at $p_T^{\text{truth}} = 25$ GeV is taken as the nominal α and β coefficients, reflecting the dependence in the p_T region where pile-up is most relevant. The pile-up-corrected p_T , after the area-based and residual corrections, is then given by

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

where p_T^{reco} refers to the EM-scale p_T of the reconstructed jet before any pile-up corrections are applied.

3.1.1.2 Absolute Monte-Carlo based calibration

In addition, a jet energy- and η -dependent correction, commonly known as “MCJES”, is applied to reconstructed jets in data and MC simulations [128]. It is derived from simulated samples of inclusive jet events and is designed to lead to agreement in energy and $|\eta|$ -direction between reconstructed jets and particle jets on average, correcting for instrumental effects of the non-compensating calorimeter response, energy losses in dead material, and out-of-cone¹ effects. The procedure to derive the MCJES for R -scan jets is modified relative to the standard procedure [105] in the following way:

¹Contribution of particles outside the jet cone.

- The standard isolation requirement to other jets is $1.5 \times R$ (i.e. 1.5×0.4). This criterion is kept for $R = 0.6$ (1.5×0.6), but it is increased for $R = 0.2$ ($1.5 \times R \rightarrow 1.5 \times 0.4$).
- The energy threshold of jets to be considered in the isolation requirement at detector level is $p_T/2$ rather than 10 GeV.

Both requirements serve to reduce the contribution of erroneously matched jets and PU at detector level.

The detector response $\mathcal{R}^2$ in E as a function of reconstructed jet η in different ranges of particle-level jet energy E_{true} is shown in figures 3.2a, 3.2c and 3.2e for $R = 0.2, 0.4, 0.6$ jets, respectively, after applying the residual PU correction from section 3.1.1.1. And in figures 3.2b, 3.2d and 3.2f the same distributions are shown but also applying the absolute MC-based calibration described above.

Before the MC-based calibration, the responses are notably below unity, especially for low E_{true} , and this trend is stronger for larger R . This difference between jets reconstructed with different R parameters is due to the higher energy density in the jet core, which is mostly captured with $R = 0.2$ jets. After applying the MC-based calibration derived here, the responses are brought into close agreement with unity. In the relevant kinematic range of $E_{T,\text{reco}} > 20, 25, 30$ GeV for respectively $R=0.2, 0.4, 0.6$ jets, a good closure within 0.5% is observed for most of the kinematic regime in $|\eta| < 2.5$, and only at low energies the closure deteriorates to a few %. This effect is consistent with what has been found in the “standard” calibration for $R = 0.4$ jets.

3.1.1.3 Global sequential calibration

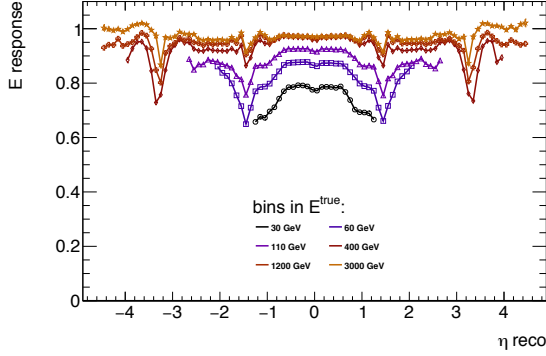
The Global Sequential (GS) calibration for R -scan jets is a series of multiplicative corrections aiming to improve the jet energy resolution. This calibration reduces the effects from fluctuations in the flavour composition of particles forming the jets, and corrects the jets not contained within the calorimeter. The corrections applied in the GS calibration are based on the following observables:

1. n_{trk} : the number of tracks with $p_T > 1$ GeV ghost-associated³ with the jet ($|\eta_{\text{det}}| < 2.5$).
2. $\mathcal{W}_{\text{trk}}$: the average p_T -weighted transverse distance in the η - ϕ plane between the jet axis and all tracks of $p_T > 1$ GeV ghost-associated to the jet ($|\eta_{\text{det}}| < 2.5$).
3. n_{segments} : the number of muon track segments ghost-associated with the jet ($|\eta_{\text{det}}| < 2.7$).

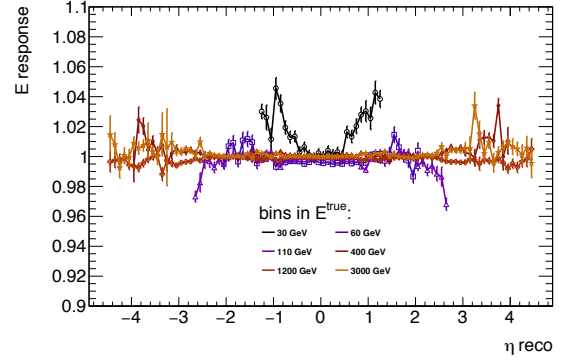
The tracking information is used to reduce the flavour dependence of the calorimeter response to jets, i.e. the difference in the observed calorimeter response to jets initiated by different parton flavours. The muon spectrometer information is used to improve the jet energy resolution of high energy jets uncontained within the calorimeter. Calorimeter-based GS corrections that are employed for jets reconstructed from EM-scale clusters

²The average energy response is defined as the mean of a Gaussian fit to the core of the $E^{\text{reco}} = E^{\text{truth}}$ distribution for jets, binned in E^{truth} and η_{det} .

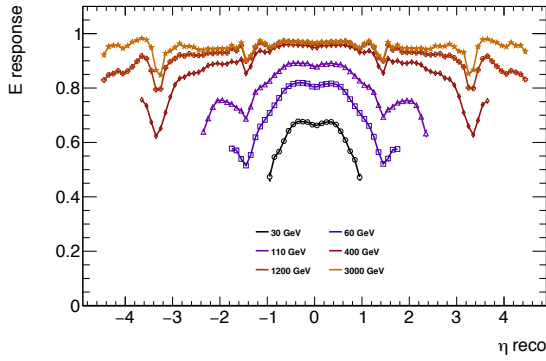
³Procedure that treats the tracks as four-vectors of infinitesimal magnitude during the jet reconstruction and assigns them to the jet with which they are clustered [127].



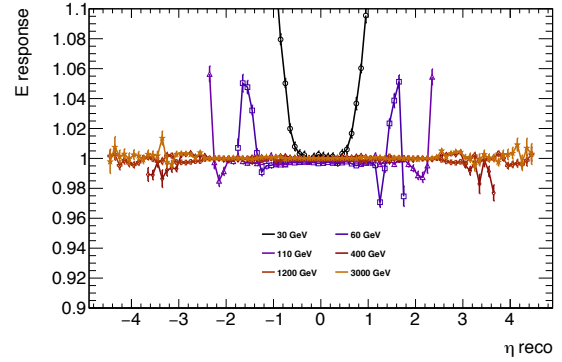
(a) $\mathcal{R}$ after applying PU correction in E for $R = 0.2$



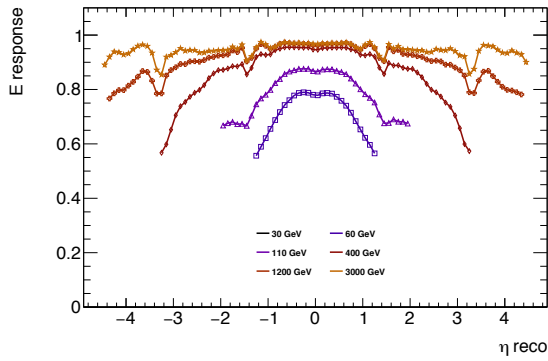
(b) $\mathcal{R}$ after applying PU and MCJES corrections in E for $R = 0.2$



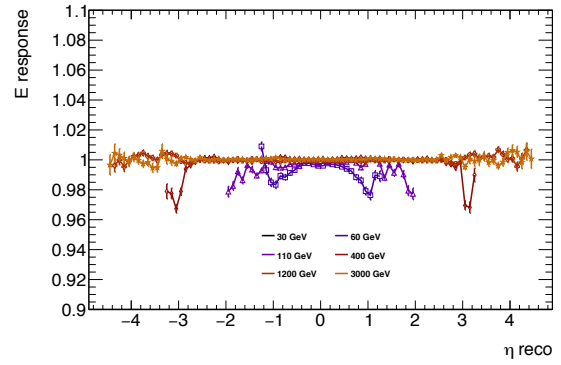
(c) $\mathcal{R}$ after applying PU correction in E for $R = 0.4$



(d) $\mathcal{R}$ after applying PU and MCJES corrections in E for $R = 0.4$



(e) $\mathcal{R}$ after applying PU correction in E for $R = 0.6$



(f) $\mathcal{R}$ after applying PU and MCJES corrections in E for $R = 0.6$

Figure 3.2: The detector response in E as a function of reconstructed jet η for different ranges in particle-level jet energy E_{true} for $R = 0.2$ (a), $R = 0.4$ (c), and $R = 0.6$ (e) jets after applying the residual PU correction is shown. The same distributions after applying also the absolute MC-based calibration are shown for $R = 0.2$ (b), $R = 0.4$ (d), and $R = 0.6$ (f). The distributions are shown for regions of parameter space where $E_{T,\text{true}} > 15, 20, 30$ GeV for $R = 0.2, 0.4, 0.6$ jets, respectively.

are not used for R -scan jets, since the local cluster weighting calibration scheme for topo-clusters is strongly correlated with these observables. By construction, the GS corrections leave the average jet energy scale in the QCD inclusive jet sample that is used to derive the calibration invariant.

The resulting improvements in the jet energy resolution⁴ after sequentially applying the above corrections are shown in fig. 3.3 for a central η bin. An incremental improvement for all observables is found, as expected.

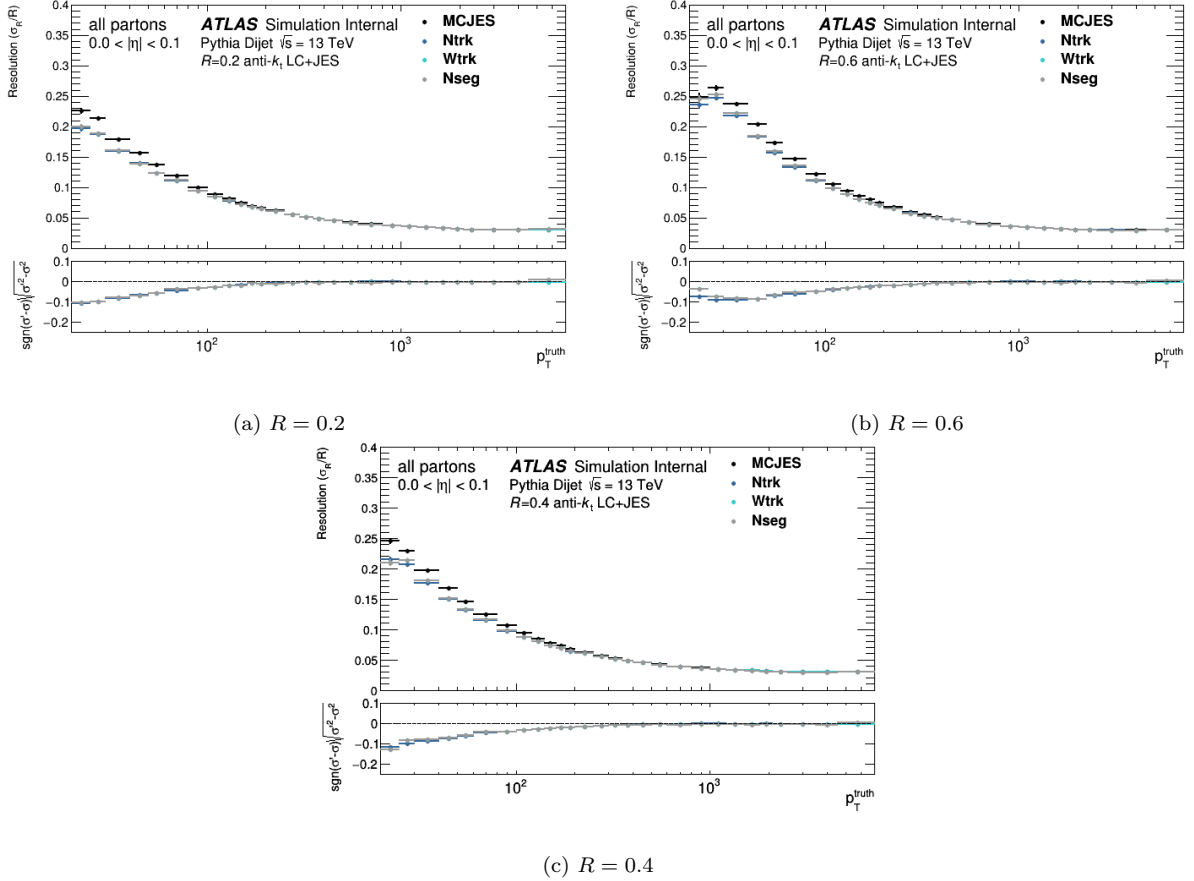


Figure 3.3: Improvements in the jet energy resolution as a function of p_T , shown step-wise for each of the GS corrections, for the very central η bin (0.0-0.1). Again for the $R = 0.2$, (a), for $R = 0.6$, (b) and for the standard jet size, $R = 0.4$, in (c).

3.1.2 In-situ calibrations

At this point, the calibration of MC jets is finished. However, a residual “in-situ” calibration is derived to correct for remaining differences between the jet energy response in data and simulation. Such differences may arise from the imperfect description of the detector response and detector material in MC simulation, as well as of the simulation of the interactions with the detector.

For standard $R = 0.4$ jets, this correction is calculated using γ +jet, Z +jet, dijet and multijet p_T -balance techniques [105, 129, 130]. In order to cover a broad p_T jet regime,

⁴The jet resolution (σ_R) is given by the standard deviation of the Gaussian fit to the jet response distribution. The fractional jet resolution $\sigma_R/R = \sigma_{p_T^{reco}}/p_T^{reco}$ is used to determine the size of the fluctuations in the jet energy reconstruction.

each of these techniques is exploited in a different and complementary p_T range. All these corrections are derived for the central jets, with $|\eta| < 1.2$ and are combined following the procedure described in refs.[105, 131].

In the case of R -scan jets, differences between data and MC simulation are quantified using a new in-situ technique known as “direct matching method”. This technique compares the p_T of an R -scan jet against a fully-calibrated *reference* jet. These reference jets are reconstructed with the anti- k_t algorithm with radius parameter $R = 0.4$ from topoclusters at the EM-scale. The reference jets are calibrated with the full jet energy scale discussed in detail in [105], which consist on dedicated MC-based calibrations following the same procedure presented as in section 3.1.1, with two extra GS corrections based on the longitudinal structure of the energy depositions within the calorimeters; and on the in-situ calibrations mentioned previously.

In the direct matching method, R -scan jets are geometrically matched to a reference jet. Two different topologies are used to derive in-situ calibrations: dijets and $Z(\mu\mu)$ +jets, in order to cover a wide jet p_T range. This is because the sample of dijet candidate events in data is statistically limited at low p_T due to the use of prescaled triggers, while the Z +jet sample in data is statistically limited at high p_T above ~ 0.5 TeV due to its production cross section.

The direct matching method differs from the standard ones used on these topologies for $R = 0.4$ jets, which focus on the imbalance in the transverse momentum between the back-to-back objects (jet/jet or Z /jet). The basic idea is that there is a well calibrated object in the event (a Z boson or a jet in a well-calibrated reference region), labeled as the reference one, and one recoiling jet, the probe one, and by comparing the p_T for each pair of objects using different techniques, correction factors can be derived.

3.1.2.1 Procedure to derive in-situ calibration factors

The procedure detailed below was used to derive calibration factors for 2015+2016 data using the dijets and Z +jet topologies.

For a given matched R -scan–reference jet pair, the following ratio is calculated:

$$\mathcal{R} = \frac{p_T^{\text{Rscan}}}{p_T^{\text{Ref}}} \quad (3.1)$$

where p_T^{Rscan} is the transverse momentum of an R -scan jet, and p_T^{Ref} is the p_T of the matched reference jet. The average ratio in data and MC simulation is extracted by fitting the p_T ratio distributions with a Gaussian in bins of η^{Rscan} and p_T^{Ref} . The size of the η^{Rscan} bins is 0.1. Then the correction factor $\mathcal{C}$ is defined by:

$$\mathcal{C}(p_T^{\text{Ref}}, \eta^{\text{Rscan}}) = \frac{\langle \mathcal{R} \rangle_{\text{MC}}}{\langle \mathcal{R} \rangle_{\text{Data}}} \quad (3.2)$$

The correction factors in equation 3.2 are derived as a function of p_T^{Ref} , but the correction is ultimately applied to the R -scan jets. By doing this, it can be assured that no bias is being introduced in the process, since p_T^{Ref} is already well defined and calibrated. Then, a mapping procedure is used to obtain the correction factors as a function of p_T^{Rscan} . The procedure consists of obtaining $\langle p_T^{\text{Rscan}} \rangle$ for each $(p_T^{\text{Ref}}, \eta^{\text{Rscan}})$ bin, as shown in figures 3.4 and 3.5 for R -scan jets with $R = 0.2$ and $R = 0.6$, respectively. The η^{Rscan} binning used for the mapping procedure is shown in table 3.1. Finally, the correction factors $\mathcal{C}$

-3., -2.8, -2.5, -1.8, -1.3, -1.0, -0.7, -0.2, 0., 0.2, 0.7, 1.0, 1.3, 1.8, 2.5, 2.8, 3.
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Table 3.1: The binning of η^{Rscan} used in the mapping procedure and in the evaluation of systematic uncertainties on the in situ calibration factors (see section 3.3).

are placed at $\langle p_T^{\text{Rscan}} \rangle$. The purpose of using a coarser η^{Rscan} binning is to have the same p_T^{Rscan} binning for the calibrations and uncertainties (see section 3.3.1).

This procedure is applied independently to the dijets and Z +jet topologies. Results are shown in the following sections 3.2.1 and 3.2.2. Subsequently, the results are statistically combined to assure adequate coverage of the entire p_T spectrum. Details on the combination procedure and results can be found in the appendix A.1.

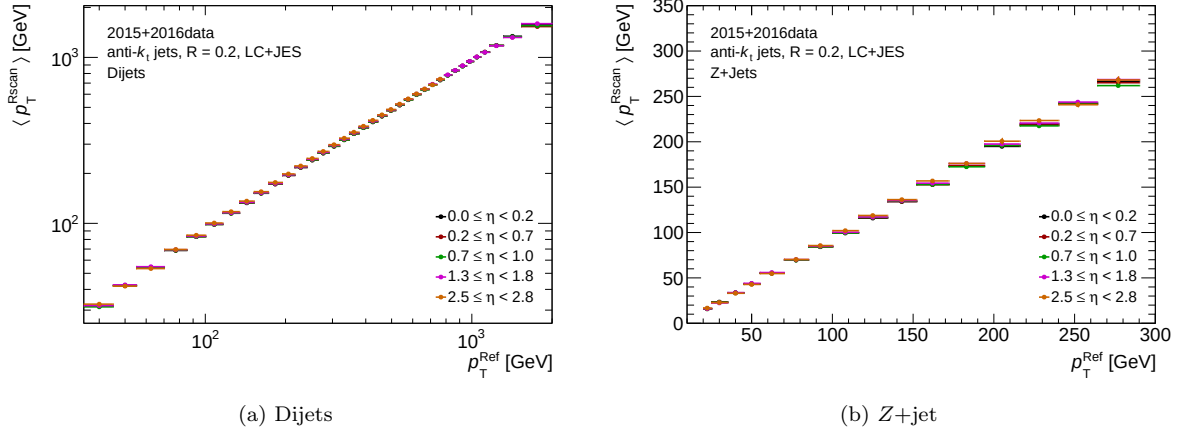


Figure 3.4: Average transverse momentum of R -scan for $R = 0.2$ jets as a function of the transverse momentum of the matched reference jet for representative η^{Rscan} bins. The asymmetric error bars in the x -axis correspond to the mapped p_T^{Ref} bins.

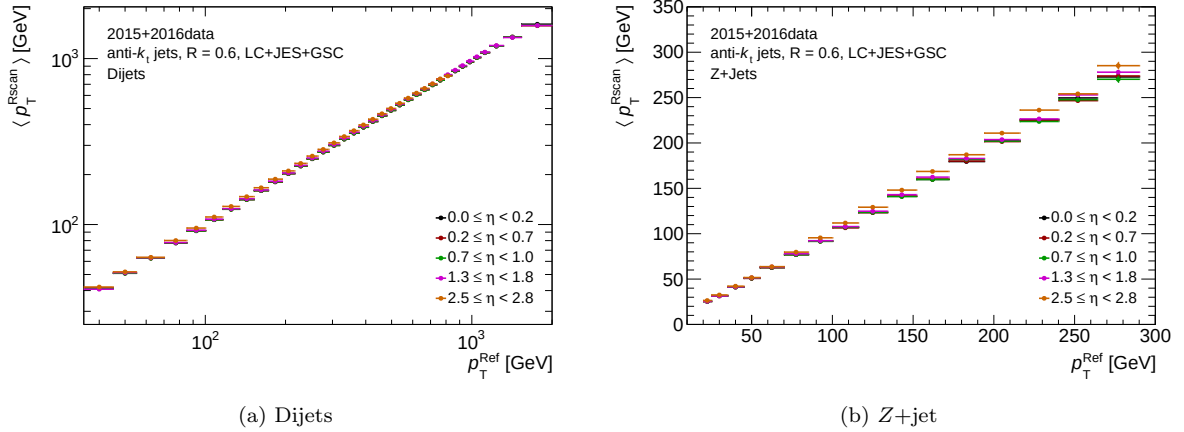


Figure 3.5: Average transverse momentum of R -scan for $R = 0.6$ jets as a function of the transverse momentum of the matched reference jet for representative η^{Rscan} bins. The asymmetric error bars in the x -axis correspond to the mapped p_T^{Ref} bins.

3.1.2.2 Event and object selection

For Z +jet, events with only two opposite-charge isolated and calibrated muons satisfying $|\eta| < 2.4$ and $p_T > 25$ GeV are selected. For the muon reconstruction (isolation), the

“Medium” (“Loose”) working point was used. In addition, events containing a Z candidate are selected. For this, the invariant mass of the two leading p_T muons, $m_{\mu\mu}$, is calculated and only events with $80 < m_{\mu\mu} < 116$ GeV are kept.

Candidate events are required to satisfy the following condition to prevent the leading pile up jets becoming reference jets:

$$\frac{0.5 \cdot (p_T^{(0)} + p_T^{(1)})}{p_T^{\text{truth}}} < 1.4$$

This typically happens for the low p_T slices only, but the requirement is applied to all MC simulation samples. Here, $p_T^{(0)}$ and $p_T^{(1)}$ are the transverse momenta of the leading and subleading reference jet candidates, while p_T^{truth} refers to the leading particle jet p_T .

For dijet as well as Z +jet events, jet quality is assured through the **LooseBad** flag definition for Run 2 [132]. The selection is designed to reject events from background processes (beam-gas or beam-halo events, cosmic ray muons and calorimeter noise) while keeping a high efficiency of selecting events produced in pp collisions. The jet quality criteria is applied only to hard-scatter jets, which are identified by the “Jet Vertex Tagger” (JVT) [133], using the “Medium” JVT working point.⁵ A jet is considered a pile-up jet if the JVT coefficient is below 0.59. Only jets with $p_T < 60$ GeV and $|\eta| < 2.4$ are examined for this. If a jet does not pass the quality criteria and is not a pile-up jet, the entire event is rejected.

For R -scan and reference, only jets with $p_T > 20$ GeV and $|\eta| < 3.0$ are selected. They must also fulfill isolation requirements. A jet i is considered isolated if it satisfies:

$$\Delta R(i, j) > 2 \times R, \quad i \neq j$$

where j runs over all other jets and R is the radius parameter of the jet. The same requirement is applied to reference and R -scan jets as well. All jets satisfying $p_T > 7$ GeV and $|\eta| < 3$ are used in the isolation requirement. For Z +jet, reference and $R = 0.2$ ($R = 0.6$) jets are further required to satisfy $\Delta R(\text{jet}, \text{muons}) > 0.35$ (0.6). Finally, an R -scan and a reference hard-scatter jet are considered matched if $\Delta R(R\text{-scan}, \text{reference}) < 0.2$.

Further technical details regarding the trigger strategy, the basic object selection and the samples used for this studies can be found in the original note [125].

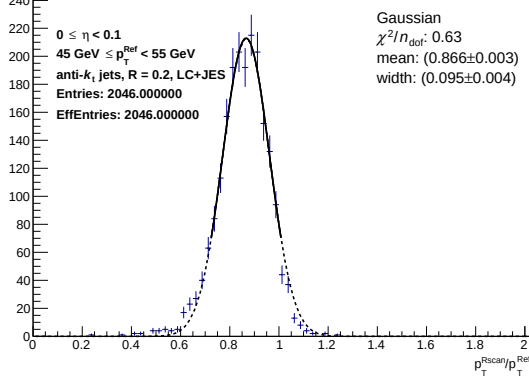
3.2 Results

3.2.1 Dijets

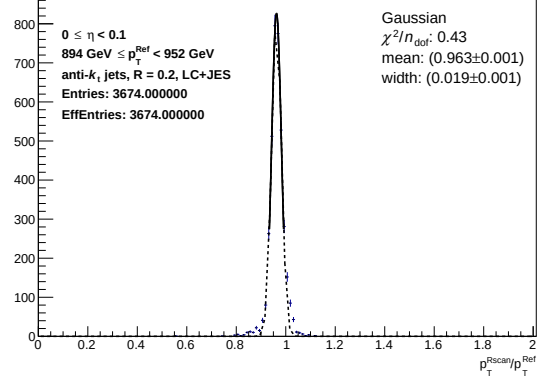
In order to get the correction factors from equation 3.2, distributions of the p_T ratio $\mathcal{R}$ defined by equation 3.1 are obtained from data (2015+2016) and MC in terms of p_T^{Ref} and η^{Rscan} bins. These distributions are fitted with a Gaussian function in order to obtain the average p_T ratio $\langle \mathcal{R} \rangle$ in a given $(p_T^{\text{Ref}}, \eta^{\text{Rscan}})$ bin. The core of the $\langle \mathcal{R} \rangle$ distributions shows a clear Gaussian behaviour in all bins considered. Figure 3.6 shows these distributions for some representative p_T^{Ref} and η^{Rscan} bins as well as their respective Gaussian fitted functions for $R = 0.2$ and $R = 0.6$ radii jets.

Figure 3.7 show the average p_T ratio $\langle \mathcal{R} \rangle$ extracted from the Gaussian fits to $\mathcal{R}$ for 2015+2016 data, MC16a PYTHIA 8 and, MC16a SHERPA as a function of p_T^{Ref} for representative η^{Rscan} bins for R -scan jets with $R = 0.2$ and $R = 0.6$. The ratios show only a

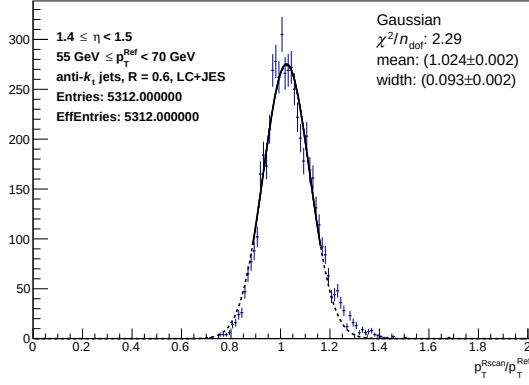
⁵The Medium JVT working point has a 92% (2%) efficiency of selecting hard-scatter (pile-up) jets.



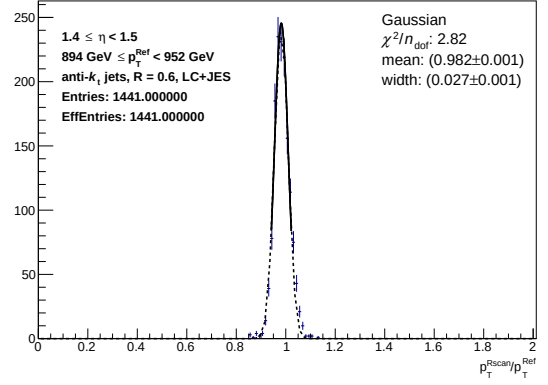
(a) $R = 0.2$, $45 < p_T^{\text{Ref}} < 55$ GeV, $0 < \eta^{\text{Rscan}} < 0.1$



(b) $R = 0.2$, $894 < p_T^{\text{Ref}} < 952$ GeV, $0 < \eta^{\text{Rscan}} < 0.1$



(c) $R = 0.6$, $55 < p_T^{\text{Ref}} < 70$ GeV, $1.4 < \eta^{\text{Rscan}} < 1.5$



(d) $R = 0.6$, $894 < p_T^{\text{Ref}} < 952$ GeV, $1.4 < \eta^{\text{Rscan}} < 1.5$

Figure 3.6: Representative distributions of the p_T ratio $\langle \mathcal{R} \rangle$ in 2015+2016 data and Gaussian fits for R -scan jets with $R = 0.2$ in the central region $0 < \eta^{\text{Rscan}} < 0.1$ and $R = 0.6$ in the $1.4 < \eta^{\text{Rscan}} < 1.5$ region, both for different p_T^{Ref} bins.

weak dependence on p_T^{Ref} , and range from 2% in the central region to 5% in the forward region.

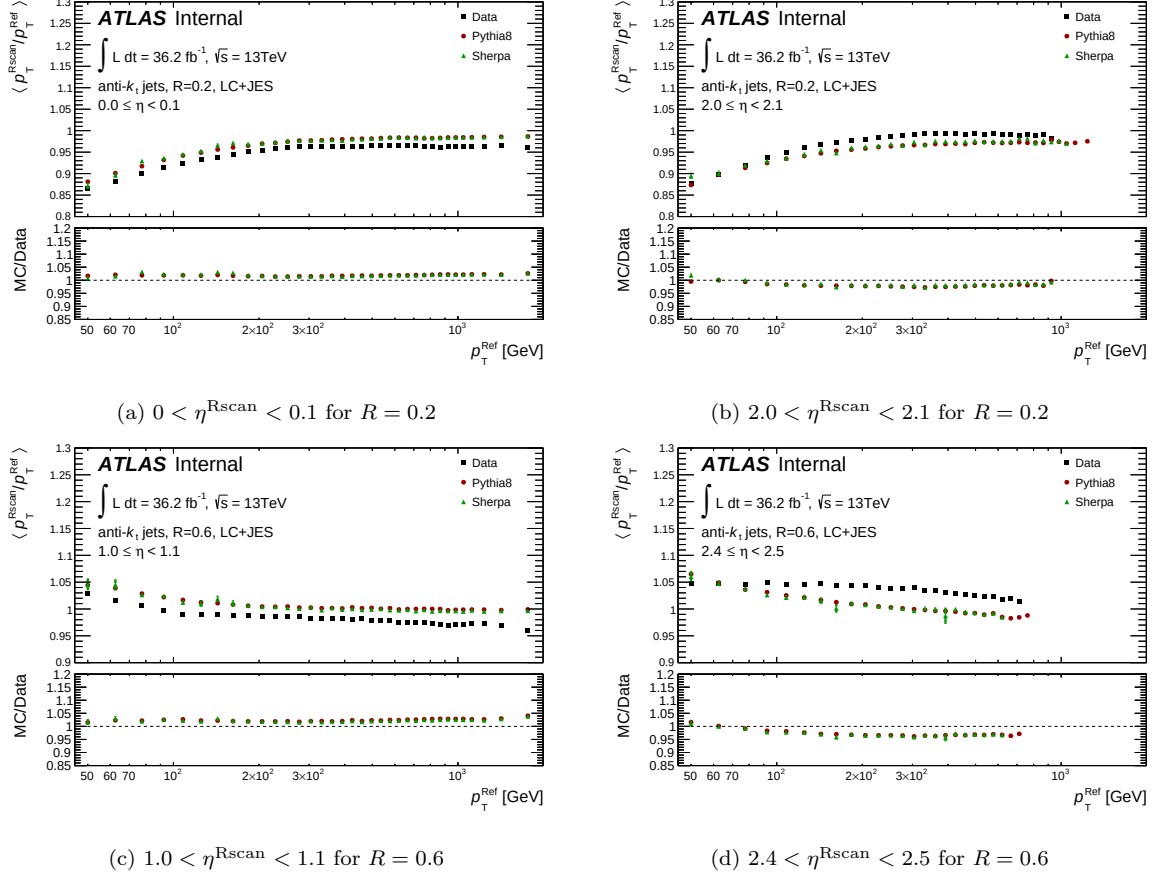
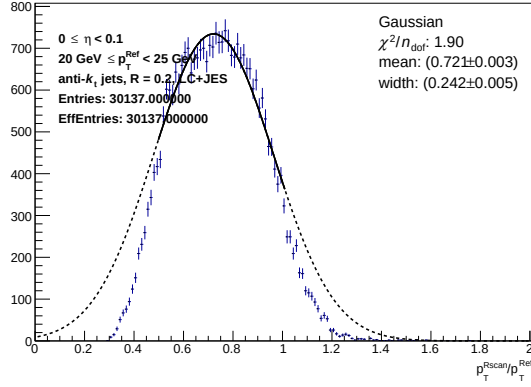


Figure 3.7: Average p_T ratio $\mathcal{R}$ as a function of p_T^{Ref} for 2015+2016 data (black squares), MC16a PYTHIA 8 (red circles) and, MC16a SHERPA (green triangles) for R -scan jets with $R = 0.2$ for (a) the $0\text{--}0.1$ η^{Rscan} bin and (b) for the $2.0\text{--}2.1$ η^{Rscan} bin. Same distributions are shown for R -scan with $R = 0.6$ for (c) the $1.0\text{--}1.1$ η^{Rscan} bin and (d) the $2.4\text{--}2.5$ η^{Rscan} bin. The bottom panels show the MC over data ratios.

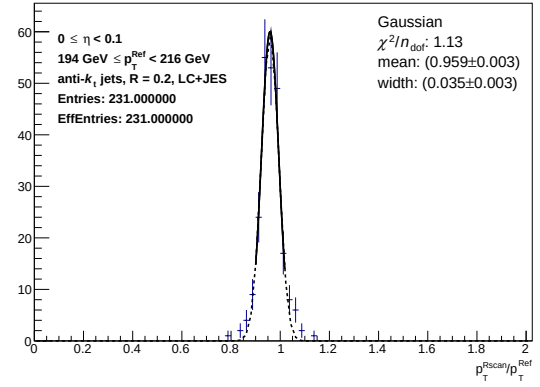
3.2.2 Z +jets

In the same way as the dijet results in section 3.2.1, results for Z +jet topology are discussed in this section. Figure 3.8 shows the distribution of the p_T ratio $\mathcal{R}$ from eq. 3.1 for 2015+2016 data in representative p_T^{Ref} and η^{Rscan} bins. Once more, the distributions are fitted to a Gaussian function in order to obtain the average p_T ratio $\langle \mathcal{R} \rangle$ in a given $(p_T^{\text{Ref}}, \eta^{\text{Rscan}})$ bin. The core of the $\mathcal{R}$ distributions shows a clear Gaussian behaviour in the vast majority of bins considered, except at low p_T^{Ref} , where, as expected, kinematic threshold effects are found to have an effect on the left shoulder of the $\mathcal{R}$ distribution. This does not significantly affect the $\langle \mathcal{R} \rangle$ extraction.

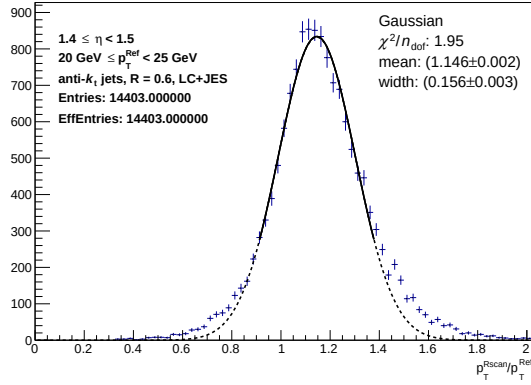
Figure 3.9 show the average p_T ratio $\langle \mathcal{R} \rangle$ extracted from the Gaussian fits to the $\mathcal{R}$ distributions for 2015+2016 data, MC16a POWHEG +PYTHIA and, MC16a SHERPA as a function of p_T^{Ref} for representative η^{Rscan} bins for R -scan jets with $R = 0.2$ and $R = 0.6$. The MC over data ratios are shown in the bottom panels. The ratios show almost no dependence on p_T^{Ref} , and range from 2% in the central region to 5% in the forward region.



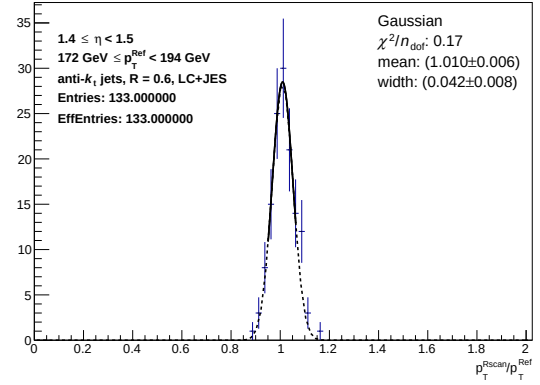
(a) $R = 0.2$, $20 < p_T^{\text{Ref}} < 25$ GeV, $0 < \eta^{\text{Rscan}} < 0.1$



(b) $R = 0.2$, $194 < p_T^{\text{Ref}} < 216$ GeV, $0 < \eta^{\text{Rscan}} < 0.1$

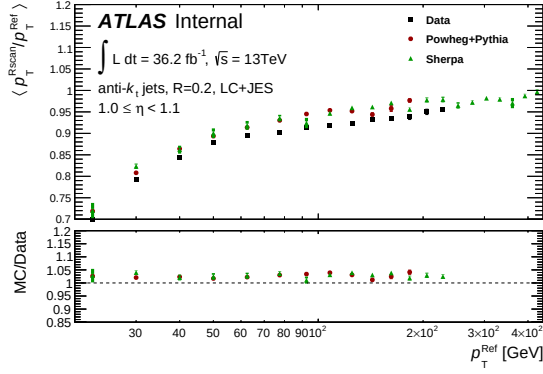


(c) $R = 0.6$, $20 < p_T^{\text{Ref}} < 25$ GeV, $1.4 < \eta^{\text{Rscan}} < 1.5$

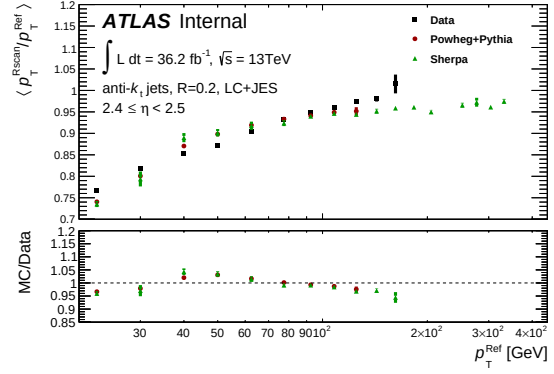


(d) $R = 0.6$, $172 < p_T^{\text{Ref}} < 194$ GeV, $1.4 < \eta^{\text{Rscan}} < 1.5$

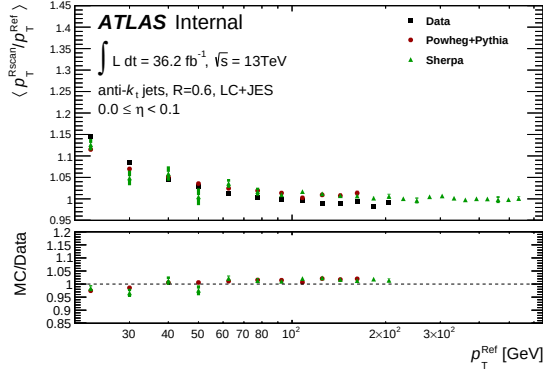
Figure 3.8: Representative distributions of the p_T ratio $\mathcal{R}$ in 2015+2016 data and Gaussian fits for R -scan jets with $R = 0.2$ in the central region and $R = 0.6$ in the $1.4 < \eta^{\text{Rscan}} < 1.5$ region, both for different p_T^{Ref} bins.



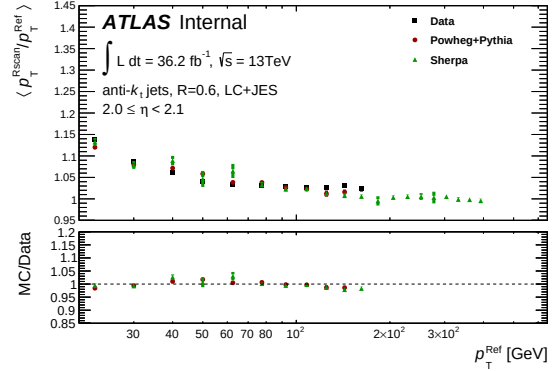
(a) $1.0 < \eta^{\text{Rscan}} < 1.1$ for $R = 0.2$



(b) $2.4 < \eta^{\text{Rscan}} < 2.5$ for $R = 0.2$



(c) $0 < \eta^{\text{Rscan}} < 0.1$ for $R = 0.6$



(d) $2.0 < \eta^{\text{Rscan}} < 2.1$ for $R = 0.6$

Figure 3.9: Average p_T ratio as a function of p_T^{Ref} for 2015+2016 data (black squares), MC16a POWHEG +PYTHIA (red circles) and, MC16a SHERPA (green triangles) for R -scan jets with $R = 0.2$ for (a) the 1.0 – 1.1 η^{Rscan} bin and (b) for the 2.4 – 2.5 η^{Rscan} bin; while $R = 0.6$ is shown for (c) the 0 – 0.1 η^{Rscan} bin and (d) the 2.0 – 2.1 η^{Rscan} bin. The bottom panels show the MC over data ratios.

3.2.3 Closure test

A standard procedure used within ATLAS to verify the correctness of any derived calibration is to perform a closure test. For this, the procedure detailed in section 3.1.2.1 is repeated but using the jets from data already corrected with the derived in-situ calibrations.

The closure test results for dijets are shown in representative η^{Rscan} bins in figure 3.10 for R -scan jets with $R = 0.2$ and $R = 0.6$.

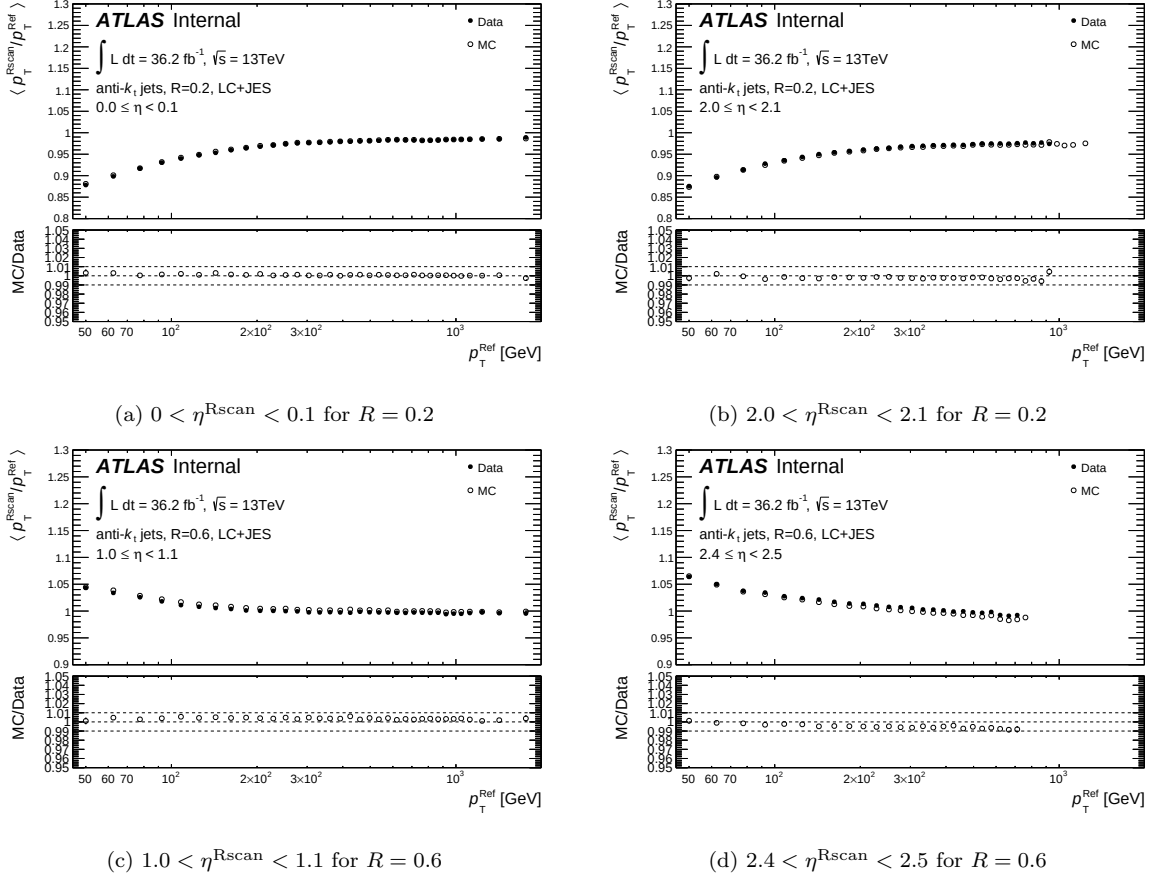
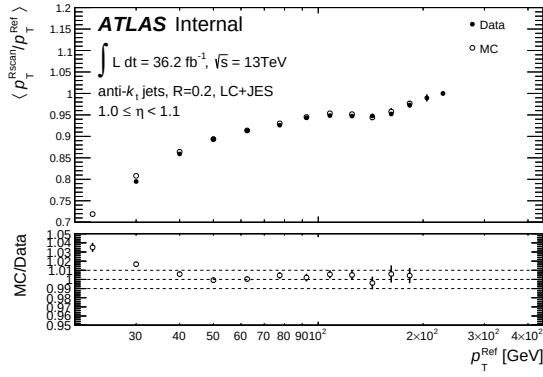


Figure 3.10: Closure of the in-situ calibration derived from dijet events for 2015+2016 data for R -scan jets with $R = 0.2$ and $R = 0.6$ in representative η bins.

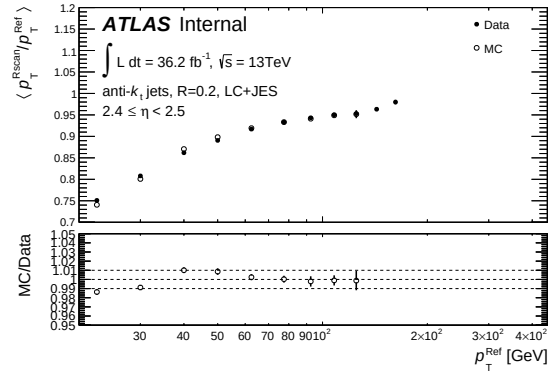
Similarly, the results for Z +jet are shown in figure 3.11 for R -scan jets with $R = 0.2$ and $R = 0.6$. For both calibrations, the non-closure is below 1%, as excepted at low p_T for Z +jet in a few η^{Rscan} bins.

After the calibration factors are obtained for each topology, the mapping procedure explained in section 3.1.2.1 takes place. The calibration results in terms of p_T^{Rscan} obtained in the dijet and Z +jet topologies are found to be consistent with each other. This can be seen for four representative η bins in figure 3.12 for R -scan jets with $R = 0.2$ and $R = 0.6$ radius parameter.

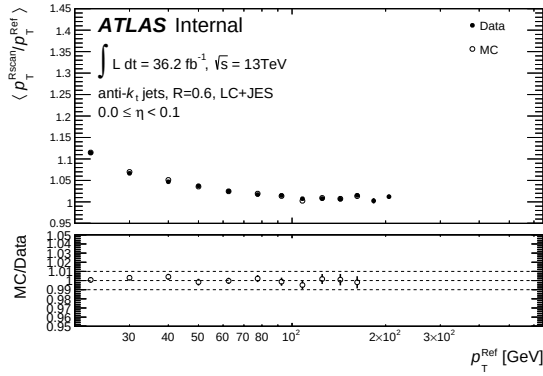
Given the consistency of the calibration results obtained in the dijet and Z +jet topologies, the two sets of calibration results can be statistically combined into a single calibration, to reduce the uncertainty and to maximise the domain of the jet calibration. Details on the statistical combination of the calibration procedure as well as the results are presented in appendix A.1.



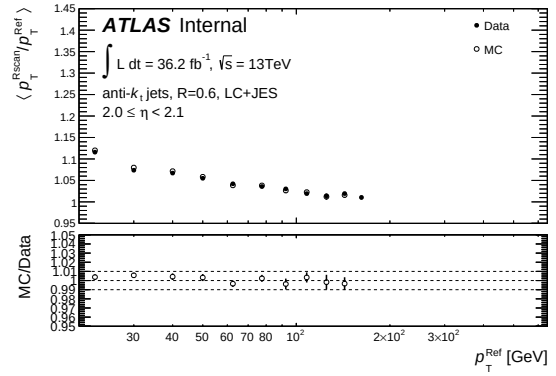
(a) $1.0 < \eta^{\text{Rscan}} < 1.1$ for $R = 0.2$



(b) $2.4 < \eta^{\text{Rscan}} < 2.5$ for $R = 0.2$

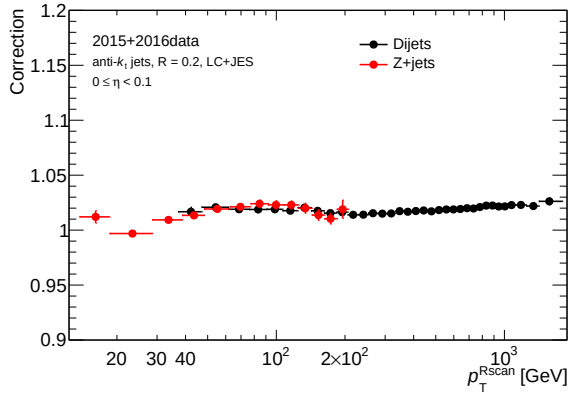


(c) $0 < \eta^{\text{Rscan}} < 0.1$ for $R = 0.6$

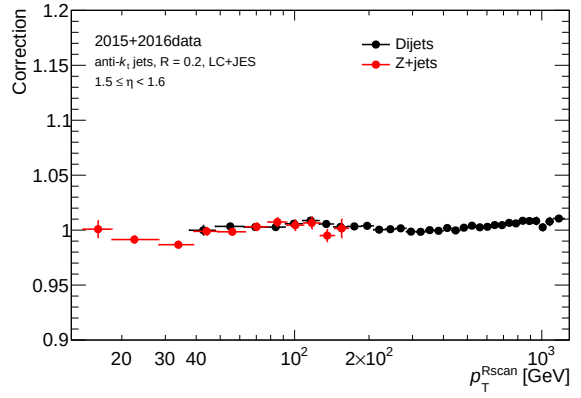


(d) $2.0 < \eta^{\text{Rscan}} < 2.1$ for $R = 0.6$

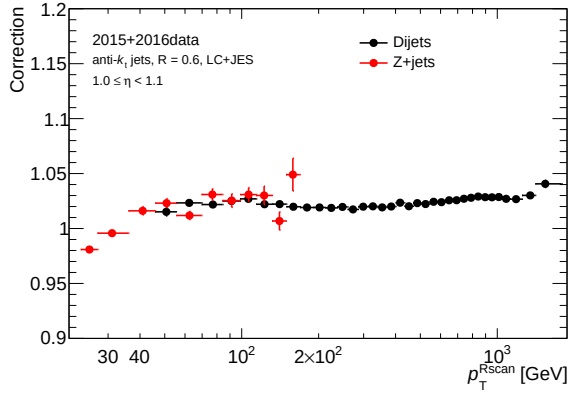
Figure 3.11: Closure of the in-situ calibration derived from Z +jet events for 2015+2016 data for R -scan jets with $R = 0.2$ and $R = 0.6$ in representative η bins.



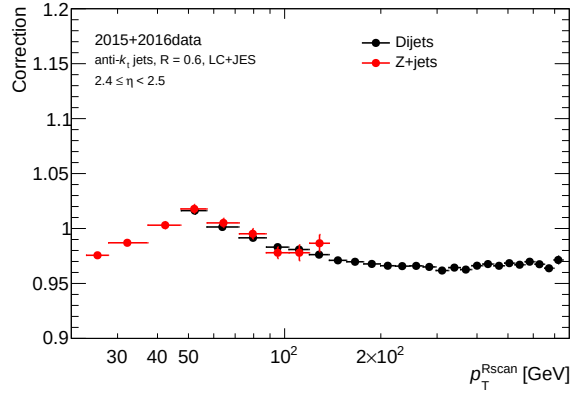
(a) $0 < \eta < 0.1$ for $R = 0.2$



(b) $1.5 < \eta < 1.6$ for $R = 0.2$



(c) $1.0 < \eta < 1.1$ for $R = 0.6$



(d) $2.4 < \eta < 2.5$ for $R = 0.6$

Figure 3.12: Comparison of the Z+jet and dijets calibrations for R -scan jets with $R = 0.2$ and $R = 0.6$ in representative η bins.

3.3 Systematic uncertainties

3.3.1 Direct matching method uncertainties

There are some parameters that are intrinsic to the direct matching method, basically the ones used to define the matching between the jets. The arbitrary choice of these parameters is varied to derive systematic uncertainties. The election of those variations is summarised in table 3.2.

Parameter	Down variation	Nominal	Up variation
dR in matching ($\Delta R(R_{\text{scan}}, \text{Ref}) < dR$)	0.1	0.2	0.3
f in isolation ($\Delta R > f \times R$)	1.5	2	2.5
JVT working point	Loose (0.11)	Medium (0.59)	Tight (0.91)

Table 3.2: Summary of the systematic uncertainties in the in-situ direct matching method, excluding those propagated from reference jets.

A MC modelling uncertainty is also considered and it is derived by comparing the nominal calibration with one evaluated using a sample with a different MC generator. Table 3.3 shows the MC samples used for each topology.

	Dijets	Z+jets
Nominal	PYTHIA 8	POWHEG +PYTHIA
Variation	SHERPA	SHERPA

Table 3.3: Summary of the MC samples used for the nominal calibration and for the estimation of the MC modelling uncertainty for dijets and Z+jets.

Due to statistics limitations, the systematic uncertainties are derived in coarser η^{Rscan} bins with respect the ones used to derive the calibration. These are shown in table 3.1. New sets of calibration factors (as a function of $p_{\text{T}}^{\text{Ref}}$) are derived by varying up and down one of the parameters or by using a different MC simulation sample, as shown in the tables above. Finally, the systematic uncertainty is defined as the relative difference between the nominal calibration and the systematically shifted one, which is then mapped to be as a function of $p_{\text{T}}^{\text{Rscan}}$, as described for the nominal calibration in section 3.1.2.1.

The statistical uncertainties on each systematic uncertainty are evaluated using a bootstrapping technique based on an ensemble of 100 pseudo-experiments. Each pseudo-experiment is constructed by reweighting each event in data and simulation according to a Poisson distribution with expectation value equal to one. This procedure preserves the correlations between jets produced in the same event. Each systematic uncertainty is evaluated for each pseudo-experiment and the statistical uncertainty is obtained by taking the square root of the means.

The evaluated systematic uncertainties are rebinning along $p_{\text{T}}^{\text{Rscan}}$ until the observed shifts are statistically significant. This avoids a multiple counting of statistical uncertainties in the systematics. The significance threshold for the rebinning was chosen to be equal to one, where the significance is defined in the following way

$$\frac{|\sum_i \text{uncertainty}_i / \text{error}_i|^2}{\sqrt{\sum_i \frac{1}{\text{error}_i^2}}}$$

where the sum is over p_T^{Rscan} bins.

In order to not remove features that could be due to physics effects, a maximum of five bins are allowed to be merged.

To illustrate the rebinning results, figure 3.13 shows a comparison of the MC modelling systematic uncertainty and their significance before and after the p_T rebinning for anti- k_t jets with radius parameter $R = 0.2$ for the dijet topology.

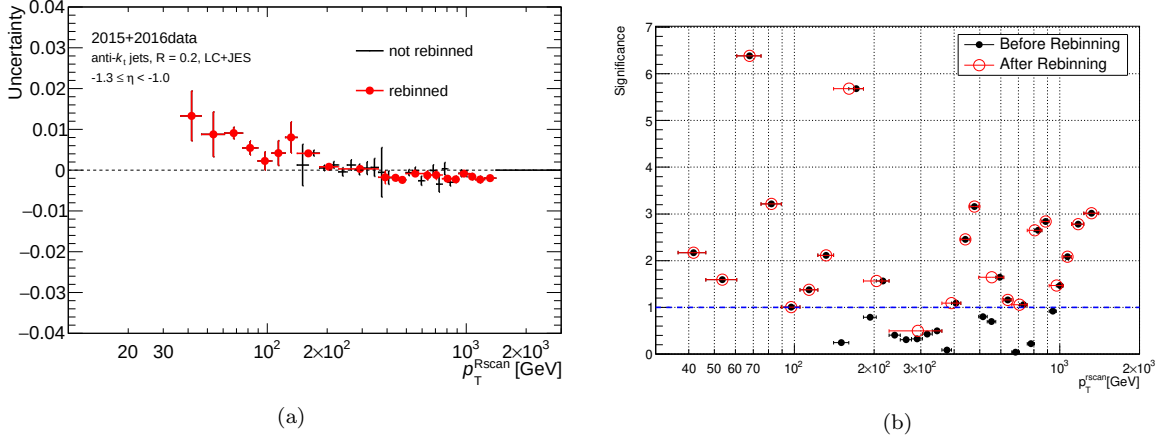


Figure 3.13: (a) In-situ MC modelling systematic uncertainty for dijets as function of p_T^{Rscan} for anti- k_t jets with radius parameter $R = 0.2$ in the $-1.3 < \eta < -1.0$ region before (black) and after (red) the p_T rebinning. (b) shows the significance before (black) and after (red) the p_T rebinning.

In addition, figure 3.14 shows a comparison of the dR down variation and JVT up variation systematic uncertainties before and after the p_T rebinning for R -scan jets with radius parameter $R = 0.2$ and $R = 0.6$ for the dijet topology. While figure 3.15 shows also this comparison but this time for the isolation down variation and MC modelling systematic uncertainties for the Z +jet case. In each case a selected η^{Rscan} bin is shown.

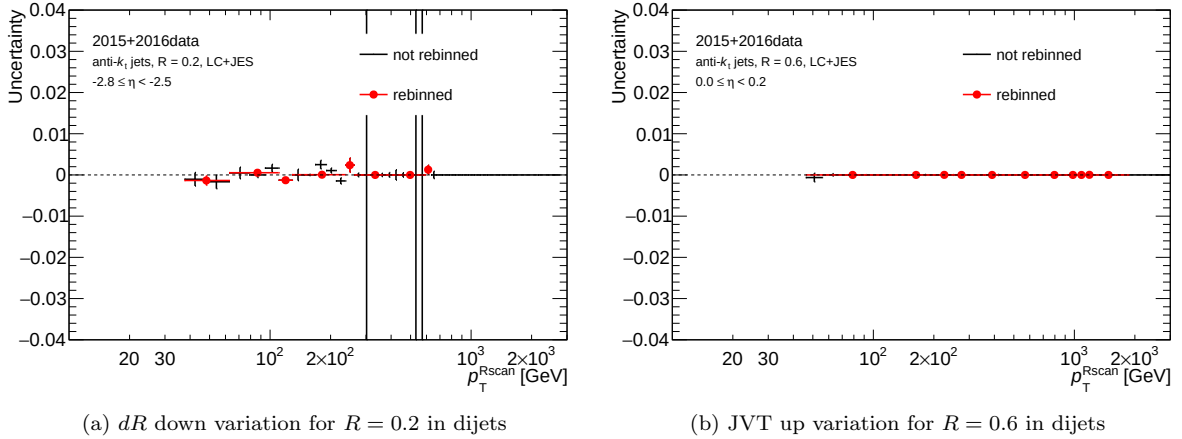
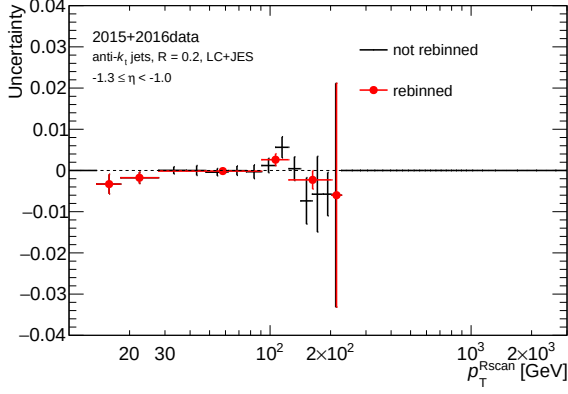


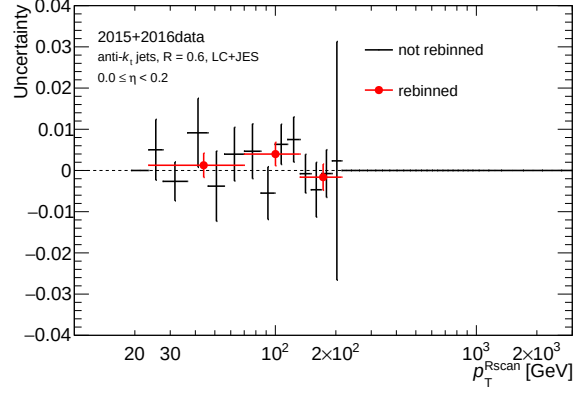
Figure 3.14: (a) In-situ systematic uncertainty for dijets accounting for the down variation of dR in the matching as function of p_T^{Rscan} for anti- k_t jets with radius parameter $R = 0.2$ with $-2.8 < \eta < -2.5$ before (black) and after (red) the p_T rebinning. The systematic uncertainty corresponding to the JVT up variation for R -scan $R = 0.6$ in dijets is also shown in (b) for the $0 < \eta < 0.2$ region.

Lastly, the final systematic uncertainties are then stored in the original p_T^{Rscan} binning and are shown for dijets and Z +jet s in figures 3.16 and 3.17, respectively.

The impact of the systematic uncertainties show a similar trend for $R = 0.2$ and $R = 0.6$, being the one related with the Monte Carlo choice (labelled as MC Sherpa) the

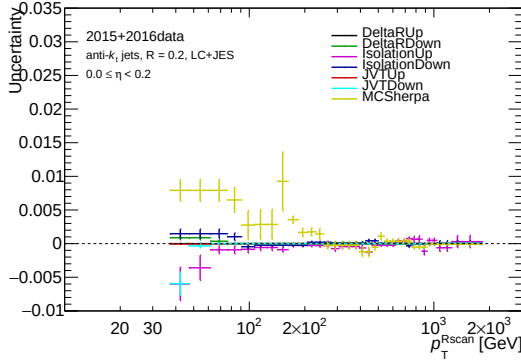


(a) Isolation down variation for $R = 0.2$ in Z +jet

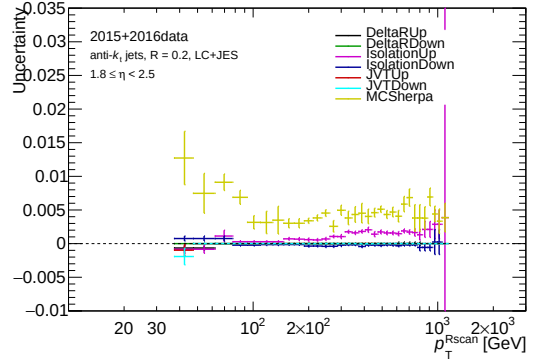


(b) MC modelling for $R = 0.6$ in Z +jet

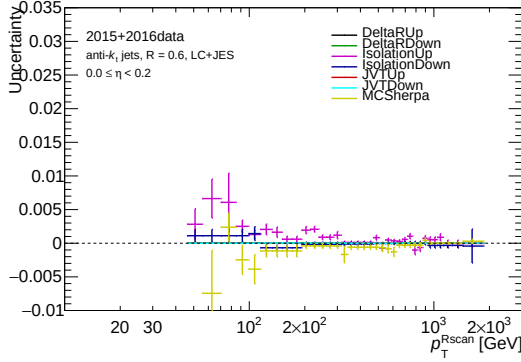
Figure 3.15: (a) In-situ systematic uncertainty for Z +jet accounting for the down variation of the isolation in the matching as function of p_T^{Rscan} for anti- k_t jets with radius parameter $R = 0.2$ with $-1.3 < \eta < -1.0$ before (black) and after (red) the p_T rebinning. The systematic uncertainty corresponding to the MC modelling for R -scan $R = 0.6$ in Z +jet is also shown in (b) for the $0 < \eta < 0.2$ region.



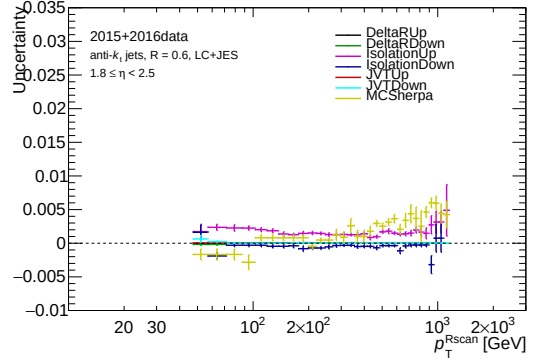
(a)



(b)



(c)



(d)

Figure 3.16: Final in-situ systematic uncertainties for dijets for anti- k_t jets with radius parameter $R = 0.2$ (a and b) and $R = 0.6$ (c and d) with $0 < \eta < 0.2$ (a and c) and with $1.8 < \eta < 2.5$ (b and d).

dominant one, follow by the one associated to the isolation requirement. As expected these uncertainties have a larger impact on the low p_T jet range where $p_T^{\text{Rscan}} \lesssim 20$ GeV.

In the same way as it is done for the nominal calibration, the systematic uncertainties are also statistically combined. The procedure and the results can be found in appendix A.1.2.

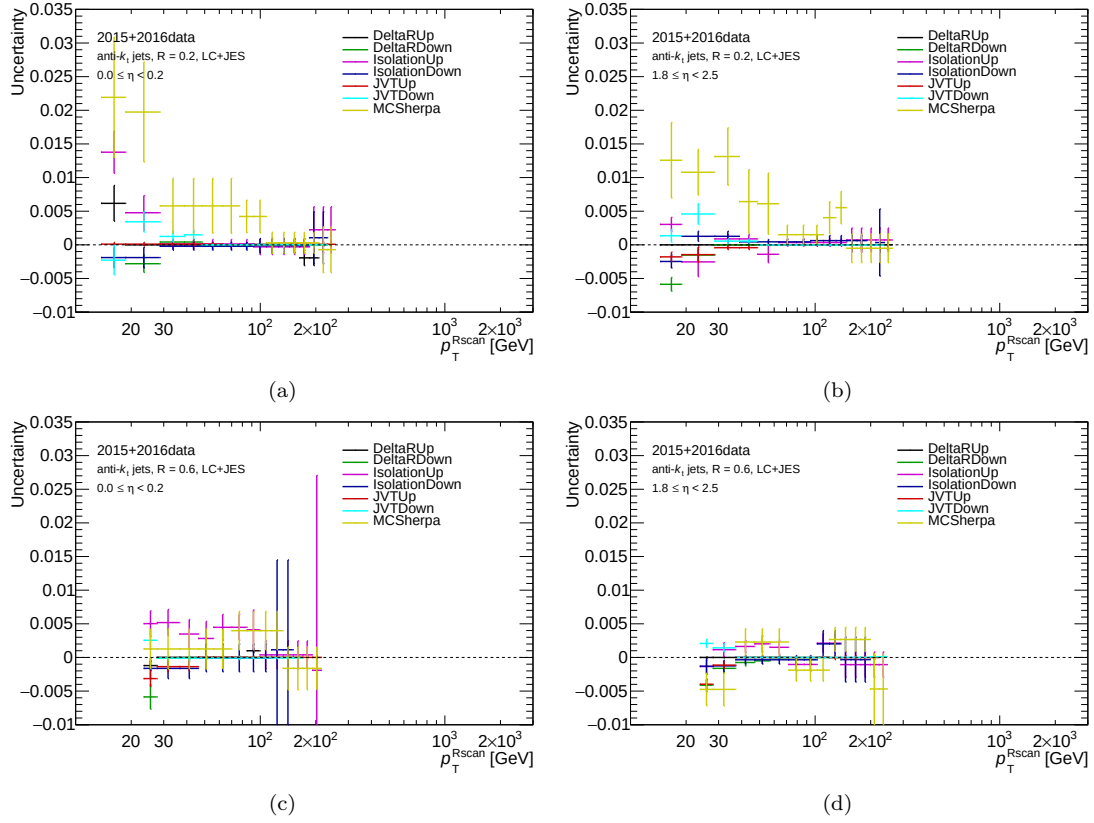


Figure 3.17: Final in-situ systematic uncertainties for Z +jet for anti- k_t jets with radius parameter $R = 0.2$ (a and b) and $R = 0.6$ (c and d) with $0 < \eta < 0.2$ (a and c) and with $1.8 < \eta < 2.5$ (b and d).

3.3.2 Other systematic uncertainties

Table 3.4 summarises all the systematic uncertainties in the JES. In addition to the in-situ uncertainties, other sources of uncertainty come from the pile-up corrections, jet flavour response and composition, contribution of particles outside the jet cone, punch-through correction and single-particle and test-beam measurements

Since well calibrated $R = 0.4$ are used for deriving the in-situ calibrations, also their respective uncertainties contribute to the overall picture and they need to be properly propagated over the R -scan in-situ calibrations. They are also considered in the table and marked with an asterisk.

In particular, the out-of-cone radiation and the residual pile-up correction p_T dependence have an important effect on the in-situ calibration method and they are further studied on the internal note [125].

Name	Description
Dijets	
ΔR matching	Variation of the matching criteria
Isolation	Variation of the isolation requirement
JVT for reference jets	Jet vertex tagger uncertainty
Statistical	Statistical uncertainty over all regions of jet p_T and η
Z+jets	
ΔR matching	Variation of the matching criteria
Isolation	Variation of the isolation requirement
JVT for reference jets	Jet vertex tagger uncertainty
Statistical	Statistical uncertainty over all regions of jet p_T and η
Pile-up	
μ offset*	Uncertainty of the μ modelling in MC simulation
N_{PV} offset*	Uncertainty of the N_{PV} modelling in MC simulation
ρ topology	Uncertainty of the per-event p_T density modeling in MC simulation
p_T dependence	Uncertainty in the residual p_T dependence
Jet flavour	
Flavor composition	Uncertainty in the jet composition between quarks and gluons
Flavor response	Uncertainty in the jet response of gluon-initiated jets
b -jet	Uncertainty in the jet response of b -quark-initiated jet
Out-of-cone	Contribution of particles outside the jet cone
Punch-through*	Uncertainty in punch-through GS correction
Single-particle response*	High p_T jet uncertainty from single-particle and test-beam measurements

Table 3.4: Summary of the systematic uncertainties in the JES, including those propagated from reference jets. Those with an asterisk are derived using $R = 0.4$ jets at EM scale.

Chapter 4

Search for resolved dijet resonances produced in association with a photon

“Imagination will often carry us to worlds that never were, but without it we go nowhere.”

Carl Sagan

Searches for new particles decaying to pairs of jets have been a fundamental part of the physics programme at collider experiments for over thirty years [134]. Since any strongly interacting new particle directly produced at a hadron collider via quarks and gluons (i.e. excepting VBF processes) must decay to them, dijet signatures offer a simple way to search for a wide array of possible new physics models. Each increase in collision energy for a given collider comes with a corresponding increase in parton luminosity, allowing searches to access higher mass ranges for possible new physics. However, this access to higher energies comes at a high cost: lower masses and smaller hypothesised couplings are rendered inaccessible by the trigger prescales required to control increasing instantaneous luminosities. Dijet searches in ATLAS at 13 TeV have excluded resonances beginning at a mass of 1.2 TeV [135, 136], 0.2 TeV [137], and an 8 TeV dijet search [138] beginning from 250 GeV was strongly limited by these same trigger prescales, while CMS excluded resonances between 50 and 350 GeV at 13 TeV [139, 140]. Low-mass resonances were studied by early experiments such as UA2 and CDF with only a very limited dataset, such that models with small couplings to SM particles were not well constrained [134, 138].

ATLAS and CMS have engaged in a programme of complementary searches targeting this low-mass, low-coupling region in several ways. The trigger-level analysis (TLA) technique evades trigger bandwidth restrictions by recording only minimal event information but at a very high rate [141, 142]. A second approach assumes the production of a high- p_T initial-state radiation (ISR) object, such as a jet or a photon, against which the new particle recoils [3]. This ISR object can be used for triggering, allowing the resonance to be reconstructed from lower- p_T jets that would not pass an unprescaled single-jet trigger. In the case that such a resonance is very light, it would be strongly boosted when recoiling against the ISR object. This scenario is studied by reconstructing the decay products as a single large- R jet [143, 144]. For a resonance of intermediate mass, too light to be

accessible to the dijet analysis and too heavy to produce a strongly boosted decay, a final state is studied consisting of two small- R jets in addition to the ISR object. A resolved final state, consisting of two jets and one photon (see figure 4.1), is the subject of this analysis presented in this chapter. It has been previously studied in several preliminary results but has never yet been published by ATLAS or CMS [145].

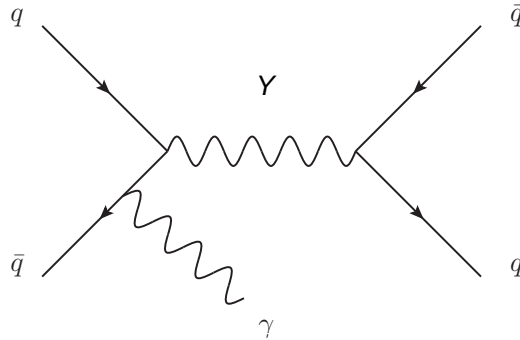


Figure 4.1: Example Feynman diagram for a generic new resonance Y produced in association with photon ISR object and decaying to two jets.

Figure 4.1 illustrates an example process for production of a generic new resonance (Y) in association with an ISR object. For this analysis, a leptophobic axial-vector mediator Z' particle is used as a benchmark model to take the place of Y as described in [4]. For some BSM models [146–148], new particles are expected to preferentially decay to third-generation quarks. Sensitivity to such models can be dramatically improved by requiring that one or both of the jets from the resonance decay be *tagged* as originating from a b -quark.

A summary of the different searches along with the latest results (including the one from this analysis, namely as *Dijet+ISR*) carried out by the ATLAS experiment is shown in figure 4.2. Dijet search contours for 95% CL upper limits on the coupling g_q as a function of the resonance mass $m_{Z'_A}$ for the leptophobic axial-vector Z'_A model are presented in it.

This analysis uses data collected with the ATLAS detector in 2015–2017 at a centre-of-mass energy of 13 TeV. This dataset corresponds to integrated luminosities between 76.6 fb^{-1} and 79.8 fb^{-1} for this analysis, depending on the particular triggers used. The invariant mass distribution of a selected pair of jets (m_{jj}) in each event is compared to a smooth SM-only background prediction taken from a fit. A model-nonspecific search phase compares the data to the expected background over the mass range 169 GeV to 1200 GeV¹ to determine whether any significant discrepancy is observed. In case the search phase does not show any significant excess, limits are then set on the benchmark Z' models for signal masses in the range 250 GeV to 1100 GeV. Four channels are analysed in total, all of which correspond to a photon ISR object. These consist of two different trigger selections, one optimised for higher m_{jj} (*combined trigger*) and the other allowing access to lower m_{jj} ranges (*single photon trigger*), and two different jet selections: b -tagged and inclusive. The results of this analysis are reported in [5].

¹The lower limit for the search is determined by the trigger requirement and the upper limit is driven by either the requirement of a low enough range for a good fit combined with the presence of a search in the same phase space, or by data statistics

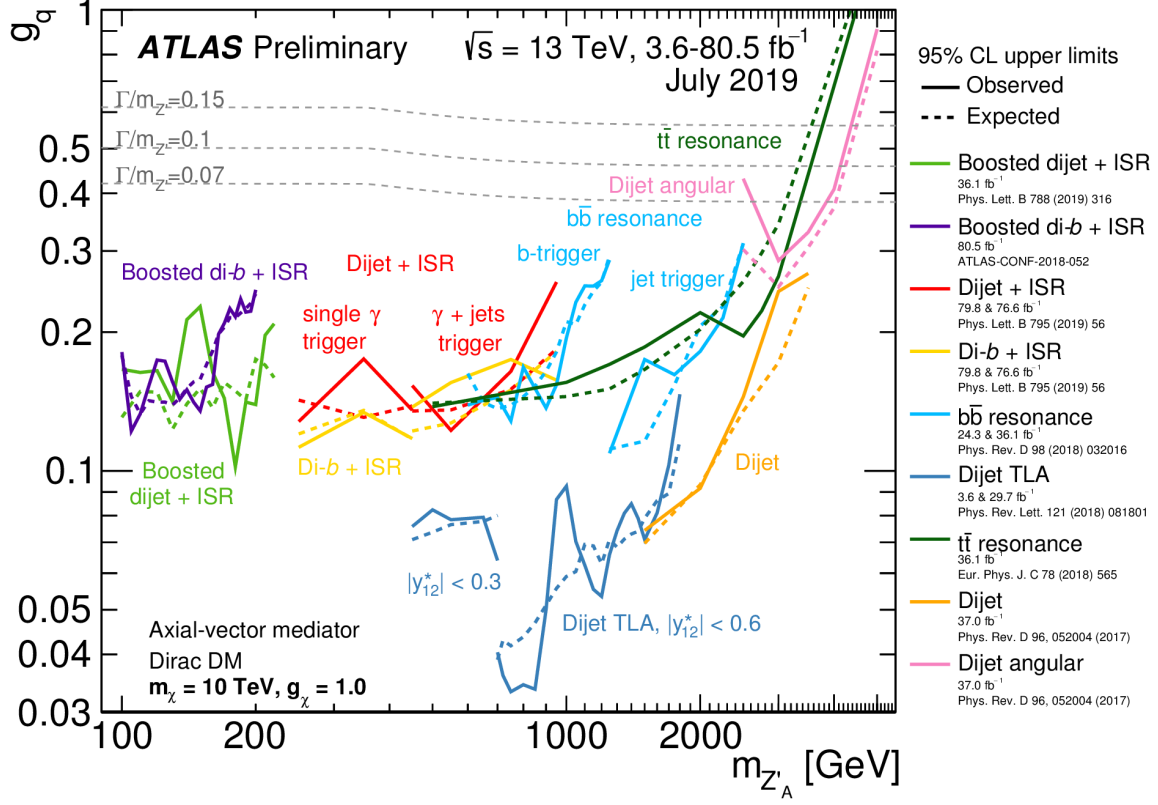


Figure 4.2: Dijet search contours for 95% CL upper limits on the coupling g_q as a function of the resonance mass $m_{Z'_A}$ for the leptophobic axial-vector Z'_A model. The expected limits from each search are indicated by dotted lines. The TLA dijet analysis has two parts, employing different datasets with different selections in the rapidity difference y^* as indicated. The dijet+ISR (γ) analysis also has two parts, each using a different trigger strategy, and each further studied in inclusive and b -tagged channels. Coupling values above the solid lines are excluded, as long as the signals are narrow enough to be detected using these searches.

4.1 Dataset and Monte Carlo simulations

4.1.1 Dataset

Studies in this analysis are based on pp collision data collected at $\sqrt{s}=13$ TeV between 2015 and 2017 inclusive, corresponding to a luminosity of 76.6 fb^{-1} and 79.8 fb^{-1} depending on the channel studied (see section 4.2.4). Events with unsuitable beam conditions or some inactive portions of the detector are removed by the application of a Good Runs List.

Between 2016 and 2017, both topoclustering thresholds and pileup conditions changed. Alteration in the LHC bunch scheme partway through 2017 also dramatically altered the pileup profile for the year's dataset. Therefore, several cross checks comparing 2016 to 2017 data, as well as both datasets to corresponding MC campaigns were performed (see section 4.3).

4.1.2 Monte Carlo samples

This analysis employs a data-driven background estimate. MC samples corresponding to background processes were only used as cross checks and for studies of the analysis strategy before unblinding. Monte Carlo samples corresponding to BSM Z' production and decay were used to optimise the analysis selection and to determine the reported limits.

All MC samples used are produced with a Geant4-based simulation, with additional pile-up interactions in each simulated event modeled by adding multiple soft pp collisions generated by Pythia 8.165 [149] with the MSTW2008 LO PDF and AU2 tune [150]. After event generation and the addition of pile-up, the response of the ATLAS detector to particles passing through the detector elements is simulated with the GEANT4 toolkit [57] and events are reconstructed using the same software used to reconstruct events in data.

Background processes

Background processes with a photon and 1, 2 or 3 jets were simulated with SHERPA as generator (NLO). MC16a and MC16d campaigns are used. More details of these samples can be found in [151].

Signals

The main benchmark model is a Z' axial vector mediator signal consistent with recent recommendations from the ATLAS-CMS Dark Matter (DM) Forum [4]. This simplified model is also used in other ATLAS and CMS searches including DM mediators as one of their benchmarks (e.g. monojet [152], high-mass dijet [136], TLA [141], other iterations of the dijet+ISR search [145]).

This benchmark signal is used in the search and limit-setting phases of the analysis and for testing the sensitivity of potential resonant signals on the search phase. It is motivated by the role that searches for dijet resonances play in constraining possible interactions between dark matter and the SM. In this analysis, we consider a pure axial-vector leptophobic Z' model in the specific scenario outlined in ref.[153], where dijet searches complement mono-jet-like searches in regions of parameter space where the decay of the Z' to invisible particles is kinematically suppressed.

In this model, the Z' arises from a simple extension of the SM with an additional $U(1)$ gauge symmetry and a Dirac fermion Dark Matter particle that has charges only under this new group. Assuming that some SM particles are also charged under this group, the Z' can mediate interactions between the SM and DM. The DM particle χ has a mass m_χ . The spin-1 Z' has mass M_{med} .

The Dark Matter Forum report models with vector or axial-vector couplings between the spin-1 mediator Z' and SM and DM fields, with the corresponding interaction lagrangians:

$$\mathcal{L}_{\text{vector}} = g_{SM} \sum_{q=u,d,s,c,b,t} Z'_\mu \bar{q} \gamma^\mu q + g_{DM} Z'_\mu \bar{\chi} \gamma^\mu \chi \quad (4.1)$$

$$\mathcal{L}_{\text{axial-vector}} = g_{SM} \sum_{q=u,d,s,c,b,t} Z'_\mu \bar{q} \gamma^\mu \gamma^5 q + g_{DM} Z'_\mu \bar{\chi} \gamma^\mu \gamma^5 \chi. \quad (4.2)$$

The parameters in the model are then

$$\{ g_{SM}, g_{DM}, m_\chi, M_{\text{med}} \}, \quad (4.3)$$

where g_{SM} is the coupling of the Z' mediator to quarks, g_{DM} is its coupling to the DM fermion, m_χ is the mass of the DM fermion and M_{med} is the Z' mass.

The two most relevant parameters of this model in the dijet search are the coupling of the Z' to quarks as it drives the intrinsic width of the resonance, and the Z' mass. The DM mass is fixed at 10 TeV and the coupling to DM to 1.5. Changing the DM-related parameters has no effect on the width of the resonance in this search, since with this choice the mediator cannot decay directly to DM. Nevertheless, a dijet search can still probe a dark interaction even though the DM particle is inaccessible to colliders.

Signal samples have been generated for ten mass points. These have been produced with at least 20,000 events with coupling constants $g_{SM} = 0.1, 0.2, 0.3$ and 0.4 . Given that this analysis is sensitive to samples with $g_{SM} \sim 2$, higher couplings than the ones produced are not necessary since the corresponding mass points would be already excluded.

The signal samples have been generated using the Madgraph generator [154] with the NNPDF2.3 LO PDF [155] and the A14 tune [53], and hadronic showers are produced in PYTHIA 8. Further details on simulated samples can be found in the internal note [156].

The width is calculated as:

$$\Gamma_{\text{Med}} = \Gamma_{\text{DM}} + \Gamma_{\text{SM}} \quad (4.4)$$

where:

$$\Gamma_{\text{SM}} = \sum_{q \in (m_q < \frac{m_{\text{Med}}}{2})} \frac{3m_{\text{Med}}g_{SM}^2}{12\pi} \times \left(1 - \frac{(2m_q)^2}{m_{\text{Med}}^2} \right)^{3/2} \quad (4.5)$$

and

$$\Gamma_{\text{DM}} = \begin{cases} \frac{m_{\text{Med}}g_{\text{DM}}^2}{12\pi} \times \left(1 - \frac{(2m_{\text{DM}})^2}{m_{\text{Med}}^2} \right)^{3/2}, & \text{if } m_{\text{DM}} < \frac{m_{\text{Med}}}{2} \\ 0, & \text{otherwise} \end{cases} \quad (4.6)$$

Further details on the signal modelling are given in appendix B.3.

This analysis is sensitive to couplings at the level of 0.1 and 0.2 and will only set limits in the regime where the width is less than 15% of the resonance mass. Signals with larger widths cannot be discovered by the search phase, and attempting to fit for these wider signals can potentially bias the background fit. For much wider signals, it would also be necessary to account for interference with the standard model.

4.2 Object reconstruction and event selection

4.2.1 Object reconstruction and calibration

In all of the events selected for analysis, all components of the detector are required to be operating correctly. In addition, all events are required to have a reconstructed primary vertex [133], defined as a vertex with at least two reconstructed tracks, each with $p_T > 500$ MeV.

Since the target final state is characterised mainly by the presence of two jets and a photon, their effective reconstruction becomes significant in order to obtain sensitive results.

Photon candidates are reconstructed from clusters of energy deposits in the electromagnetic calorimeter [157], and their energy corrected by applying energy scale factors measured with $Z \rightarrow e^+e^-$ decays [158].

The trajectory of the photon is reconstructed using the longitudinal segmentation of the calorimeters along the shower axis (shower depth) and a constraint from the average collision point of the proton beams. Candidates are restricted to the region $|\eta| < 2.37$, excluding the transition region between the barrel and endcap calorimeters to ensure that they arise from well-calibrated regions of the calorimeter. An additional requirement is applied on the transverse energy of the photon candidate after reconstruction, which is required to have $p_T > 10$ GeV. Later selection to ensure trigger efficiency is much tighter; no event without at least one photon of $p_T > 95$ GeV will enter the analysis.

Quality requirements are applied to the photon candidates to reject events containing misreconstructed photons arising from instrumental problems or from non-collision backgrounds. A default overlap removal procedure is applied to separate photons from jets, following the recommendations of the analysis harmonisation taskforce [159]. This ensures that if a jet and a photon are found within $\Delta R < 0.4$ of one another, the jet is removed. Further *tight* identification requirements are applied to reduce contamination from π^0 or other neutral hadrons decaying into two photons [157]. The photon identification is based on the profile of the energy deposits in the first and second layers of the electromagnetic calorimeter. In addition to the tight identification requirement, candidates must meet *tight isolation* criteria using calorimeter and tracking information, requiring that they be separated from nearby event activity [160, 161]. This specifies that the sum of energies of all EM-scale topoclusters in a $\Delta R < 0.4$ cone around the photon must satisfy the following: $\text{topoetcone40} < 2.45 \text{ GeV} + 0.022 \cdot E_T^\gamma$. An additional requirement is placed on tracks such that the sum of track p_T in a $\Delta R < 0.2$ cone around the photon must be a small fraction of the total photon p_T : $\text{ptcone20}/p_T^\gamma < 0.05$. Converted photon candidates matched to one track or a pair of tracks passing inner-detector quality requirements [157] and satisfying tight identification and isolation criteria are also considered. Any pair of matching tracks must form a vertex that is consistent with originating from a massless particle.

When it comes to jets, these are reconstructed using the AntiKt4EMTopo algorithm with radius parameter $R = 0.4$ from clusters of energy deposits in the calorimeters [109]. Quality requirements are applied to remove events containing spurious jets from detector noise and out-of-time energy deposits in the calorimeter from cosmic rays or other non-collision sources [162]. Jet energies are calibrated to the scale of the constituent particles of the jet and corrected for the presence of multiple simultaneous (pile-up) interactions [105, 126].

After reconstruction, jets with transverse momentum $p_T > 25$ GeV and rapidity $|\eta| < 2.8$ are considered. To suppress pile-up contributions, jets with $p_T < 60$ GeV and $|\eta| < 2.4$ are required to originate from the primary interaction vertex with the highest summed p_T^2 of associated tracks. If a jet and a photon candidate are within $\Delta R = 0.4$, the jet candidate is removed.

4.2.2 Trigger strategy

A combination of a single- and multi-object triggers is implemented in the analysis. Each shows an advantage: a multi-object triggering strategy provides greater sensitivity where both options are available, while a single-photon triggering strategy allows the inclusion of

a larger m_{jj} range. Ultimately, trigger choice was dictated by a combination of sensitivity, available m_{jj} range, and ease of fitting the resulting spectrum (see section 4.2.4).

The single-photon trigger strategy aims to use the most inclusive set of cuts which allows full efficiency in the lowest unprescaled single-photon triggers across the 2015, 2016, and 2017 datasets. In all three periods, the appropriate trigger is `HLT_g140_loose`. The efficiency of this trigger with respect to the offline reconstruction is studied by bootstrapping from the `HLT_g60_loose` trigger and as a function of the transverse momentum of the leading isolated photon passing loose identification. This means that the efficiency is determined by taking the ratio of events passing both triggers from those that passed only the reference trigger, which is fully efficient for isolated photons passing tight identification with $p_T > 70$ GeV. This procedure allows to build a turn-on curve to study the efficiency of the trigger. It is also important to determine from this curve the lowest threshold for the leading photon p_T where the turn-on curves reaches the plateau ($\sim 99\%$), since it is translated into a cut on the photon p_T for the final event selection. This assures that we are working on the turn-on efficiency plateau, where $\sim 99\%$ of the times the selected event has actually passed the trigger considered. A more accurate assessment of the turn-on is then determined by fitting the curve with a modified error function:

$$p_0 \cdot \left(1 + \operatorname{erf} \left(\frac{x - p_1}{\sqrt{(2)p_2}} \right) \right)$$

Figure 4.3 shows the turn-on curve for the single photon trigger with analysis cuts applied.

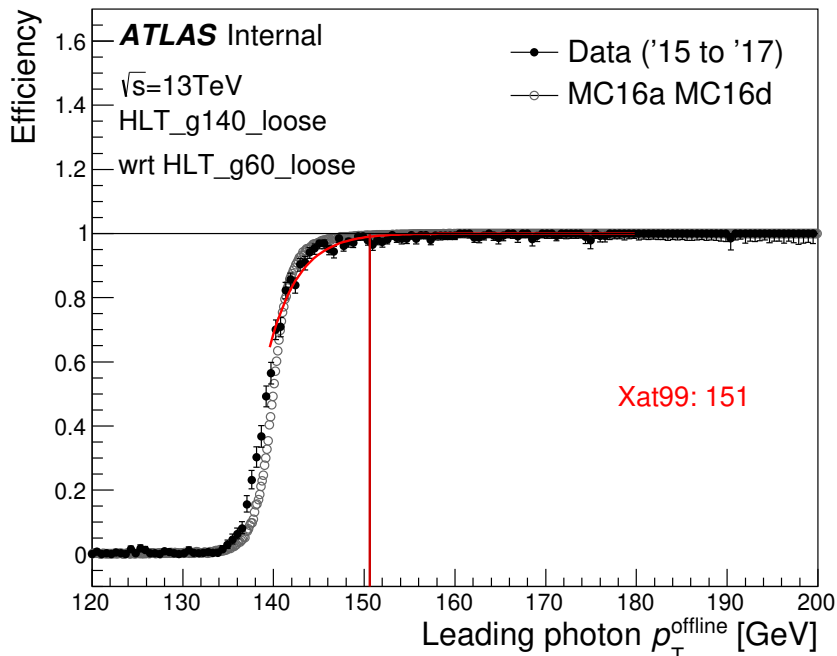


Figure 4.3: Turn-on curve in 2015–2017 data for the `HLT_g140_loose` trigger. The efficiency is found with reference to the prescaled `HLT_g60_loose` trigger, which is fully efficient within the p_T range considered. All analysis cuts are applied. `HLT_g140_loose` is found to be $> 99\%$ efficient for leading photon $p_T > 149$ GeV.

As the thresholds of this trigger did not change at any point during the considered data taking periods, and since this photon trigger is relatively pile-up insensitive, the performance is found to be essentially identical for the three years as shown in figure 4.3.

The multi-object trigger strategy on the other hand, is based on two HLT triggers: `HLT_g75_tight_3j50noL1_L1EM22VHI`, running unprescaled in 2016, and `HLT_g85_tight_L1EM22VHI_3j50noL1`, running unprescaled in 2017. Both are seeded by the L1 trigger `L1_EM22VHI`, which ran unprescaled during both years. At HLT, these triggers require the presence of at least three jets with $p_T > 50$ GeV and at least one photon with $p_T > 75$ or 85 GeV, respectively, passing the tight identification criteria. Since there is no jet-photon overlap removal algorithm in the HLT, it is assumed that the photon fakes one of the three jets. The result corresponds to an offline selection containing two jets and a single photon, resulting in a *dijet+ γ combined* trigger. Unfortunately, there was no equivalent multi-object selection running unprescaled during 2015 data taking. As a result the 2015 dataset is not included in the multi-object trigger selection, decreasing the total dataset by $\sim 3 \text{ fb}^{-1}$ of data.

As for the single-photon trigger, the efficiency of the trigger with respect to the offline reconstruction is studied by bootstrapping from the `HLT_g60_loose` trigger. The `HLT_g60_loose` trigger is fully efficient for the full set of events passing the multi-object (combined from now on) trigger, but since it is heavily prescaled and quite close in p_T range, the statistics in the following plots are somewhat low. The efficiency of the combined trigger was studied as a function of the transverse momentum of the leading isolated photon passing tight identification and of the two leading jets after photon-jet overlap removal.

As this particular trigger requires both a photon and jets, its efficiency depends on the photon and subleading jet momenta.

Let's take 2017 trigger `HLT_g85_tight_L1EM22VHI_3j50noL1` for instance. The jet component of the trigger reach a plateau for subleading jets with $p_T > 65$ GeV. Figure 4.4a shows the efficiency in terms of the leading photon p_T after requiring that the subleading jet is fully efficient for the jet part. In addition, requiring that the photon has $p_T > 95$ GeV² makes the whole trigger fully efficient. The same conclusion can be reached by reversing the selection. The result of first applying a photon $p_T > 95$ GeV cut without a selection on the subleading jet p_T cut is shown in figure 4.4b. There the trigger becomes fully efficient for subleading jets with $p_T > 65$ GeV.

The above figures show that the 2017 combined trigger is fully efficient for events with an offline isolated photon with $p_T > 85$ GeV passing tight identification and two jets with $p_T > 65$ GeV. Additionally, no issues are seen with the HLT approximation of the photon-jet overlap removal where every photon is assumed to fake a jet.

Figure 4.5 shows the efficiency of `HLT_g85_tight_L1EM22VHI_3j50noL1` in 2017 data with no kinematic selection applied and the same distribution after the final analysis cuts are applied.

A similar behaviour is observed with the `HLT_g75_tight_3j50noL1_L1EM22VHI` trigger in the 2016 dataset. Fully efficiency is achieved by requiring subleading jet $p_T > 65$ GeV and leading photon $p_T > 85$ GeV. Since the turn-on curves show a similar behaviour as the ones already presented, thus coming to the same conclusions for 2016 and 2017 combined triggers, these figures are not shown here but they can be found in the internal note [156].

²The p_T values where each trigger is fully efficient, for both photon and jets, are taken from the ATLAS respective trigger groups recommendations.

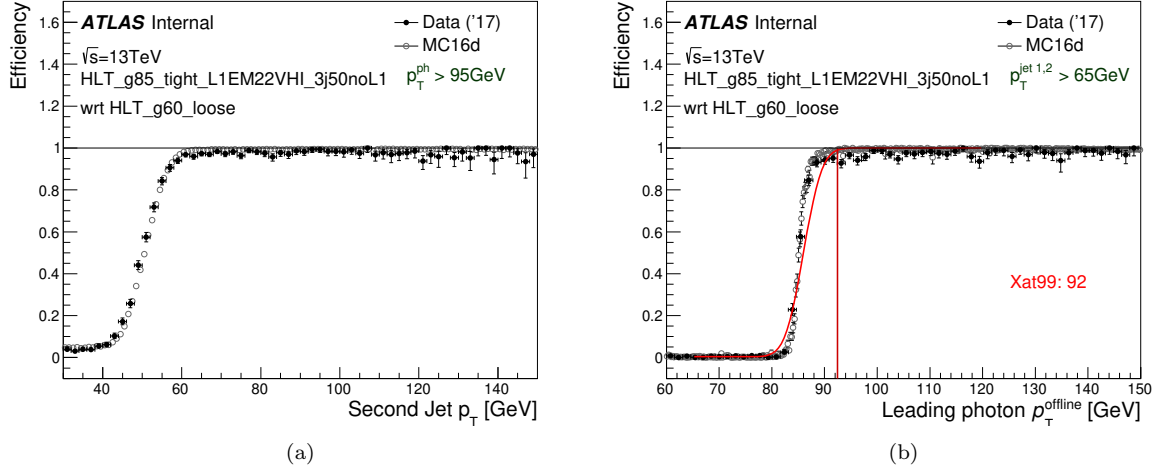


Figure 4.4: The efficiency of the combined trigger (4.4a) as a function of subleading jet p_T after overlap removal, with the leading photon p_T required to be above 95 GeV; (4.4b) as a function of leading isolated photon p_T passing tight identification criteria, with the subleading jet p_T required to be above 65 GeV. The efficiencies in 2017 data and MC16d are shown. The dashed line corresponds to full efficiency.

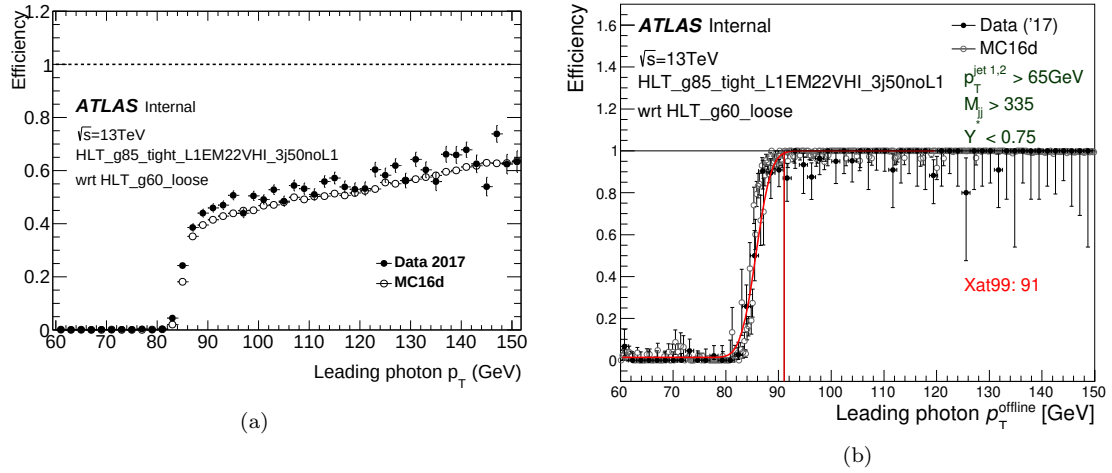


Figure 4.5: The efficiency of the combined trigger as a function of leading isolated photon passing tight identification criteria (4.5a) without any kinematic selection and (4.5b) with the subleading jet $p_T > 65$ GeV and the final analysis cuts in y^* and m_{jj} applied. The efficiency in 2017 data is shown. The dashed line corresponds to full efficiency. It can be seen that the plateau is reached for leading photon $p_T > 95$ GeV.

In order to be able to smoothly combine 2016 and 2017 data, a single unified set of cuts is defined such that both triggers will be on their plateaus. This requires an offline isolated photon with $p_T > 95$ GeV passing tight identification and two jets with $p_T > 65$ GeV. Nonetheless it is clear from figure 4.5 that the analysis selection does not achieve truly full efficiency even after application of these jet and photon p_T cuts. To account for this, an uncertainty is estimated by looking at trigger efficiency as a function of m_{jj} . For details on this uncertainty see section 4.5.2.

Figure 4.6 compares the shapes of the background distributions using a single-photon triggering strategy versus the multi-object triggering strategy, while the sensitivities of the two analysis strategies are shown in figure 4.7 (details in section 4.2.5).

Two key points are illustrated by these plots:

1. The single-photon triggering strategy leads to a sharper m_{jj} distribution which could be fit from a lower mass, while the multi-object triggering strategy leads to a distribution with a noticeable shoulder which could not be fitted until ~ 300 GeV or higher in m_{jj} .
2. The multi-object triggering strategy provides better analysis sensitivity than the single-photon triggering strategy.

As it is key that this analysis should be able to set limits on signal masses as low as 200 or 250 GeV in order to leave no uncovered region with respect to the boosted dijet+ISR analysis, the additional mass range available through the single-photon trigger must be included. However, it would be unfortunate to lose the sensitivity gained by the multi-object trigger, where it is available. This analysis will therefore use both selections. A spectrum will be created with each triggering strategy and fitted independently. For masses where the multi-object trigger selection can be fitted and used to constrain signal points, those will be the nominal results. Where this spectrum is not yet smoothly falling, the single-photon trigger result will be used. This conclusion is summarised and the relevant luminosities for each selection are recorded in the event selection discussion later in this section (see table 5.3).

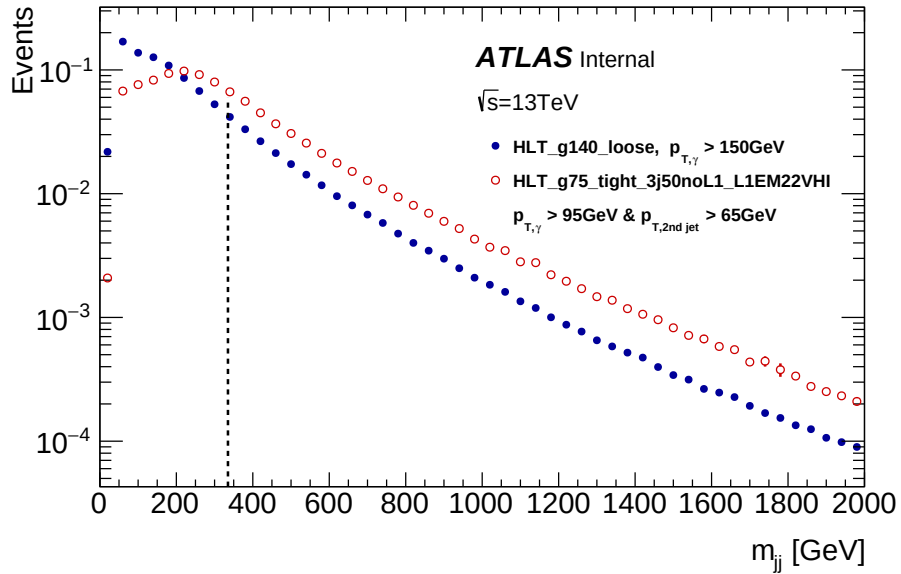


Figure 4.6: Invariant mass distribution for Sherpa multijets requiring on one side events to pass HLT_g140_loose trigger and leading photon $p_T > 150$ GeV (single-photon trigger); and on the other hand, events to pass HLT_g75_tight_3j50noL1_L1EM22VHI trigger, leading photon $p_T > 95$ GeV and two leading jets $p_T > 65$ GeV (combined trigger) . No y^* cut is applied.

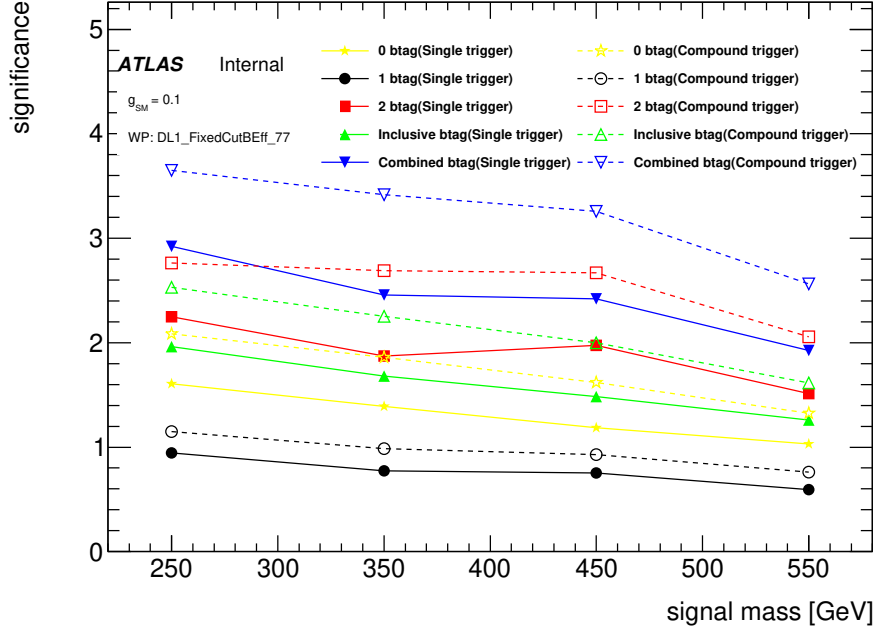


Figure 4.7: Comparison of analysis sensitivity (based on the definition in equation 4.7) to a benchmark Z' with couplings $g_q = 0.1$ for a multi-object trigger strategy versus a single photon trigger strategy. For the doubly b -tagged result, the DL1 tagger at the 77% fixed efficiency working point is used (see section 4.2.5). The luminosities are scaled to represent the full Run 2 dataset including the 3 fb^{-1} loss from the multi-object trigger strategy. These results show that for masses where both triggering strategies can be fitted, the multi-object trigger strategy provides improved analysis sensitivity, even when accounting for the loss of the 2015 dataset. Here *compound* makes reference to the combined trigger.

4.2.3 Discriminating variables optimisation

Since this type of search looks for an excess of events (signal) by fitting a well modelled SM m_{jj} observable (background), it is very important to keep potential signal events. This can be achieved by applying an optimised event selection. Kinematic cuts are applied on the reconstructed objects (see section 4.2.4) but there are also more complex variables, that given the different topologies on the signal and background events, can be also used to define a more effective signal candidate region.

The signal significance gives a relationship between the number of signal events related to the amount of background and can be increased with an appropriate cut selection. An optimal cut value is obtained at the maximum point on a significance distribution. A study has been carried out with the goal of increasing the sensitivity by finding one or multiple discriminant variables to cut on. These cut values will also have an impact on the smoothness of the m_{jj} range that would be properly fit. So even if a certain cut improves the signal significance, it has to be verified that it does not change the m_{jj} distribution in a way that it makes it impossible to fit.

This study used four target mass points: 250, 350, 450 and 550 GeV, each with a range of ± 50 GeV. It aims for selection cut values that are identical for all mass ranges. In addition, only the trigger requirement and a cut on the p_T value where it reaches the 99% the efficiency are applied.

Several discriminant variables were considered and, after comparing their respective significances (computed as $(S/\sqrt{B})$), two of them were found to be the most promising

ones. On one side, the asymmetry in p_T between the two signal jets ($A = \frac{(|p_{T,1}| - |p_{T,2}|)}{(|p_{T,1}| + |p_{T,2}|)}$), which is expected to be smaller on average for signal than for background. And y^* , a key discriminating variable for dijet analyses. y^* is a measure of rapidity difference between the two signal jets $y^* = \frac{y_1 - y_2}{2}$. Signal should be produced roughly isotropically, but multijet production preferentially generates forward jets. Therefore, the requirement that the two selected jets are relatively central in their centre-of-mass frame makes y^* an effective discriminant³.

These variables along with their optimal cut values are shown in figure 4.8 for a single representative mass point of 550 GeV.

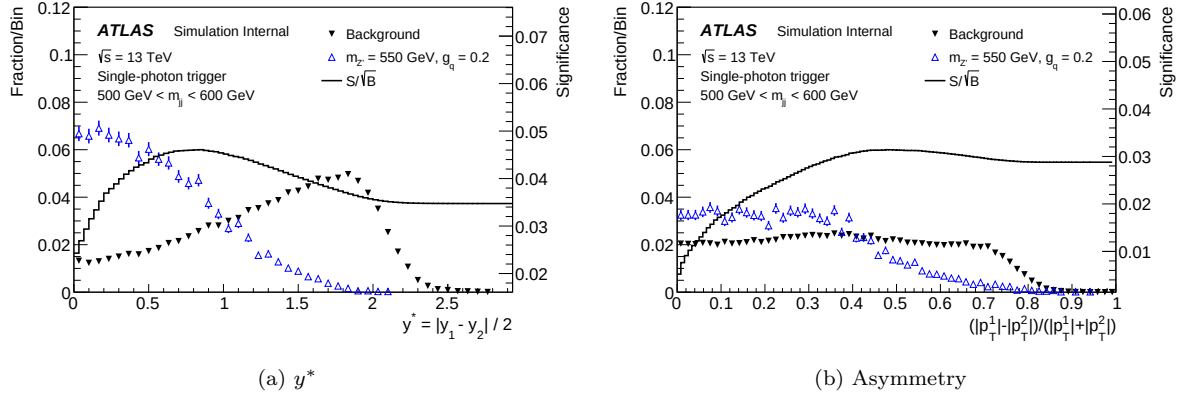


Figure 4.8: Signal (S) and background (B) distributions of the discriminant variables (asymmetry, and y^*), along with the cumulative distribution $S/\sqrt{B}$, for the two leading jets in photon+jet events in the 500 GeV to 600 GeV mass range. Optimal cut values are shown in legend.

Distributions for additional mass points and other variables considered can be found in the internal note [156].

Since many effective discriminant variables were found, the toolkit for Multivariate Data Analysis from ROOT (TMVA) [117] was used for different subsets of these variables aiming to find a powerful discriminating combination of them. Some of the methods tested were Fisher, Likelihood, and rectangular cuts. The first two multivariate discriminant methods provided a new variable to cut on that unfortunately presented very different optimal values for each mass range, which effectively results in different variables for different ranges. Hence, this study only focuses on the third method which determines optimal rectangular cuts on variables without the necessity of introducing new composite variables with different performance across mass ranges.

Finally, it was found that all variables were sufficiently correlated that almost no additional sensitivity was gained by using multiple variables instead of simply the more powerful of them: y^* . It was therefore concluded that a multivariate technique offered no additional power over a rectangular cut based technique.

The goal was then to determine a cut value in y^* which maximises the significance across all mass ranges. The criteria employed was to use the cut value that optimises the mass range with the lowest significance value among all the masses, and verify that it did not significantly reduce the significance value for the other masses. Ultimately, $y^* \leq 0.75$ was found to be this value.

³Future iterations of the analysis would do well to study this variable or equivalents in the context of $2 \rightarrow 3$ processes, as its use has been developed and mostly informed by $2 \rightarrow 2$ process searches like the dijet analysis.

4.2.4 Event selection

Events entering the analysis are required to pass basic quality requirements like being properly included in the GRL, pass standard cleaning requirements [163] and jet cleaning criteria [162]. These events also have to pass the relevant triggers listed on table 5.3 below.

Trigger	Year	High-level Trigger	Lumi. [fb ⁻¹]
Combined	2015	–	–
	2016	HLT_g75_tight_3j50noL1_L1EM22VHI	33.009
	2017	HLT_g85_tight_L1EM22VHI_3j50noL1	43.586
Single-photon	2015 – 2017	HLT_g140_loose	79.826

Table 4.1: Triggers used for each channel and each year’s datasets. While the various triggers change in each year, they allow for a consistent set of analysis cuts across the entire dataset. An additional signal region using single-jet triggers allows an extension of the search range to lower masses, albeit at lower sensitivity. Luminosity, accounting for LAr veto and live fraction, was calculated using Luminosity DB tag `Of1Lumi-13TeV-010` via [164] with trigger chain information taken from [165].

These triggers are used in each of the specified cases, in accordance with the studies presented in section 4.2.2. The total luminosity result is thus 76.595 fb⁻¹ for $m_{jj} > 335$ GeV (*combined* trigger) and 79.826 fb⁻¹ for $m_{jj} < 335$ GeV (*single photon* trigger).

Signal region definition

The analysis selection is described in table 4.2. The jet and photon multiplicity and p_T cuts are necessary to ensure each trigger is fully efficient. Optimal cuts in y^* were determined as described in section 4.2.3. The m_{jj} cuts are determined by the shape of each spectrum and are chosen such that this can be described by a smooth fit above the cut.

Cut	Single-photon trigger	Combined trigger
Number of jets	$n_{\text{jet}} \geq 2$	$n_{\text{jet}} \geq 2$
Number of photons	$n_{\gamma} \geq 1$	$n_{\gamma} \geq 1$
Lead γ p_T	$p_T^{\gamma} > 150$ GeV	$p_T^{\gamma} > 95$ GeV
Lead & sublead jet p_T	$p_T^j > 25$ GeV	$p_T^j > 65$ GeV
Centrality	$ y_{12}^* < 0.75$	$ y_{12}^* < 0.75$
Invariant mass	$m_{jj} > 169$ GeV	$m_{jj} > 335$ GeV

Table 4.2: Analysis search region cuts.

After the full selection is applied, approximately 1.25% (1.9%) of the initial number of events are kept for the single (combined) trigger in the inclusive channel. These values decrease for the b -tagged channel, where only the 0.01% of the initial events are kept for both options of trigger. Cutflows for data and MC, as well as simulated signal samples can be found in B.1.

4.2.5 b -tagging studies

The analysis is further divided into two searches, one inclusive in jets and one retaining only events where the two jets used to form the candidate resonance are b -tagged. This section describes the choice of tagging criteria and justifies the addition of the b -tagged channels.

Out of the many taggers available, only two were considered following the official recommendations from the flavour tagging group. These are MV2c10 and DL1. Each had eight supported working points (WP): 60%, 70%, 77%, or 85% efficiency as either a fixed cut or hybrid working point⁴. Several studies took place in order to determine which combination was optimal for the search.

The optimal choice of tagger and WP was determined by comparing signal sensitivity for each choice across the full range of Z' mass points. The significance was defined as follows [166]:

$$Z = \sqrt{\sum_i^{bins} Z_i^2}, \text{ where } Z_i = \sqrt{2 \left[(s+b) \log\left(1 + \frac{s}{b}\right) - s \right]} \quad (4.7)$$

The full analysis selection was used in the nominal MC samples. Additionally, the requirement was imposed that the two jets forming the candidate Z' both passed the relevant tagging requirements.

Figure 4.9 compares the significance for a range of taggers and for all available fixed WP for the most promising available tagger. In all cases, the Z' $g_{SM} = 0.2$ points are used for the tests. For the full set of plots for all taggers, working points, and coupling values the internal note [156] can be consulted.

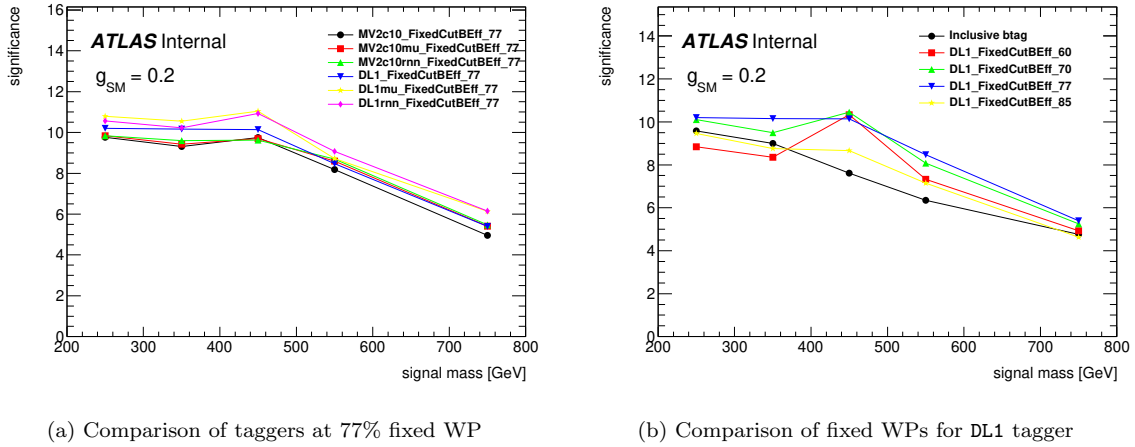


Figure 4.9: Signal significance in two- b -tagged channel for 4.9a various taggers at the same fixed working point and 4.9b various fixed working points for the most promising supported tagger. The selection corresponds to the combined trigger. Signals with a coupling of $g_q = 0.2$ are shown.

Only the fixed cut WP are shown in figure 4.9, but the same results in terms of the optimal tagger and WP were concluded from hybrid WP signal significances [156].

For all mass points, the DL1 tagger outperforms the MV2c10 tagger. Relative significances for various WP change significantly across the mass range, for various values of

⁴Hybrid working points correspond to a fixed cut working point at low b -jet p_T and a fixed efficiency working point at high b -jet p_T .

signal coupling, but it is found that the optimal efficiency WP is 77% for both, the fixed and the hybrid WP. The decision between these two working points still needs to take into account the possibility of introducing features or sharp changes in the composition of the m_{jj} spectrum.

In order to ensure that the final tagged spectra can be fitted properly, one key criterion which must be met is that the b -tagging efficiencies and fake rates must vary smoothly as a function of mass. Sharp increases and decreases in the rate could lead to localised excesses and deficits in the data spectrum, which would at best present challenges to the fit and at worst could fake signals. After checking these distributions, it was found the fixed efficiency WP at 77% was the safest choice since it showed potentially less problematic non-smoothness on the b -tagging efficiency. Details on these checks can be found in the internal note [156].

Now that optimal b -tagging configuration for the analysis has been chosen, it is time to define how can these b -jets improve the sensitivity of the signal region. Since there are two jets on the final state, there are a few combinations of b and light jets that could be used.

Figure 4.10 shows the significance for representative tagging choices in each of five cases:

- **Inclusive** No tagging requirements are made in the selection
- **0-tag** Explicitly require that neither jet from the candidate resonance is b -tagged
- **1-tag** Require that exactly one jet from the candidate resonance is b -tagged
- **2-tag** As in the optimisation studies, require that both jets from the candidate resonance are b -tagged
- **Combined** A simple combination is performed between the 0, 1, and 2-tagged channels:

$$Z_{comb} = \sqrt{Z_0^2 + Z_1^2 + Z_2^2}$$

As figure 4.10 shows, the 2-tagged selection offers a noticeable increase in sensitivity over the inclusive channel. It is nonetheless still important to keep the inclusive spectrum since it is the most general case and is the simplest option for reinterpretation. The 2-tagged channel provides additional information which is already interesting for some models, but not all. A statement about sensitivity in the exclusive versus combined tagged channels would, additionally, be a very model-dependent statement. For models which decay preferentially to heavy flavours, the 2-tagged channel alone will already be interesting. A combined result would only be re-interpretable if all three exclusive tagging channels (0, 1, and 2) were provided, since the branching ratios can vary from model to model, and a simpler result is preferred for this analysis including b -tagging. Therefore, the option of showing only two results in each channel (inclusive and 2-tagged) is preferred.

To summarise, the analysis will be presented in two channels per trigger selection: inclusive and 2-tagged. For this last one, the DL1 tagger at the 77% fixed efficiency working point is used. At this threshold, only 0.7% light-flavour jets and 25% c -jets are retained. Both the leading and subleading jets are required to pass this tagging requirement.

Once the final b -tagging configuration and the channels are decided, a last check needs to be made to verify how the m_{jj} spectrum changes after the final signal region selection is applied.

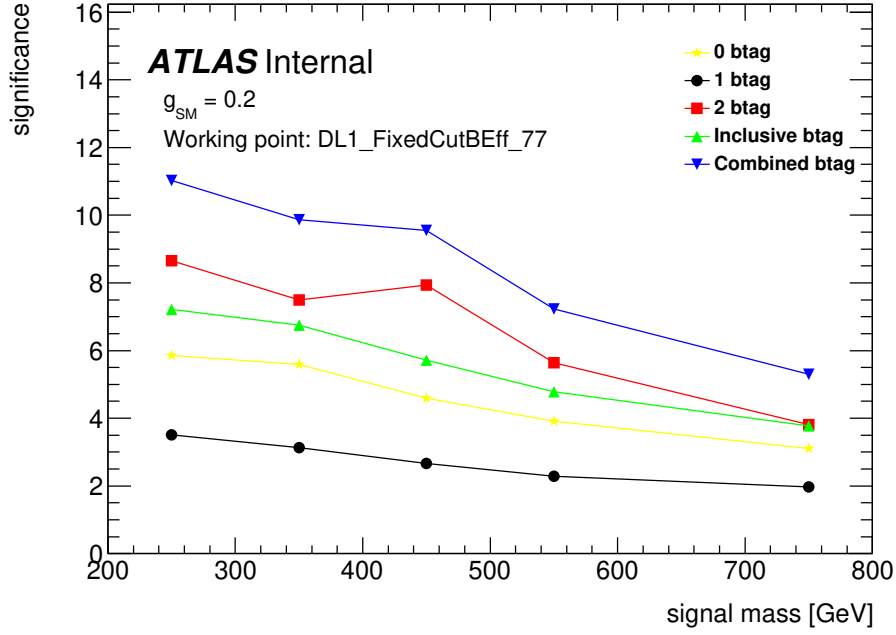


Figure 4.10: Signal significance versus mass in the inclusive, 0-tag, 1-tag, and 2-tag channel as well a combination of 0, 1, and 2-tags. The DL1 tagger is used at the 77% fixed efficiency WP. Z' signals with coupling $g_q = 0.2$ are used.

The m_{jj} distribution in Sherpa MC16d after all analysis cuts in the inclusive and 2-tagged cases is shown in figure 4.11. The selection corresponds to the single photon trigger, and the spectra are broken down by flavour to illustrate changes in the composition as a function of m_{jj} . The inclusive spectrum is dominated by light jets in roughly equal proportion for all masses. The 2-tagged spectrum illustrates the decrease in b -tagging performance as a function of mass, with a higher proportion of true di- b events at lower masses and a composition dominated by mis-tagged light jets at higher masses. These plots use the DL1 tagger at the 77% fixed cut working point. Additional plots of the compositions of various jet kinematic distributions can be found in [156].

Understanding the composition of the tagged spectra is key to understanding whether it will be possible to describe it with a fit-based background estimate. Similarly to the tagging efficiencies and mistag rates, a smooth variation in the flavour composition helps prevent the formation of sharp corners in the tagged spectrum. These plots show that changes in composition are smooth within the statistical uncertainties of the MC samples.

Figure 4.11b also indicates the highest masses to which this analysis can reasonably report limits in the 2-tagged channel. Above approximately 1200 GeV, the composition of the 2-tagged spectrum is no longer dominated by true b -jet pairs. Thus we propose that 1200 GeV be the maximum mass used in the analysis.

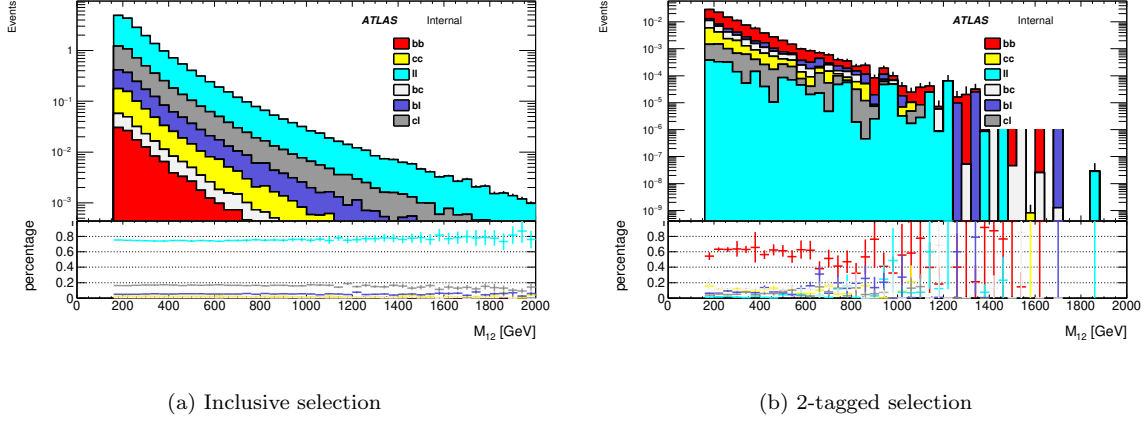


Figure 4.11: Flavour composition breakdown of m_{jj} spectrum in Sherpa MC16d for the inclusive selection 4.11a and for the 2-tagged selection 4.11b. The fraction represented by each flavour pairing is shown in the ratio plot. The single photon trigger signal region is used.

4.3 Kinematic checks

Since ultimately the analysis consists into looking for an excess of events over data based on a fitting to the background distribution that was optimised for MC simulations, it is important to perform some checks on basic kinematic distributions to ensure that the data were well understood. Comparisons for the most important quantities are given here, while additional plots can be found in [156].

Figure 4.12 shows the p_T and η distributions for the leading photon in the inclusive channel for both trigger options. Figures 4.13 and 4.14 show the same distributions for the leading and subleading jets respectively.

These same distributions can be found in appendix B.2 for the 2 b -tagged categories.

No significant discrepancies are observed between the data and MC distributions. The largest differences are observed in the photon p_T spectrum for the combined trigger and in the subleading jet p_T spectrum for the single photon trigger. Since the photon does not enter the final analysis observable, differences of the magnitude observed in its p_T are not overly concerning. For the subleading jet p_T with the single photon trigger, the data/MC difference is smooth and changes slowly, indicating that it will not be able to introduce an m_{jj} -dependent feature into the final result. It is concluded that the analysis kinematics in the inclusive channel are sufficiently well understood for these datasets.

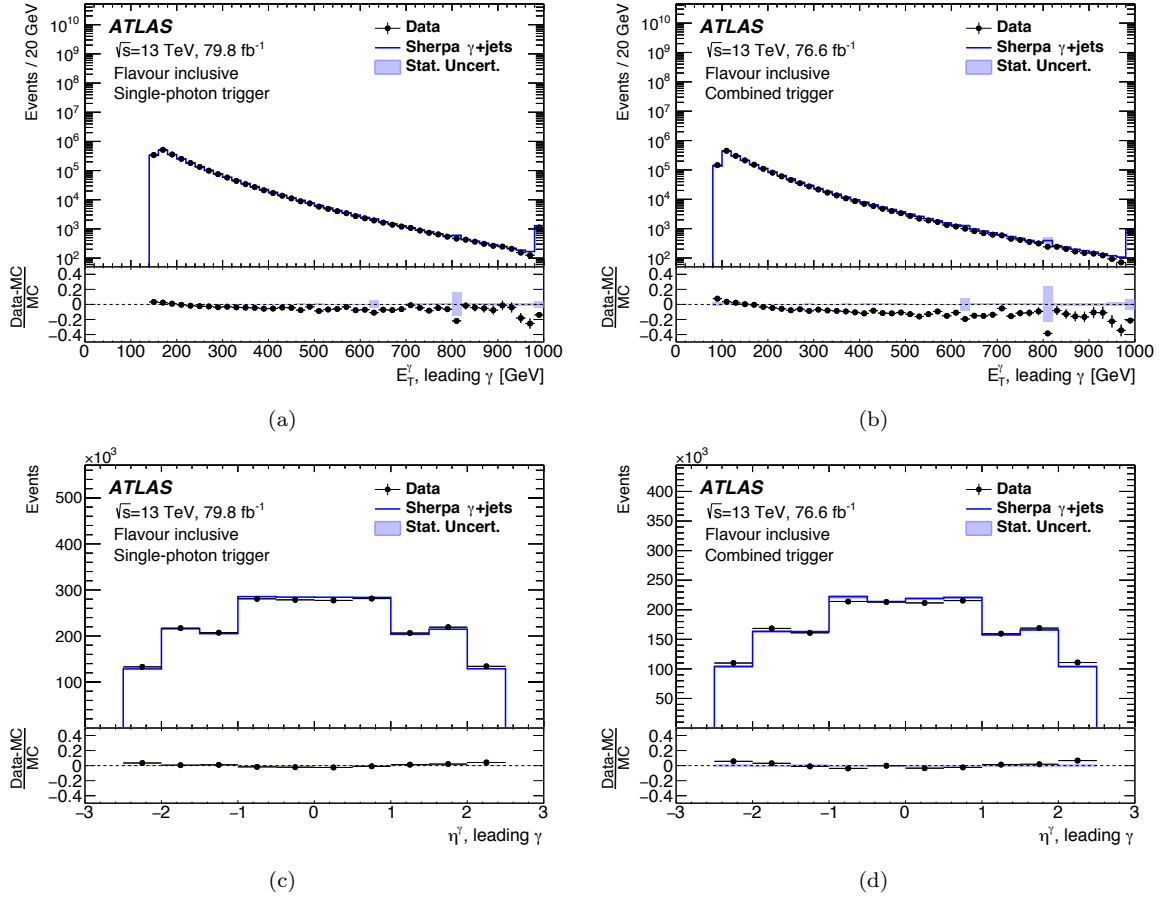


Figure 4.12: Comparisons of data to MC for the photon p_T and η distributions of the flavour-inclusive categories. Figs.(a) and (c) show the single-photon-trigger data while (b) and (d) show the combined-trigger data.

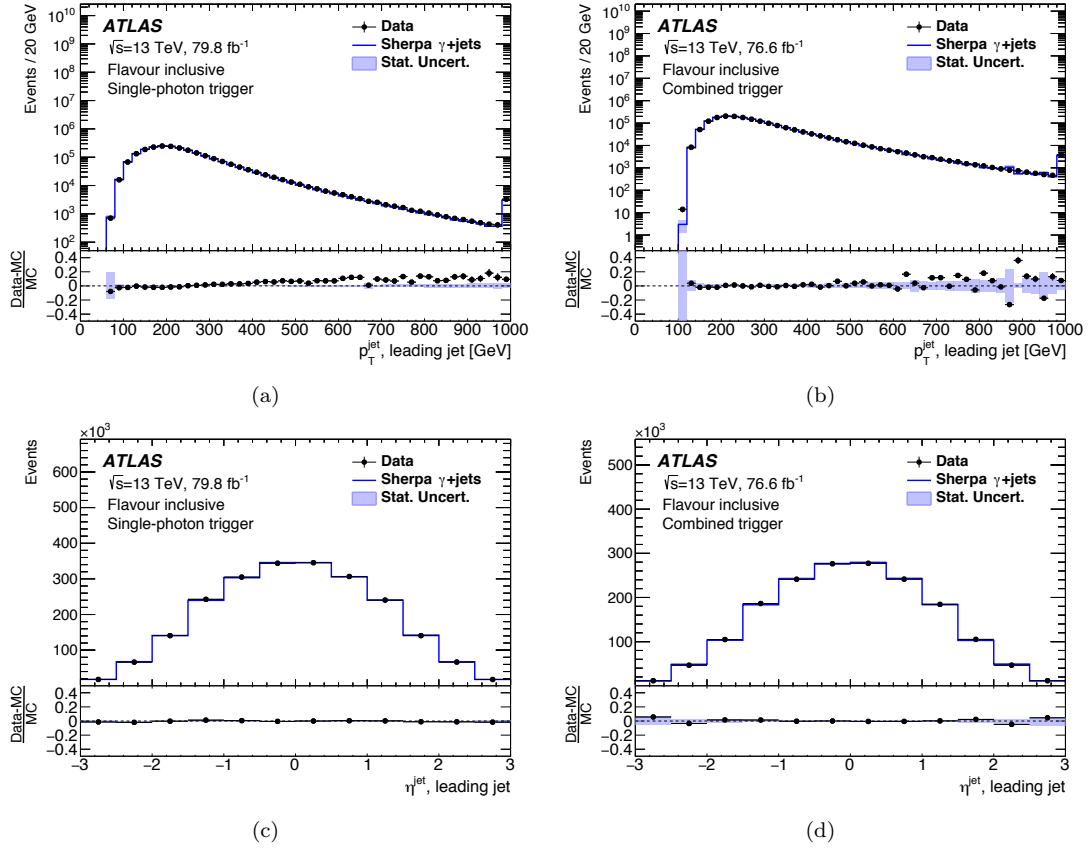


Figure 4.13: Comparisons of data to MC for the distributions of p_T and η of the highest- p_T jet in the flavour-inclusive categories. Figs.(a) and (c) use the single-photon trigger while (b) and (d) use the combined trigger.

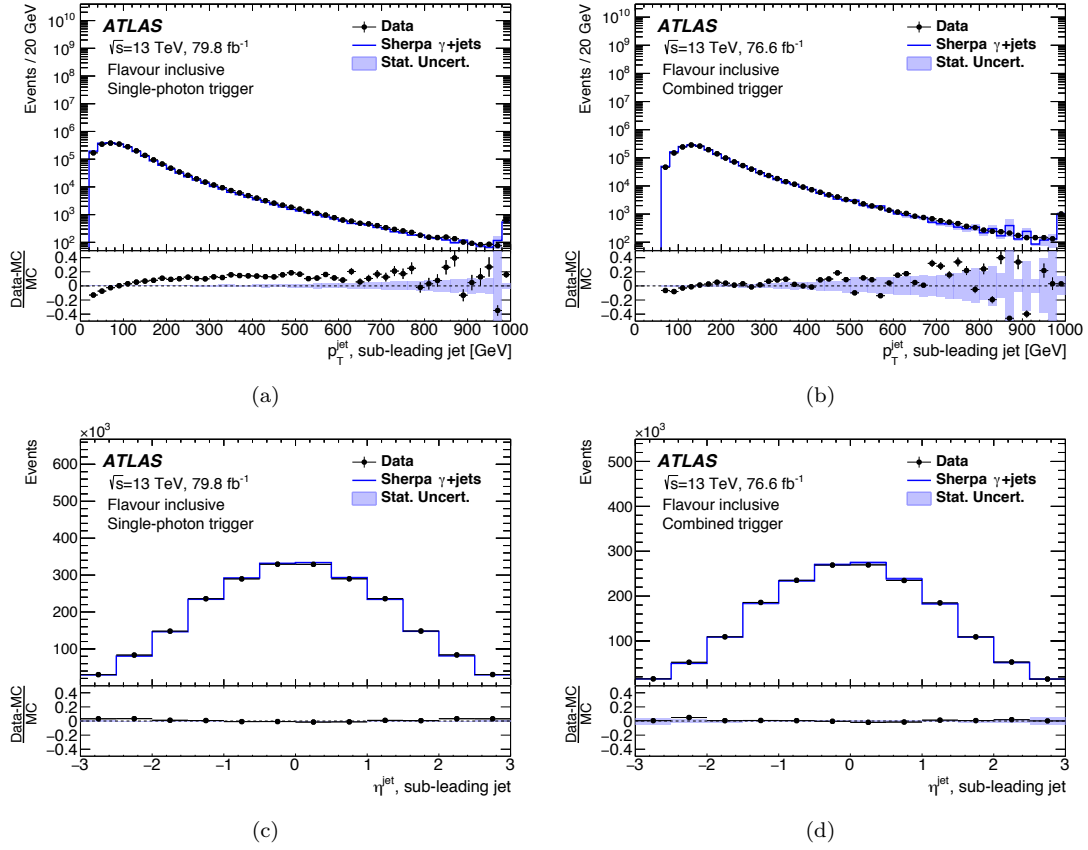


Figure 4.14: Comparisons of data to MC for the distributions of p_T and η of the second-highest- p_T jet for the flavour-inclusive categories. Figs.(a) and (c) show the single-photon-trigger data while (b) and (d) show the combined-trigger data.

4.4 Background estimation

The background estimate for this analysis is performed using a parametric fitting procedure. The background to be modelled consists of QCD processes with a complex mixture of PDFs, parton showering, and the effects of detector response and kinematic selection.

Many dijet searches at ATLAS use a “global fit” method, which fits a single, few-parameter analytic function to the observed dijet mass distribution over the entire search range. And, according to the most recent analyses, data analysed so far can be described with the functions in table 4.3.

Functional form	Citation	Label
$f(x) = p_1(1-x)^{p_2}x^{p_3}$	[135]	our3param
$f(x) = p_1(1-x)^{p_2}x^{p_3+p_4 \ln x}$	[138]	our4param
$f(x) = p_1(1-x)^{p_2}x^{p_3+p_4 \ln x+p_5(\ln x)^2}$	[138]	our5param
$f(x) = p_1x^{-p_2}e^{-p_3x-p_4x^2}$	[167]	UA2

Table 4.3: Functional forms explored for fitting the QCD background, with citation to previous results in which they have been used to fit similar distributions and label for reference in the rest of the text.

where $x = m_{jj}/\sqrt{s}$ and p_i are free parameters determined by fitting the m_{jj} distribution with the binning detailed in appendix B.4, which was inherited from the previous version of the analysis [145].

These functions have been studied and tested in various spectra relevant to the analysis, composed of both MC and subsets of non-sensitive data. The analysis strategy will create the nominal background estimate from whichever function performs the best in real data, and will define an uncertainty on that function selection using the second-best of the four functions.

Traditionally, resonance searches in dijet channels have been conducted by looking for a localised excess above a smooth background which is obtained by fitting the entire dijet mass spectrum with these ad-hoc functions. However, these functions are approximations to the underlying mass distribution, and with increasing data their approximate nature becomes apparent and obtaining a background model from a global ad-hoc fit to the data becomes increasingly challenging, especially when the data span several orders of magnitude. Thus, for this analysis a sliding window fit (SWiFt) is chosen instead, as described in [168]. This is a background estimation method which looks for localised excesses by sliding over the data spectrum of a given half-width (corresponding to a number of bins termed as window-half-width or “whw” in the following) in small, overlapping windows. This allows the analysis to move away from an assumption that low and high ranges of m_{jj} are strongly correlated. The unblinding strategy will consider the possibility of a global fit and, if the fit quality is too low, will move to a sliding window fit and iteratively narrow the window until the background can be adequately described.

Sliding window fits, however, pose potential issues for analyses due to their increased flexibility. The narrower the window used for the fit, the more flexibility the fit has, and the sensitivity decreases proportionally (refer to sec. 8.2.3 of the TLA backup documentation [169]). Thus the widest window still able to accommodate the spectrum shape should be selected for the analysis.

The maximum usable window width can be found by fits to the Monte Carlo spectra, where it is certain that no signal exists. To do so, the window half-width can be increased one bin at a time until a pre-determined fit quality criterion reaches a certain threshold.

Following previous iterations of this analysis, the criterion is set to be for the background estimation to have a χ^2 p -value > 0.05 when compared to data, if necessary after excluding the window containing the largest excess, putting in evidence that this criterion ties discovery to background estimation.

Tests in MC can also be complemented by tests in a dataset equivalent to that used for the 2015+2016 data preliminary result, which yielded a null result [145]. These tests are mostly useful for narrowing down the set of fit functions, and rule out window widths that are too large for a dataset that is smaller than the full dataset used for the analysis.

On the other hand, the minimum acceptable window width can be determined via signal injection tests, as discussed in section 4.4.2.

Neither the MC nor the data statistics of the two datasets above is representative of the full dataset included in this analysis. For this reason, the sliding window size is determined directly on data during the unblinding procedure⁵. These datasets are only used as a first attempt to test the different fit functions and the possible window sizes for the SWiFt method.

4.4.1 Fitting tests

All fits should be tested in Monte Carlo spectra, regardless the lack of statistics for certain processes. Their success is not enough to guarantee success in data, but any failures not attributable to very low statistics could indicate failure in data. These tests can also provide an indication of the widest sliding window widths likely to succeed on the unblinded spectra.

Two fits are shown to the inclusive MC spectra, for the single photon trigger in figure 4.15a and the combined trigger 4.15b. The MC samples are normalised to the luminosities expected in the full 2015–2017 dataset. These use the five-parameter dijet function as a global fit and with a SWiFt window half-widths of 16. The summary of the χ^2 p -values in MC for the two inclusive channels is shown in table B.6 on appendix B.5

A similar test was carried out in the doubly b -tagged channel, but in this case the equivalent MC statistics are even worse than in the inclusive case. Only limited conclusions can be drawn from the plots, which are challenging to fit or evaluate due to the presence of sporadic high-weight MC events.

Another way of testing the background estimation process is to run the fitting procedure in a dataset that is equivalent to the one from the last public result (2015+2016), where no signal was found. The selected dataset has a luminosity of approximately 15 fb^{-1} .

This test is useful to gather a first idea on the maximum possible window that can be used for the sliding window fit, with about a quarter of the dataset.

At a first glance, it was seen that all functions already provide a good description of the 15 fb^{-1} data for the single photon trigger with a global fit in the inclusive channel. If the full dataset behaves similarly to the smaller one, there will be no need to use a sliding window fit. On the other hand, for the combined trigger spectrum, a sliding window fit is needed. The various p -values and test results are summarised in table B.7 on appendix B.5.

This dataset does not include any b -tagging selection, as that signal region is still unexplored and blind, but instead uses the ABCD method to reweight the inclusive sample

⁵Unblinding makes reference at the procedure where the actual data that will be analysed for the final results is used.

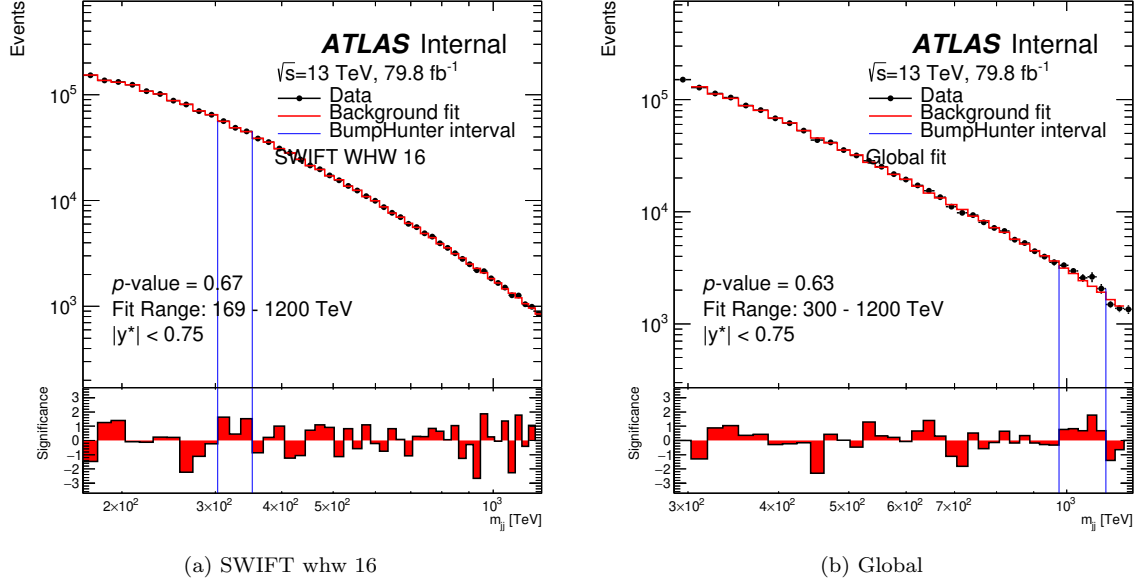


Figure 4.15: Fits to the inclusive selection in Sherpa Monte Carlo. 4.15a is shown for the single photon trigger channel with a fit using the five-parameter function for SWiFt whw 16 settings. 4.15b shows the same distribution on the combined trigger channel, using the same fitting function for the global fit settings. Samples are normalised to the full analysis luminosity.

(more details can be found on appendix C of [156]).

The ABCD method allows the data-driven estimation of a background rate when events are selected by a pair of cuts in a plane of two uncorrelated variables such that both of the cuts enhance the signal to background ratio. By making a cut in each of the two variables, four non-overlapping regions are defined, of which one is the signal region, labelled region A. Ideally, most signal events are concentrated in region A, while the other regions B, C and D are the control regions dominated by background events. Using the event yields in the four regions, the background in the signal region is determined.

This method shows that, even though the statistics of the Sherpa 2-tagged spectrum is not sufficient to draw any statistically firm conclusion, there is a general deterioration of the closure of the method starting from 600 GeV. This is a possible explanation on why the fitting tests are not successful on the full range up to 1.2 TeV, and we have to restrict the fit range to 800 GeV and 1 TeV. Nevertheless, in data the full range is used and the unblinding procedure is followed.

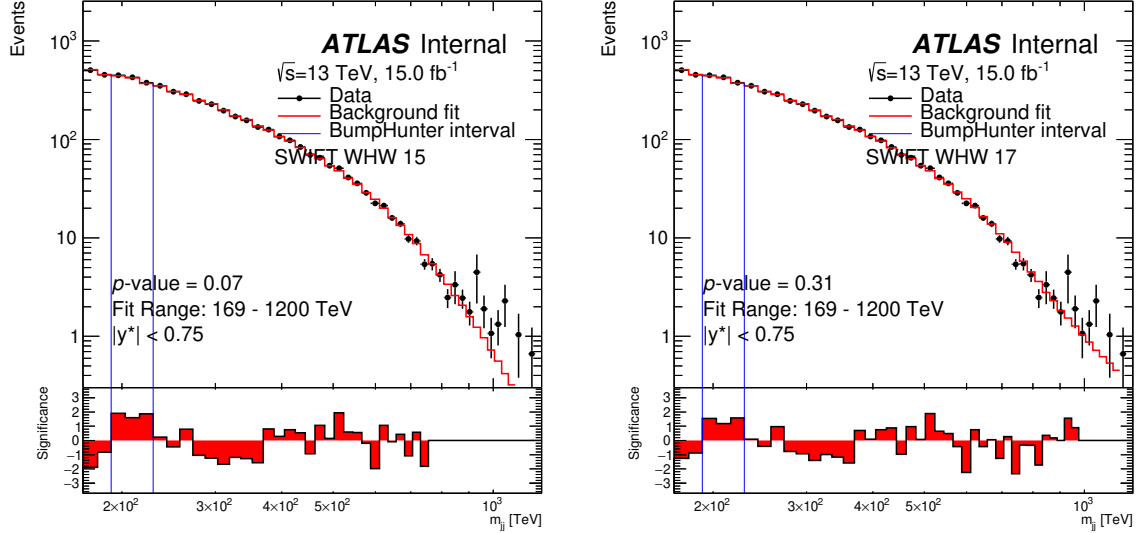
For the ABCD 2-tagged spectrum, results are shown in figure 4.16 and table B.8 on appendix B.5 for two different background estimation ranges (1 TeV and 800 GeV) showing that we would have at least two functions with a window width above 14 bins of half-width.

More fits in MC and the 15 fb⁻¹ dataset with the whole variety of fitting functions as well as many different SWiFt whw sizes can be found on the internal note [156].

4.4.2 Signal injection tests

Any fit-based background estimation technique needs to fulfill certain requirements of robustness to be reliable for a new physics search. These are:

- The background estimation must not exhibit localised excesses or deficiencies due



(a) Single photon trigger, ABCD 2-tagged spectrum, end point 800 GeV, `our4param` (b) Single photon trigger, ABCD 2-tagged spectrum, end point 1 TeV, `our5param`

Figure 4.16: Examples of fits in 15 fb^{-1} of data in an ABCD-scaled 2-tagged spectrum, using the `our4param` and `our5param` functions.

to differences between the QCD shape and background estimation.

- If the background estimation is significantly affected by the presence of signal, the signal must be identified and the signal window excluded for further analysis.
- If the signal is present but at low levels such that it is not identified, the predicted background values must not be significantly affected, neither in the region neighboring the signal nor globally.

Several studies are performed to verify that those requirements are met. The sliding window fit is used for this, and the minimum window half-width obtained from the MC studies before is used as a starting point.

Signal injection studies are performed as described next to prove that the background estimate will not be biased by the presence of a signal.

To achieve this, Gaussian signals are injected on the background in order to study the dependence of the signal sensitivity in the search phase on the SWiFT window width and validate the robustness of the background fit in presence of signal (more details on this kind of studies can be found in [169]).

The injected signals have a relative width of 5% to 15% and are injected at all tested mass points in the fit mass range. In this study, the signal normalisation is iteratively tuned to exceed the BumpHunter p -value threshold (0.01) set to remove the interval of highest excess of the mass spectrum from the fit.

BumpHunter [170, 171] is a statistical framework designed to identify mass resonances with a narrow natural width that would appear as gaussian bumps on top of the SM background. The algorithm locates the most significant bump, where the data are most deviant from the null hypothesis (H_0) which is taken to be only background. Based on this bump, the test returns a p -value, corresponding to its Type-I error probability. This test is designed to be sensitive to local excesses of data.

The background is derived from pseudo-experiments from a smooth fit to the 15 fb^{-1} data spectra, drawing pseudo-data with statistics equivalent to the statistics of the full dataset. The signal-plus-background distribution is then fitted using the SWiFt algorithm with different window widths. The shape of the fitted background with signal injected is then compared to the shape of the background without any signal injected, allowing to check the bias given by the possible signals against the statistical uncertainties.

Figure 4.17 is given as example. Here the curves in the main panel indicate the ratio to the background without any signal injected, for the case in which the signal normalisation is below the BumpHunter 0.01 p -value threshold for removal of the window corresponding to the excess (“just above”, green graphs) and in the case when it does not (“just below”, blue graphs). The bottom panels show the bin-by-bin significance of pseudo-data vs background estimation in the two cases, with the light red area superimposed representing the significance from a fit to the pseudo-data without any signal injected.

The “just below” case represents the bias to the background from having a signal-like fluctuation without being able to discover any signal, while the “just above” case represents the case where the signal is found and removed, and the pseudo-data distribution is then refitted. The bias from the “just above” case is expected if a signal is found and the corresponding window removed to be smaller than for the case where the window is not removed, so the minimal acceptable signal window is decided using the “just below” case. The bias in the “just below” case is considered acceptable when contained within 3σ of the statistical uncertainties of the background model. Figure 4.17a shows a case in which the bias is not acceptable, in the case of a wide signal close to the start of the fit range (400 GeV mass vs 300 GeV for the fit’s starting point). While for figure 4.17b the bias is acceptable, in the case of a narrow signal in the middle of the fit range (750 GeV mass vs 250 GeV for the fit’s starting point).

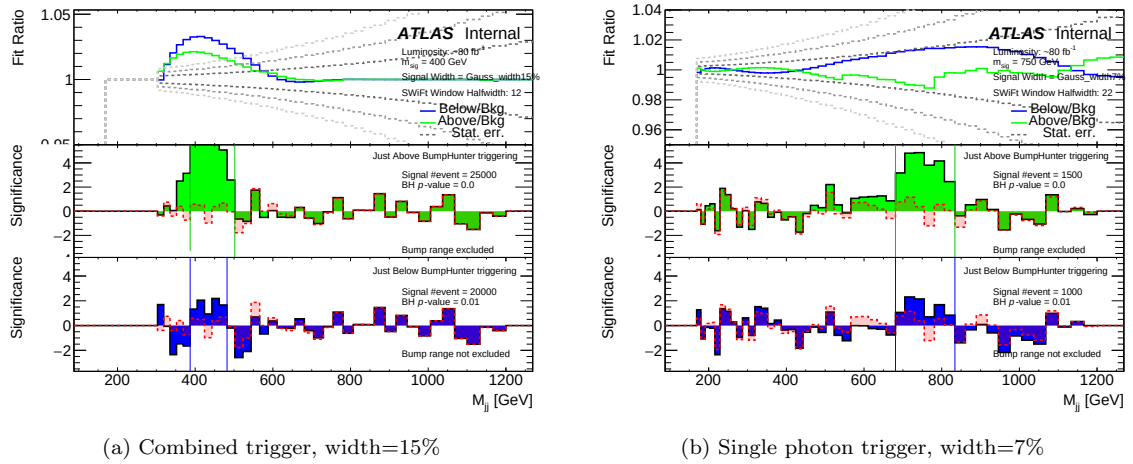


Figure 4.17: Comparisons of the fit in cases of inclusion/exclusion of the bump region for different Gaussian signals injected at the 400 GeV mass point for the combined trigger (left) and 750 GeV mass point for the single photon trigger (right). The green and blue curves on the top panel represent the ratios between background without any signal injected to the background with signal injected, in the green case after removing the most discrepant bins in all SWiFt fits and in the blue case without bin removal, mimicking the case in which the signal is just below the discovery threshold. The bottom two panels show the significance of signal+background with respect to the estimated background in the two cases (with and without signal exclusion, respectively). The significance of the deviations of the (pseudo-)data with respect to the background estimated starting from a distribution where there was no injected signal is overlaid in red, showing the intrinsic statistical fluctuations of the dataset.

This test was repeated for all SWiFt half-window widths from 22 bins to 12 bins, for

all signal mass points considered in the analysis (250 GeV to 1100 GeV) and for the three Gaussian widths of 7%, 10% and 15%, and for each of the two inclusive channels. It was not performed for the b -tagged channel since the MC statistics was insufficient.

The conclusions drawn from these plots affect both search and limit setting phase, since the presence of a non-detectable signal biasing the background estimation would mean a model-independent search is not sensitive to it. Based on the results it was decided to:

- Set the minimum acceptable SWiFt window half-width to 14 bins, as that ensures that the bias for signals of 7% and 10% in each of the two trigger selections remains below the threshold.
- If the SWiFt window half-width is smaller than 19 bins, Gaussian limits will not be set for widths of 15% for the single photon trigger, neither for widths of 13% for the combined trigger region.
- If the minimum acceptable SWiFt window half-width of 14 bins is reached, the search region will be restricted and the signals probed to 1 TeV rather than 1.2 TeV.

4.4.3 Unblinding

All the tests performed give reason to believe that the unblinded spectra in all four channels ought to be well described using a sliding window fit with one of the selected functions and either a global fit or a window half-width of at least 14 bins. Nonetheless, a well-specified procedure is needed to define the parameters of the background estimation during the unblinding.

The unblinding procedure will follow these steps:

1. Fit chosen signal region using a global fit from the lowest starting points considered viable (169 GeV for the single photon trigger spectra, and 335 GeV for the spectra triggered by the combined trigger), and subsequently a sliding window, for the 5-parameter, 4-parameter and UA2 functions. For the sliding window fit, start with a window with a wide half-width, ideally the largest which the data and MC tests indicate might be useable, but necessarily one which gives a χ^2 p -value > 0.05 in the tests (B.7).
2. In case of the global fit, check whether two fit functions converged. In case of the sliding window fit, check whether the individual sliding window fits converged for at least two of the functions. If not, move to a sliding window or reduce the window size and start over.
3. For the fit functions that converged, check whether the global data-background χ^2 p -value > 0.05 .
 - if yes, refit allowing for window exclusion and proceed with regular search and limit setting phase (BumpHunter p -value, if above a threshold of 0.01 proceed to set limits)

- if not, the distinction between a bad background description and an excess needs to be made, so a refit is performed excluding the most discrepant window and let the background for that window be estimated using the sidebands. Then the BumpHunter p -value is checked considering the whole spectrum, and the χ^2 and BumpHunter p -values for the compatibility of the data and estimated background excluding the most discrepant window.

At this point the procedure branches into two cases.

If the p -values of both χ^2 and BumpHunter for the spectrum excluding the most discrepant window are above the predefined thresholds of 0.05 and 0.01, and the BumpHunter p -value including the window is below 0.01, respectively, then there is an indication of an excess that lies in the excluded window. So the systematic uncertainties are applied to the background in the search phase⁶. If systematic uncertainties still do not account for this excess, a set of checks that has been established by the TLA analysis when facing a similar situation are performed, as described in appendix A of [169]. These tests will give confidence that the excess is coming from an s-channel resonance or from a new process.

If the p -values of both χ^2 and BumpHunter for the spectrum even excluding the most discrepant window are still below the predefined thresholds of 0.05 and 0.01, they are the indication of a bad background estimation. In this case, the window half-width is decreased by one bin, and the procedure repeated. The procedure continues until there are two functions satisfying the criteria above, with the same window width. If the window half-width becomes so narrow that the sensitivity to the signals is lost as shown from the signal injection tests, then the procedure is repeated removing one bin from the lowest mass region at a time.

The best performing function defined by the χ^2 p -value will be used as the nominal description of the background, and the second best will be the alternative one used to estimate an uncertainty accounting from the fit function choice (see section 4.5).

4.5 Systematic uncertainties

This section describes briefly the full set of systematic uncertainties, their impact on the analysis results and the procedure used to estimate them. Further details along with illustrative figures are given in appendix B.6.

Some uncertainties, such as jet energy scale, must be applied only to the background or to the signal, but not to both, in order to properly assess their impact. Thereby, only uncertainties relevant to the fitting procedure are applied to the background estimate. While the rest of the uncertainties recommended for application in Monte Carlo are applied to the signal samples.

4.5.1 Uncertainties applied to the background estimate

There are basically two systematic uncertainties associated with the background estimation method: one comes from the choice of the fit function used by the sliding window

⁶In the tradition of dijet searches, this search does not apply systematic uncertainties in the search phase, given that correlated systematic uncertainties (such as those connected to the absolute scale) are irrelevant to the outcome of the data-driven background estimation strategy and that the influence of uncorrelated systematic uncertainties (such as those connected to smoothness) was assumed to be negligible.

fit, and the other one from the fit quality itself. The last one is the dominant of the two and is related to the statistical uncertainty of the dataset being fitted. Below are some details of each uncertainty.

Function choice. This uncertainty is associated with the choice of fit the function. As mentioned in section 4.4, the function with the best χ^2 p-value in the unblinding procedure is taken as the “nominal” function that best describes the background. However, at least two functions are required to pass the criteria for an acceptable fit and the one that performs worst is taken as an “alternative” function for each channel. The difference between the selected nominal and alternative fit functions is used to define an uncertainty which is allowed to vary between the fit function and its alternative, maintaining a directionality from one to the other so that physically motivated functional forms are maintained even if the nominal and alternative functions cross. A detailed description of how this uncertainty is implemented in the limit setting can be found in [172].

Fit quality. This uncertainty is associated directly with the quality of the fit. Since the confidence interval on a function is meant to represent the 1σ region within which the fit would fall in the large-number limit of repeated trials, it can also be computed by throwing pseudoexperiments and fitting each. The pseudoexperiments are generated using Poisson statistics based on H_0 so only the fit itself is required. H_0 is defined from the nominal fit, the fit to the real data. A large number of these pseudo-datasets are generated, each is fit using the same starting conditions as the observed data, and the error on the fit in each bin is defined to be the RMS of the function value in that bin for all the pseudoexperiments.

In both cases, the final uncertainty depends on the channel and the characteristics of the m_{jj} spectrum, and it varies from 0.5% to 10%.

Figure 4.18 shows the two uncertainties for a sliding window fit with window half-width of 23 bins. A dataset sample of 15 fb^{-1} is analysed with the inclusive selection for the combined trigger. Here, the nominal fit corresponds to the dijet 4-parameter function, while the UA2 function is taken as the alternate. The statistical uncertainty (fit quality) is dominant across the m_{jj} range. There are noticeable variations in the function choice uncertainty for different mass ranges, this is a clear example of the average differences between the fit functions in different regions of m_{jj} .

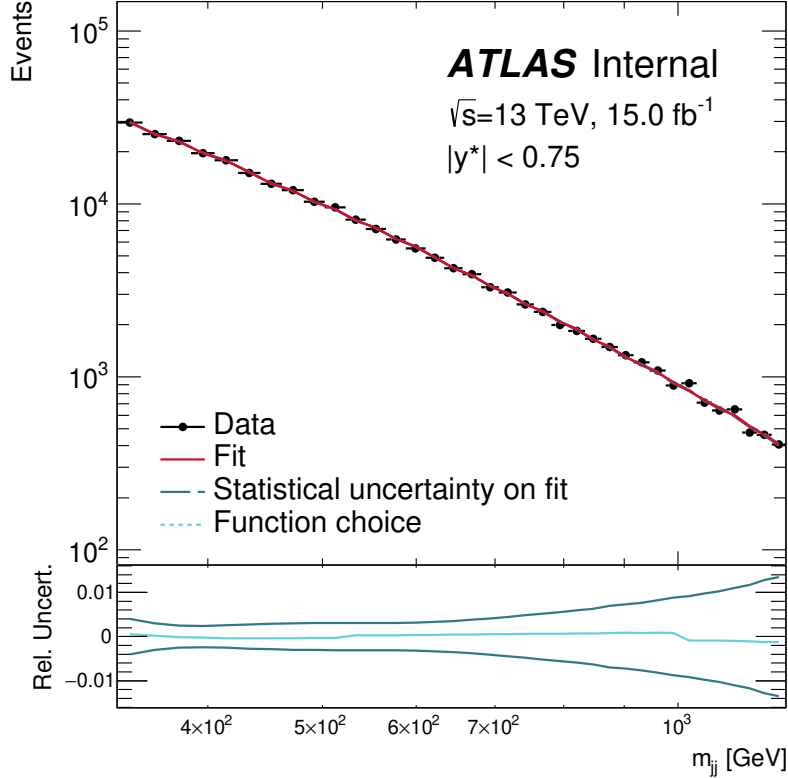


Figure 4.18: Fit quality uncertainty (dark blue) and fit function choice uncertainty (light blue) in an example fit to a statistically non-sensitive data sample using the combined trigger and inclusive selection. The fit quality uncertainty is symmetric while the fit function choice uncertainty is treated as asymmetric to preserve the directionality when the two fits cross one another.

4.5.2 Uncertainties applied to the signal

Jet energy scale and resolution. A jet energy scale (JES) uncertainty is applied to the signal templates, following the latest official recommendations [173]. A strongly-reduced four nuisance parameters (NP) configuration is used, each for a different component. The JES uncertainty ranges from around 8% for jets of $p_T \sim 25$ GeV to 1% for jets of $p_T \sim 750$ GeV.

All four uncertainties act not on the acceptance (roughly speaking, the number of events or the normalisation) but rather on the peak location of the invariant mass spectrum, moving it to higher or lower m_{jj} as events move between bins. This effect is accounted for in the limit setting procedure by using MC templates for $\pm 1, 2, 3\sigma$ in each of the uncertainties and allowing all four to be marginalised independently. This approach is only valid for the Z' model-dependent limits. The Gaussian limits require an approximation of this effect which is discussed later in this section.

The uncertainty on the jet energy resolution (JER) is also calculated by varying signal templates. But, unlike the JES, the effect is to widen the peak somewhat instead of changing its location. The impact can be hard to see bin-by-bin, as the statistics of affected bins are quite low and the fluctuations vary dramatically, so rather than use the variation between the templates and propagate very statistically dependent effects, average trends are examined to look for a single treatment that can be applied across samples. In order to do this, the binning on m_{jj} is increased to 50 GeV and the weighted

average effect between all samples is taken as the value in each bin. This is sufficient to reduce the statistical fluctuations and extract the size of the underlying uncertainty. A linear fit is performed to the resulting distribution. Based on the fits, a flat 3% JER uncertainty will be applied in both channels.

Photon ID, energy scale and resolution. The photon energy scale and resolution uncertainties are determined in accordance with the official recommendations. A simplified correlation scheme is used, reducing the various input uncertainties to two nuisance parameters corresponding to overall photon energy scale and resolution. Both of these uncertainties can affect signal acceptance by determining whether or not a photon passes the trigger-based offline p_T requirement. However, as the photon energy is not used to reconstruct the variable of interest (m_{jj}), these uncertainties do not affect signal shape. So their effects alter the normalisation of the sample but not the peak shape or location.

Since the uncertainties evaluated within each sample are statistically limited, a method was sought for deriving a value of the uncertainty which could be applied to all signal samples, instead of relying on the differences between MC templates like for the JES/JER uncertainties. To this end, the variation in each signal point due to the systematics were plotted together to understand the overall behaviour and determine if it could be used to derive a statistics-robust evaluation of the uncertainty as a function of m_{jj} .

As expected, the uncertainties are larger for the single photon trigger than for the combined one since the former selection depends entirely upon the photon in the event while the latter selection leans more heavily on the jets.

The photon ID scale factor uncertainty affects the MC weights of the events which have passed selection, thus varying the normalisation of the signal templates. It therefore shows less statistical fluctuation than the energy scale and resolution uncertainties, which vary which events pass selection rather than their weights. They are nevertheless assessed using the same technique as the previous uncertainties in order to determine a single consistent treatment across the signal samples.

Finally, to remove the statistical fluctuations and understand the overall trend in the photon uncertainties, the sum in quadrature of the three photon-related uncertainties per signal sample is taken, and a per bin weighted average of these total uncertainties for the different signal samples is then obtained. A linear fit is performed to the resulting points which shows that the size of the uncertainty does not change with m_{jj} . Thus the effects of photon energy scale, resolution, and ID scale factor are treated purely as acceptance uncertainties, with a single fixed size covering all three uncertainties of 2% for the single photon trigger and 1.4% for the combined trigger. One nuisance parameter is used to scale the number of events in the signal template.

Trigger efficiency. From the studies in section 4.2.2, it was visible that the combined trigger never achieves a perfect plateau of 100% efficiency even after all analysis cuts are applied. To study this effect and determine whether a trigger inefficiency uncertainty should be applied, the trigger efficiency as a function of m_{jj} is calculated for both choices of trigger. In both cases, all analysis cuts except for minimum m_{jj} are applied, including relevant photon and jet p_T cuts as well as the y^* cut. Ideally this distribution would look flat around 1, so a fit is performed and any shift from the unity can be assessed as an uncertainty. No obvious dependence of the efficiency on m_{jj} came out from the study. So, based on these fits, an uncertainty of 3% is applied in the combined trigger channel to account for trigger inefficiency. No such uncertainty is applied for the single photon trigger where the efficiency is essentially 100%.

***b*-tagging scale factors.** Correction factors are applied to the simulated event samples to compensate for differences between data and simulation in the *b*-tagging efficiency for *b*, *c* and light-jets. Approximately 25 individual scale factor uncertainties are provided by the flavour-tagging group and signal templates varied according to each have been produced. Since each of the 25 uncertainties is very small, a conservative simplification is made by taking the sum in quadrature of all of them and applying the result parameterised by a single nuisance parameter. The impact of that nuisance parameter was determined using a method very similar to that of the photon energy uncertainties: first the impact on each signal sample was assessed to ensure it changed only normalisation and not shape. Next the impact bin by bin of each individual scale factor uncertainty was plotted for all signal samples, to ensure the size of the effect depended only on m_{jj} and not on the individual sample being considered. Finally the quadrature sum of the impact of all 25 uncertainties was averaged across the signal samples and a parameterisation found for it which could be used on each sample, thereby producing an uncertainty robust against statistical fluctuations in the individual samples.

The sum in quadrature of all 25 uncertainty components inherits the dependence on m_{jj} of the individual components. The total uncertainty is relatively flat until about m_{jj} of 300 GeV, when it begins to increase in a fairly linear way. To assess this m_{jj} dependence in more detail, a weighted average of the values in each bin is plotted, and a linear fit is performed from 300 GeV to 1200 GeV. A flat value of 5% can be used from 170 GeV to 300 GeV.

Thus the total *b*-tagging uncertainty used in both single photon trigger and combined trigger 2 *b*-tagged channels is 5% for $m_{jj} < 300$ GeV and $0.0001115(m_{jj} - 300) + 0.05$ for $300 \text{ GeV} < m_{jj} < 1200 \text{ GeV}$.

Luminosity. The uncertainty on the integrated luminosity is derived, following a methodology similar to that detailed in [174], from calibrations of the luminosity scale using x-y beam-separation scans. It is treated as a single normalisation uncertainty applied to the signal templates as a scale factor. For the single trigger photon channels, its value is taken to be $\pm 2.0\%$ by combining the result of the scans from 2015, 2016 and 2017, using the ATLAS luminosity working group recommendation. The integrated luminosity uncertainty for the combined trigger photon channels is $\pm 2.3\%$. This is the luminosity-weighted uncertainty calculated from the $\pm 2.2\%$ integrated luminosity uncertainty corresponding to the 2017 dataset and the $\pm 2.4\%$ integrated luminosity uncertainty corresponding to the 2016 dataset.

PDF choice and parameters. PDF uncertainties largely affect the normalisation of the signal rather than the shape of its distributions. To determine the effect, events are generated using the ensemble of PDFs provided by the NNPDF group using [175]. The differences in acceptance are calculated for each member of the ensemble and, following the ATLAS official recommendation [176], the standard deviation of all acceptance variations is assigned as a systematic uncertainty. For this purpose, the mass distribution after the analysis selection and all relevant weights as a function of mediator mass is calculated for each pdf variation. Comparing this result with the total weighted number of events before the analysis selection, the relative acceptance for each PDF variation is computed. The results shown that the systematic uncertainty is less than 1% everywhere, so a 1% flat systematic was applied on the signal normalisation.

JES uncertainty for model-independent limits. When setting limits on generic

Gaussian shapes instead of benchmarks generated with Monte Carlo, the JES uncertainty becomes more poorly defined. The uncertainties on the background estimate are unchanged between model-dependent and model-independent limits, and the other uncertainties can all be applied to Gaussian shaped signals in exactly the same way as to the Z' samples. The PDF uncertainty is not applied to Gaussian limits at all, since it is a theory-dependent uncertainty.

To simulate the effects of JES on a real signal for use with the Gaussians, the impact on the m_{jj} value of the signal peak due to the uncertainty must be measured and can then be applied to move the mean of the Gaussian template. To this end, a Gaussian fit is performed to the core of each signal template as well as to the $\pm 3\sigma$ variations in each JES uncertainty component.

The equivalent fit is repeated for each point and the resulting shift in the fitted mean location is added in quadrature across the four independent nuisance parameters. The fits are less reliable in the 2 b -tagged channel due to the very low statistics, and in particular tend to fail for the $+3\sigma$ variations due to the shape of the signal. Thus the larger shifts in the -3σ direction should be taken as the more reliable estimate of the uncertainty size. In every case, the shift in the mean is found to be $\leq 2\%$. Therefore this value is chosen for use in the model-independent Gaussian limits.

4.5.3 Summary of uncertainties

A summary of all uncertainties for each channel is presented in table 4.4.

Uncertainty	Inclusive, single γ trig.	Inclusive, combined trig.	2 b -tagged, single γ trig.	2 b -tagged, combined trig.
Fit statistics	0.5% - 10% of background, depending on channel and m_{jj}			
Fit function choice	0.5% - 10% of background, depending on channel and m_{jj}			
JES	Templates for Z' , 2.0% shift in Gaus. mean for model-indep. limits			
JER	3.0%	3.0%	3.0%	3.0%
Photon related	2.0%	1.4%	2.0%	1.4%
Trigger efficiency	–	3.0%	–	3.0%
b -tagging SFs	–	–	$\sim 5.0\%$ - 15.0%	$\sim 5.0\%$ - 15.0%
Luminosity	2.0%	2.3%	2.0%	2.3%
PDF	1.0% Z' , none for model-indep. limits			

Table 4.4: Summary of all uncertainties used in limit setting, by channel.

4.6 Results

4.6.1 Search phase

Figure 4.19 shows the results of fitting each of the observed distributions, as described in section 4.4. For each distribution, the functions with the highest χ^2 p -value (shown in the figure), in absence of localised excesses, is chosen as the nominal function for the fitting method. The function with the lowest χ^2 p -value which still results in a p -value larger than

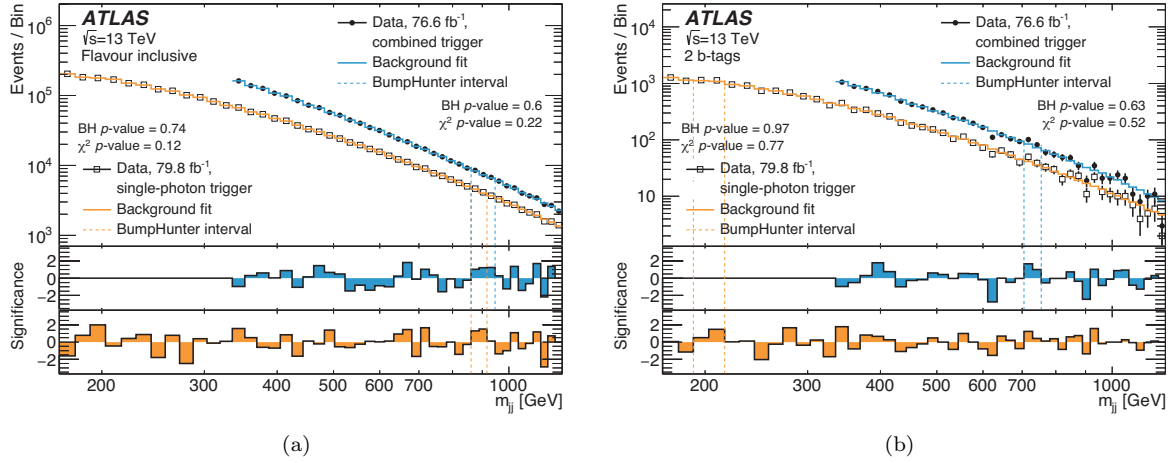


Figure 4.19: Distribution of dijet mass for events selected as in the main text, for the flavour-inclusive (a) and b -tagged (b) categories separately. The upper (filled circles) events are collected with the combined trigger and contain a $p_T > 95$ GeV photon and two $p_T > 65$ GeV jets. The lower (hollow squares) events are collected with the single-photon trigger and contain a $p_T > 150$ GeV photon and two $p_T > 25$ GeV jets. Solid lines indicate the best fit function. The bottom panels show the significances of bin-by-bin differences between the data and the fits for the combined trigger (middle) and single-photon trigger (bottom). These Gaussian significances are calculated from the Poisson probability, considering only statistical uncertainties.

0.05 is chosen as an alternative function. The primary and alternative functions for each of the four search categories are shown in table 4.5 along with the fit and BumpHunter results. The alternative function is used to estimate the systematic uncertainty of the background prediction due to the choice of function, as described in section 4.5.

Channel	Nominal function	Alternative function	Fit low edge	Fit high edge	SWIFT whw	BH p -value	χ^2 p -value
Single γ trigger, Inc.	our5param	our4param	169 GeV	1200 GeV	19	0.74	0.11
Combined trigger, Inc.	our4param	UA2	335 GeV	1200 GeV	23	0.60	0.23
Single γ trigger, $2b$ -jets	our4param	our3param	169 GeV	1200 GeV	23	0.97	0.75
Combined trigger, $2b$ -jets	our3param	our5param	335 GeV	1200 GeV	23	0.63	0.53

Table 4.5: Results for the fitting for each channel.

Without including systematic uncertainties, the BumpHunter p -value – the probability that fluctuations of the background model would produce an excess at least as significant as the one observed in the data, anywhere in the distribution – is $p > 0.5$ for all distributions. Thus, there is no evidence of a localised contribution to the mass distribution from new phenomena.

4.6.2 Limits

4.6.2.1 Setting procedure

In absence of signal, limits are set on the possible number of events from resonant new physics processes.

For the Z' mediator being studied, Monte Carlo samples have been simulated at a number of selected mass points. The Bayesian method is applied to data at these same mass points to set a 95% CL limit on the cross section times acceptance, $\sigma \times \mathcal{A}$, for the NP signal as a function of m_{NP} .

To set an upper limit to the Z' cross section the Bayesian method, originally designed by the DØ collaboration [177], is implemented. Let's consider a bin i in the m_{jj} distribution. The likelihood of observing n_i events for a given luminosity $\mathcal{L}$ is given by:

$$L(x_i|\sigma) = \frac{(a_i \mathcal{L} \sigma + b_i)^{n_i}}{n_i!} \exp[-(a_i \mathcal{L} \sigma + b_i)]$$

where σ is the unknown cross section times the branching ratio, $\sigma(pp \rightarrow Z') \times \mathcal{B}(Z' \rightarrow q\bar{q})$; a_i is the signal acceptance and b_i represents the expected number of events for the background.

The likelihood of measuring a certain m_{jj} distribution is obtained then by multiplying the likelihoods for all possible bins $L(\vec{x}|\sigma) = \prod_{i=1}^N L(x_i|\sigma)$.

$L(\vec{x}|\sigma)$ can be translated into a posterior probability $P(\sigma|\vec{x})$ by the Bayes Theorem. For an uniform prior, only for positive values of the cross section, it becomes

$$P(\sigma|\vec{x}) = \prod_{i=1}^N \frac{(a_i \mathcal{L} \sigma + b_i)^{n_i}}{n_i!} \exp[-(a_i \mathcal{L} \sigma + b_i)] \times H(\sigma) \quad (4.8)$$

where H is the Heavyside function and $P(\sigma|\vec{x})$ represents the bayesian probability for the cross section to have a σ value given the experiment result $\vec{x}$. The upper limit at a 95% CL (σ_{95}) can be found by integrating the posterior probability

$$\int_0^{\sigma_{95}} P(\sigma|\vec{x}) d\sigma = 0.95$$

In order to determine the expected upper limit, meaning the upper bound for σ in an experiment that has obtained a measure that is compatible with the background, the number of events n_i is replaced by b_i in each bin on equation 4.8.

The statistical error of this limit can be obtained by tossing pseudo-experiments where the measured number of events for each bin is treated as a random Poisson variable with parameter b_i . The 0.5 quantile from this distribution corresponds to the expected limit, while the $\pm 1\sigma$ and $\pm 2\sigma$ uncertainties are extracted from the $0.5 \pm (0.682/2)$ and $0.5 \pm (0.954/2)$ quantiles respectively.

The analysis uncertainties discussed in section 4.5 are incorporated into the method by varying all the sources according to Gaussian probability distributions and convolving these with the Bayesian posterior probability distribution. Credibility intervals are then calculated numerically from the resulting convolutions.

The limit on $\sigma \times \mathcal{A}$ from data is interpolated logarithmically (linearly in the log of the cross section) between mass points to create a continuous curve versus m_{jj} . The exclusion limit on the mass of the given NP signal occurs at the value of m_{jj} where the limit on

$\sigma \times \mathcal{A}$ from data is the same as the theoretical value, which is derived by interpolation between the generated mass values.

Limits are also set where a generic signal is approximated using a Gaussian line shape. This provides a limit on the cross section times acceptance times efficiency times branching ratio which can be applied to any model which would approximate this shape after the analysis selection, as described in detail in the appendix of ref.[138].

This form of analysis is applicable to all resonant phenomena where the NP couplings are strong compared to the scale of perturbative QCD at the signal mass, so that interference with QCD terms can be neglected.

4.6.2.2 Model dependent limits

This section shows the limits set on the benchmark Z' model following a Bayesian procedure. All uncertainties discussed in section 4.5 have been accounted for when calculating these results, and the signal samples were generated in both MC16a and MC16d weighted according to the proportion of luminosity made up by each year of data taking. The limits as a function of Z' mass are calculated independently for the two values of the SM quark coupling g_{SM} which are above and below the theoretical excluded cross section. These limits are shown in figures 4.20–4.22.

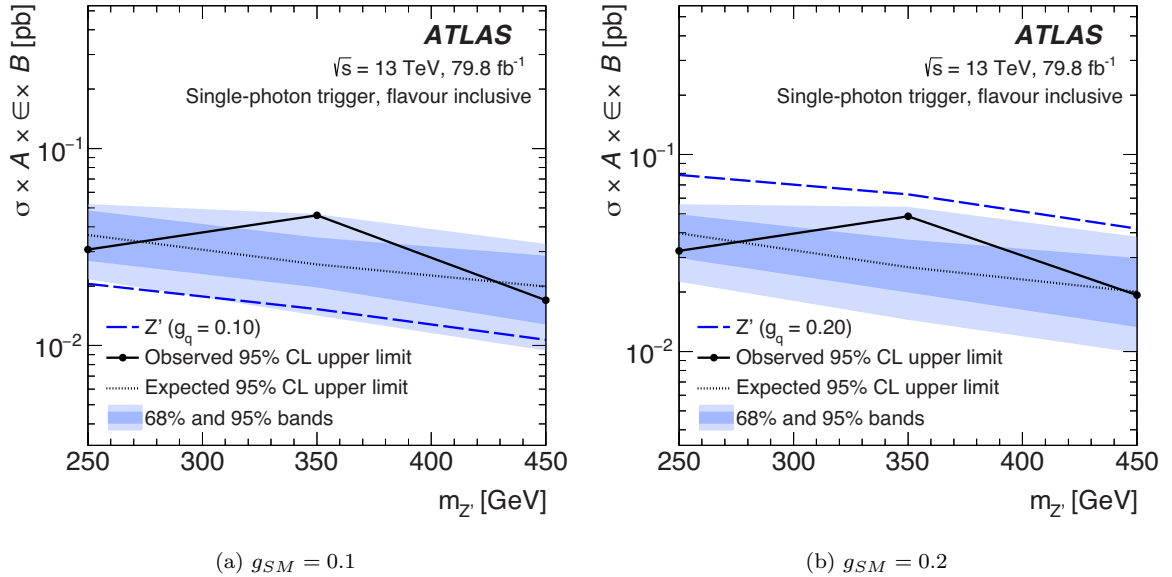


Figure 4.20: Limits on the product of cross-section, acceptance, efficiency, and branching ratio for the Z' model with either $g_q = 0.1$ (4.20a) or $g_q = 0.2$ (4.20b) for the single-photon trigger and the flavour-inclusive selection. The black points represent observed limits computed for discrete values of masses $m_{Z'}$. The black dotted line represents the 95%-CL expected limit, as calculated from pseudoexperiments, assuming observations match the mean background prediction. Also shown are green and yellow bands indicating the $\pm 1\sigma$ and $\pm 2\sigma$ variation of limits expected for observations fluctuating around the mean background prediction. The blue dotted line shows the theoretical prediction for the model.

A single summary exclusion across all coupling values can be seen in figure 4.23. The results from the single and combined triggers are combined in each channel to produce a single plot, and the different coupling possibilities are combined by interpolating the limit results across coupling as well as mass. The final result is a single two dimensional plot of limit versus coupling and m_{jj} for each of the inclusive and two b -tagged selections. The

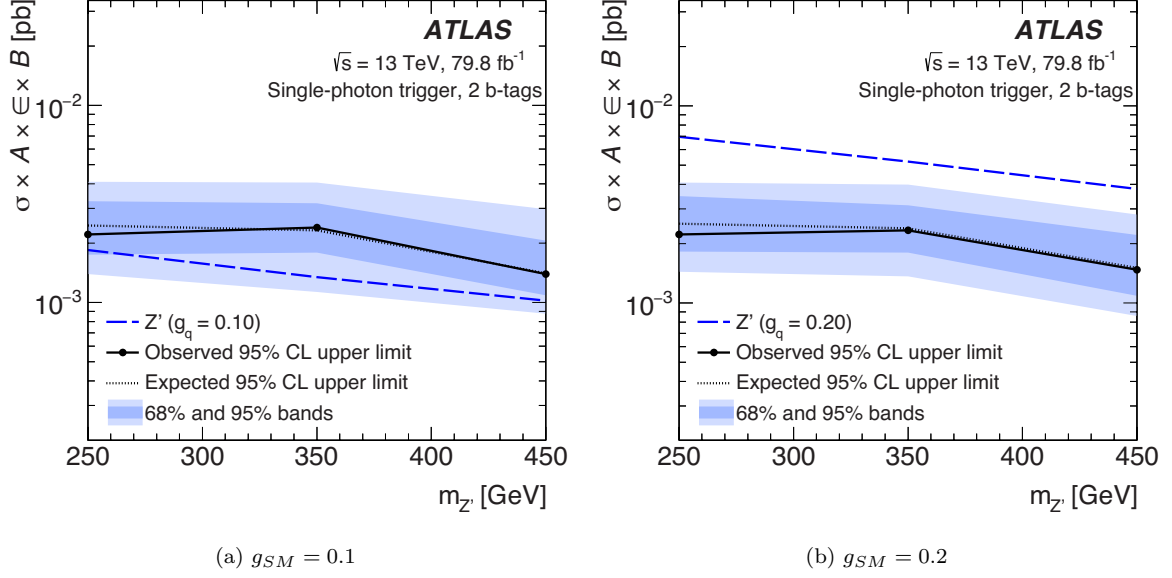


Figure 4.21: Limits on the product of cross-section, acceptance, efficiency, and branching ratio for the Z' model with either $g_q = 0.1$ (4.21a) or $g_q = 0.2$ (4.21b) for the single-photon trigger and the b -tagged selection. The black points represent observed limits computed for discrete values of masses $m_{Z'}$. The black dotted line represents the 95%-CL expected limit, as calculated from pseudoexperiments, assuming observations match the mean background prediction. Also shown are green and yellow bands indicating the $\pm 1\sigma$ and $\pm 2\sigma$ variation of limits expected for observations fluctuating around the mean background prediction. The blue dotted line shows the theoretical prediction for the model.

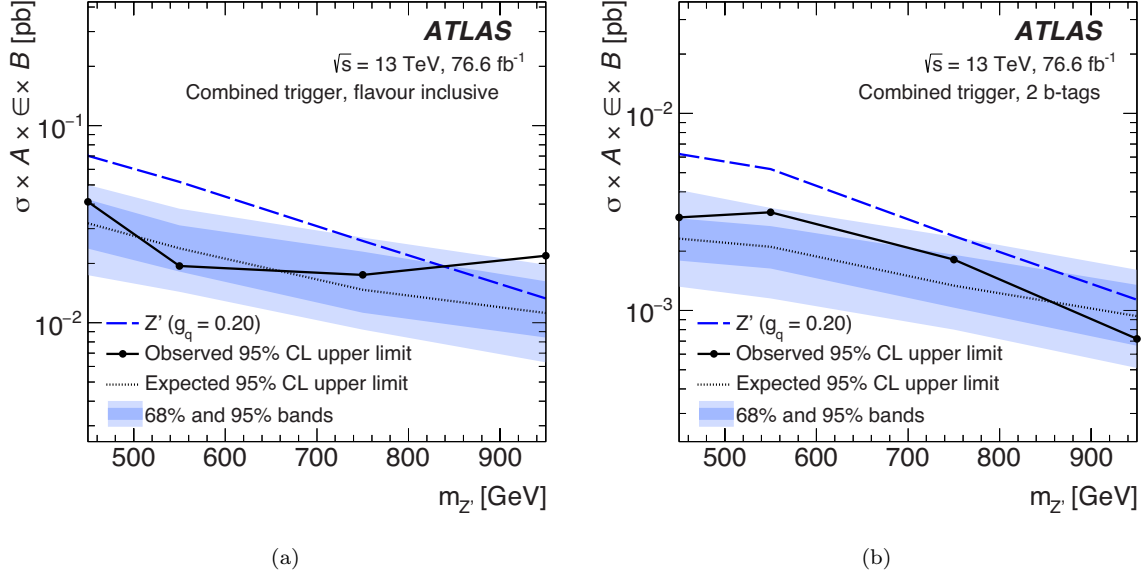


Figure 4.22: Limits on the product of cross-section, acceptance, efficiency, and branching ratio for the Z' model with $g_q = 0.2$ for the combined trigger with the flavour-inclusive selection (4.22a) and the b -tagged selection (4.22b). The black points represent observed limits computed for discrete values of masses $m_{Z'}$. The black dotted line represents the 95%-CL expected limit, as calculated from pseudoexperiments, assuming observations match the mean background prediction. Also shown are green and yellow bands indicating the $\pm 1\sigma$ and $\pm 2\sigma$ variation of limits expected for observations fluctuating around the mean background prediction. The blue dotted line shows the theoretical prediction for the model.

limits from the plots shown above, with couplings of $g_q = 0.1$ and $g_1 = 0.2$, are used as inputs.

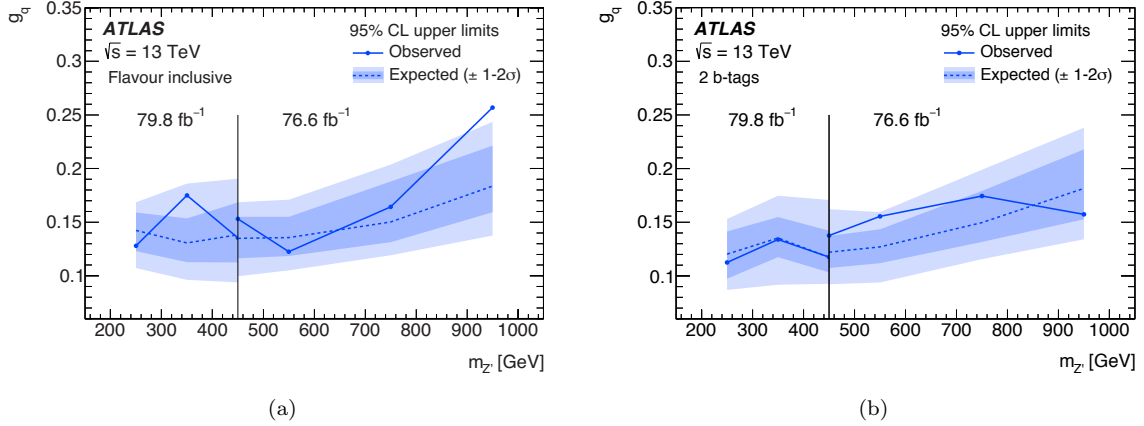


Figure 4.23: Limits on Z' mediators as a function of coupling and mass, using the inclusive 4.23a and the 2 b -tagged 4.23b selection. Limits up to masses of 450 GeV are set using the single photon trigger; above this mass the combined trigger is used. All uncertainties are applied.

4.6.2.3 Model independent limits

Model independent limits are set using Gaussian template shapes in place of the signal Monte Carlo samples. These limits represent the maximum cross section times analysis acceptance times efficiency times branching ratio for any process which, after application of the analysis selection, has a shape which can be fairly approximated as a Gaussian. Signal-related uncertainties are equivalent to those used for the model-dependent limits.

Figure 4.24 shows the Gaussian limits including all relevant uncertainties in each channel. The systematic shift is dominated by the b -tagging scale factor uncertainty in the channels with 2 b -jets, and even in the inclusive channel the addition of another small scale factor to the existing combination of luminosity $\oplus$ photon E/R $\oplus$ JER $\oplus$ PDF should be negligible.

While the y axis is shared between the two selections in these plots, the signal acceptance varies, and thus the two sets of limit points relate to two different interpretations of $\sigma \times A \times \epsilon \times \mathcal{B}$. For example, after accounting for the difference in filter efficiency between the samples used for the two triggers, the acceptance for a Z' of mass 550 GeV is about twice as large for the combined trigger as for the single photon trigger.

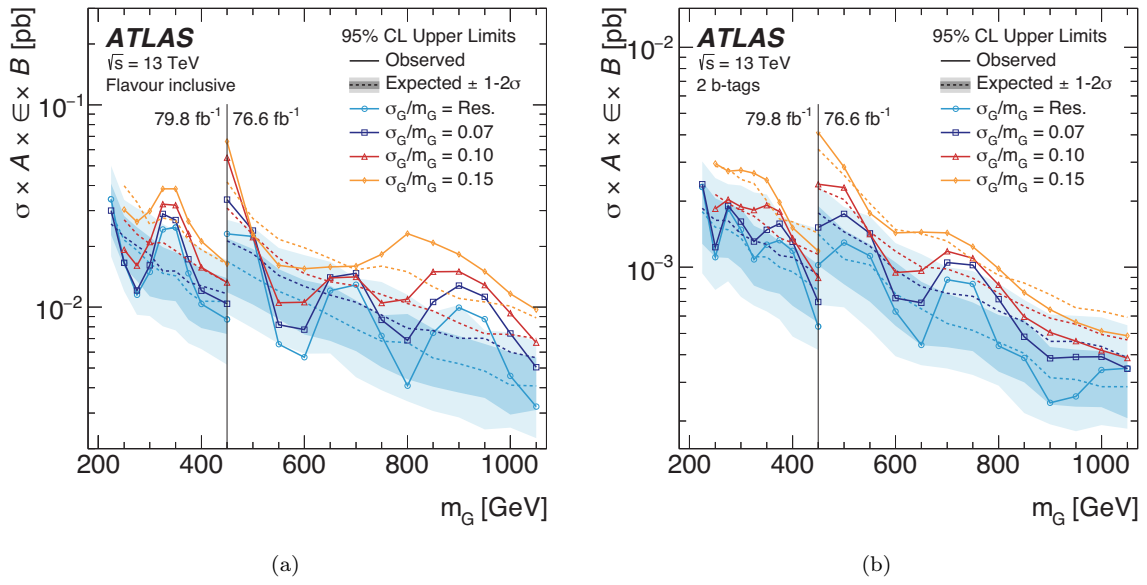


Figure 4.24: Limits on generic Gaussian shaped signals of 15%, 10%, 7% or m_{jj} resolution width using the inclusive (4.24a) and the 2 b -tagged (4.24b) selection. Limits up to masses of 450 GeV are set using the single photon trigger; above this mass the compound trigger is used due to its greater sensitivity. All uncertainties are applied. The acceptances of the two selections shown are different and must be accounted for when comparing the sensitivity.

Chapter 5

Search for top-quark decay to a charged Higgs boson and a b -quark

In 2012, a boson with a mass about 125.09 ± 0.24 GeV [178] was discovered at the CERN LHC with its properties subsequently shown to be consistent with those of the Standard Model (SM) Higgs boson. Although the last missing particle of the SM has been discovered, several questions remain, including the nature of dark matter, and the origin of neutrino masses inferred from the observation of neutrino oscillations. Several hypotheses beyond the SM have been introduced to answer these questions, and many of them include more than one Higgs doublet. Models with two Higgs doublets, so-called two-Higgs doublet model (2HDM) [6], result in five Higgs bosons: two charged ($H^\pm$) and three neutral (A, H, h). In the 2HDM context, the Higgs boson discovered at the LHC can be one of the CP-even neutral bosons (H or h). Unlike the SM, in general 2HDM allows flavour changing neutral current (FCNC) at tree level. To suppress such tree level FCNC, all fermions with the same electric charge are required to couple to one Higgs doublet only [179, 180]. The 2HDM is typically categorised into four different types: type-I, type-II, lepton-specific (type-III), and flipped (type-Y, also known as type-IV), depending on the assignment of up/down-type quark and lepton couplings to each Higgs doublet, as specified in table 5.1.

Model	Type I	Type II	Lepton-specific	Flipped
Φ_1	-	d, ℓ	ℓ	d
Φ_2	u, d, ℓ	u	u, d	u, ℓ

Table 5.1: The four possible assignments of fermion couplings to two Higgs doublets (Φ_1, Φ_2) that satisfy natural flavour conservation. Here u, d and ℓ represent the up- and down-type quarks and charged leptons, respectively.

This analysis presents a search for charged Higgs bosons. Hereafter, it is referred to them as $H^\pm$, but charge conjugate states are always implied. In the 2HDM, the mass of the charged Higgs boson ($m_{H^\pm}$) is an unconstrained parameter. Regardless of its mass, $H^\pm$ is expected to have a large coupling to the top quark unless a specific condition is being considered as in refs. [181, 182]. If the charged Higgs boson is light enough, $m_{H^\pm} < m_{top}$, it can be produced in rare decays of the top quark $t \rightarrow H^\pm b$. In this mass regime the charged Higgs boson will predominantly decay into a charm-quark and a bottom-quark, $H^\pm \rightarrow cb$, in a charm-quark and a strange quark, $H^\pm \rightarrow cs$ or a τ and ν_τ pair $H^\pm \rightarrow \tau \nu_\tau$.

The LEP experiments [183] excluded the mass of charged Higgs below 80 (72.5) GeV

for type-II (type-I for pseudo-scalar masses above 12 GeV) scenario at 95% confidence level (CL).

Previous direct searches for a light H^+ in decays of a top quark have been performed at hadron collider experiments in different channels. Since no indication of a H^+ was observed, the best upper limits on the branching fraction of $t \rightarrow H^+ b$ were placed at $\mathcal{O}(1\%)$. These are the following:

$H^+ \rightarrow \tau\nu$: previous results from CDF and DØ collaborations [184–186] were published. ATLAS set up limits for Run 1 [187, 188] and Run 2 [189]; and CMS did the same for Run 1 [190] and Run 2 [191] as well.

$H^+ \rightarrow c\bar{s}$: first results were delivered by CDF and DØ [192, 193]. For Run 1, both ATLAS [194] and CMS [195] set limits on this channel.

The $H^+ \rightarrow cb$ process is the dominant decay channel in the type-Y (flipped) 2HDM [7–9], and this signal could be a signature of models with more than two Higgs doublets [196, 197]. This can be seen in figure 5.1, where the flipped and the Type-II models branching ratios are shown as a function of $\tan\beta$ ¹ for two fixed mass values m_{H^+} of 80 GeV and 130 GeV. Figure 5.2 shows the branching ratios as a function of m_{H^+} for three different values of $\tan\beta = 1, 5$ and 50 in the flipped 2HDM model.

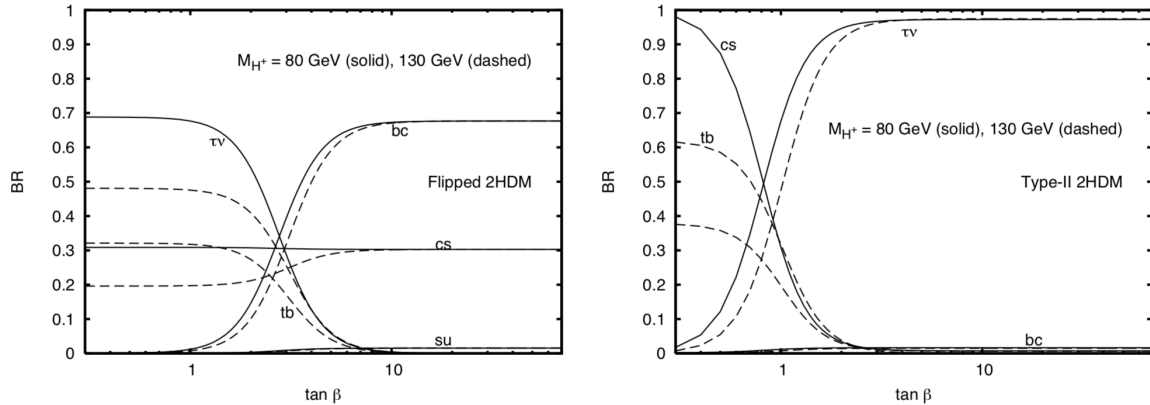


Figure 5.1: Charged Higgs branching ratios as a function of $\tan\beta$ for $m_{H^+} = 80$ GeV (solid lines) and 130 GeV (dashed lines) in the flipped (left) and Type-II (right) 2HDMs. Image taken from [8].

The most consistent feature in both models is the turn-on of decays to $t\bar{b}$ at the kinematic threshold at $m_{H^+} \sim 180$ GeV. Above this threshold, decays to $t\bar{b}$ dominate for both the flipped and Type II models, for all values of $\tan\beta$.

Below the $t\bar{b}$ threshold, the effect of the different $\tan\beta$ dependence of the lepton couplings in the flipped and Type II models becomes apparent. For $\tan\beta = 1$, the branching fractions of H^+ in the flipped model are identical to those in the Type-II model. As $\tan\beta$ increases, the branching fraction to $\tau\nu$ is suppressed in the flipped model due to the $\cot\beta$ dependence of the lepton Yukawa couplings [8]. For $\tan\beta = 5$, decays to $\tau\nu$ reach at most $\sim 5\%$ in the flipped model, while they dominate below the $t\bar{b}$ threshold in the Type II model. For $\tan\beta = 50$, the branching fraction to leptons is below 10^{-4} . Instead, the dominant decay mode of H^+ for $\tan\beta \gtrsim 3$ is into $c\bar{b}$ with a branching fraction of about $2/3$, followed by $c\bar{s}$ with a branching fraction of about $1/3$.

¹ $\tan\beta = \Phi_2^0/\Phi_1^0$, where $\Phi_{1,2}^0$ represent the vacuum expectation values for each Higgs doublet.

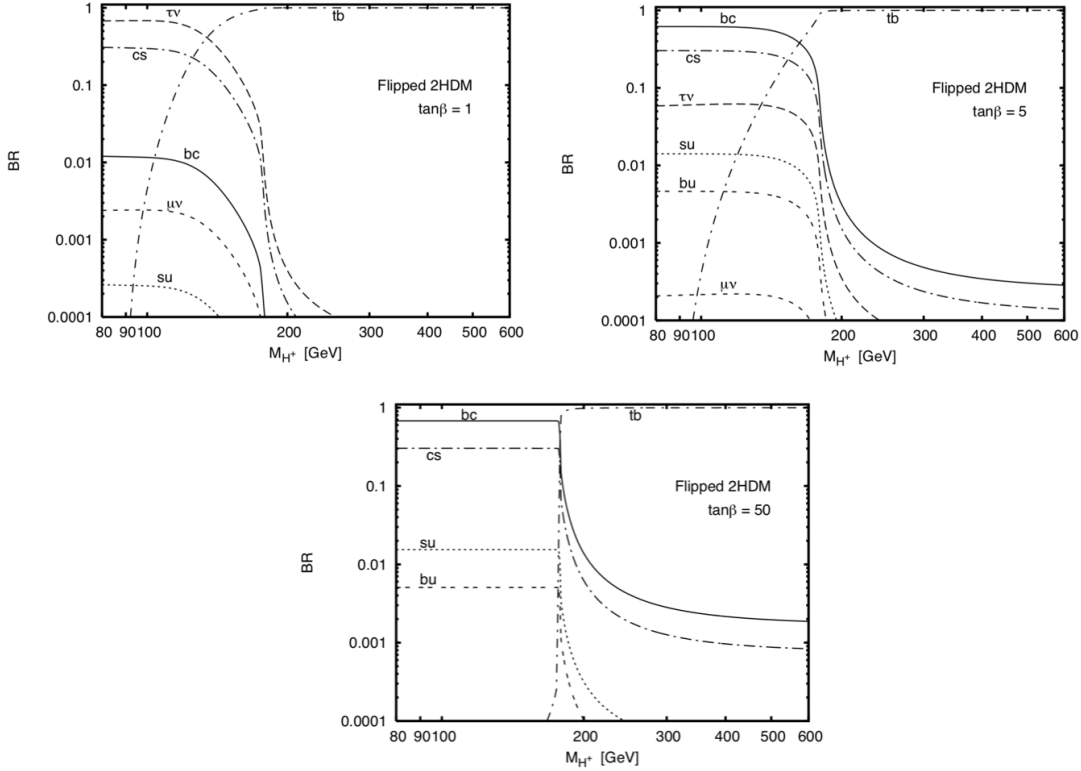


Figure 5.2: Charged Higgs branching ratios as a function of m_{H^+} for $\tan\beta = 1, 5$ and 50 in the flipped 2HDMs model. Image taken from [8].

Previous searches of this kind have been carried out by the CMS collaboration [198] based on the Run 1 dataset. This search reports upper limits at 95% confidence level of 0.8-0.5% on the branching fraction $\mathcal{B}(t \rightarrow H^+ b)$, assuming $\mathcal{B}(H^+ \rightarrow cb) = 1.0$ for the charged Higgs boson mass range 90-150 GeV. ATLAS has not published results for this channel yet.

This search is performed assuming $\mathcal{B}(H^+ \rightarrow cb) = 1.0$ without any other model-dependent assumption, and for a m_{H^+} range between 80-160 GeV.

In this context, one of the top quarks is required to decay into Wb , while the other top quark decays into $H^+ b$, yielding $t\bar{t} \rightarrow Wb t\bar{t} \rightarrow Wb H^+ b$.² This leads to a lepton-plus-jets final state with high b -jet multiplicity, which can be effectively exploited to suppress the overwhelming $t\bar{t}$ background. Only events with an electron or muon, including those produced via leptonically decaying taus, are considered. So the final state is characterised by at least four jets (at least two of which originate from b -quarks), a charged lepton (muon or electron), and missing transverse momentum. If a light $H^+ (\rightarrow cb)$ is produced in top quark decays, the $t\bar{t}$ event would have one more jet to be identified originating from a b -quark due to the H^+ decays, as shown in figure 5.3.

This search follows closely the analysis strategy developed for the Run 1 and early Run 2 searches [199–202] for an FCNC search, and takes advantage of some features that were already optimised during the previous analyses.

Due to the similarity of both signals, this search focuses on $t\bar{t} \rightarrow Wb H^+ b$ in the charged Higgs boson decay channel $H^\pm \rightarrow cb$. The two signal benchmarks share similar

²In the following $Wb H^+ b$ is used to denote $W^- \bar{b} H^+ b$. Similarly, $Wb W b$ is used to denote $W^+ b W^- \bar{b}$.

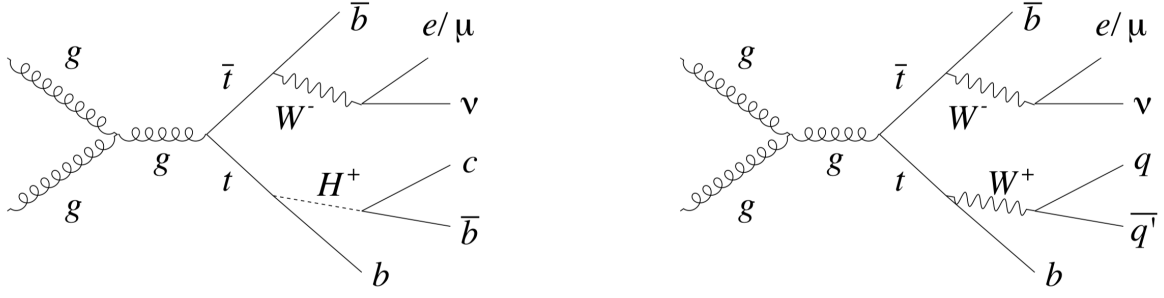


Figure 5.3: Feynman diagrams of the H^+ production in top quark pair events (left) compared to the standard model production of $t\bar{t}$ in lepton+jets final states (right).

jets flavour content and kinematic features for some values of H^+ masses, the latter being defined by how close the SM Higgs boson and assumed H^+ mass are.

Finally, the search uses a profile-likelihood fit to multiple regions defined by jet and b -jet multiplicity.

Signal to background discrimination is achieved by means of a neural network classifier which incorporates pseudo-continuous b -tagging information in the training in order to further suppress the background originating from $t\bar{t}$ production. The neural network is trained simultaneously on all signal benchmarks with a signal label as training feature; this allows to retain high performance, simplicity and to smoothly interpolate across all investigated signals when performing hypothesis testing on a given signal benchmark.

The main background for this search is SM $t\bar{t}$, including $t\bar{t}$ production in association with heavy-flavoured jets ($t\bar{t}b\bar{b}$, $t\bar{t}c\bar{c}$). Other considered backgrounds are single top production, multijet, W/Z +jets and diboson production, and $t\bar{t}$ production in association with an $H/Z/W$ boson.

Unfortunately, we experienced some constraints and throwbacks along the working process, that has already started more than a year and a half ago, that would not allow us to have definitive results by the time this thesis is being written, since we did not unblind data yet. When the time comes, datasets from 2015 to 2018 will be used resulting in a total integrated luminosity of 138.9 fb^{-1} . Nevertheless, the analysis strategy is almost finalised and it has already been optimised and tested in MC simulations and some blinded data. This chapter presents the latest version of the analysis along with some preliminary results. Some features are still under discussion.

5.1 Signal and background modelling

This section briefly describes the setup used to simulate the signal and background events, and their respective validations. Both, signals and background samples also include a simulation of pile-up interactions, and are processed through a full GEANT4 detector simulation and the same reconstruction software as the data. A complete list of datasets used can be found in appendix A of the internal note [203].

5.1.1 Signal

The $t\bar{t} \rightarrow WbH^+b$ signal simulation is done using POWHEG [204] interfaced to MADSPIN and PYTHIA 8 [205] with the A14 tune for the parton shower, hadronisation and multiple parton interaction generation. The $t\bar{t}$ production is modelled in POWHEG at NLO using NLO NNPDF3.0 PDF [206]; while the top-quark decays are modelled in MADSPIN for both the SM, $t \rightarrow Wb$, and BSM, $t \rightarrow H^+b$, decays. The $t \rightarrow H^+b$ top quark decays are generated based on the LO 2HDM UFO model. The charged Higgs boson decays are generated inclusively with PYTHIA 8 and the generated decay topology assumes branching ratio $\mathcal{B}(H^+ \rightarrow cb) = 1.0$.

Nine signal samples of 1.5 million events are generated corresponding to different charged Higgs masses (m_{H^+}). The mass grid goes from 80 to 160 GeV with a 10 GeV step³. The samples are generated without any filter, instead the full decay chains interesting for this analysis are directly generated: the $W \rightarrow \ell\nu$ decays are generated directly in MADSPIN as part of the decay chain of the SM decaying top quark.

Several checks are performed in order to validate these signal samples. In order to check the expected signal acceptance for kinematic cuts similar to those implemented in the analysis, a particle level cut-flow is performed; this relies on application of suitable kinematic cuts on jets, electrons, muons, tau-leptons particle level objects at truth level on the simulation.

Example of validation plots are shown in figures 5.4 and 5.5. The modelling of basic kinematics distributions is fully consistent across all generated H^+b signal samples.

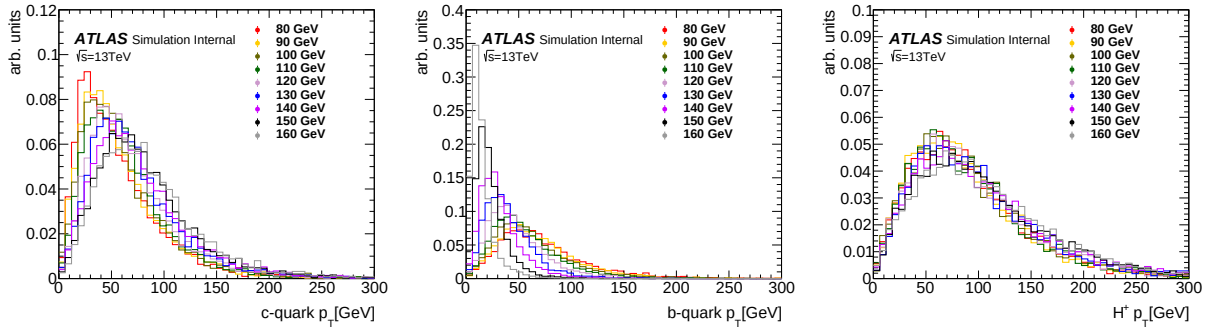


Figure 5.4: Parton level distributions of the (left) charm-quarks p_T , (middle) b -quarks p_T , and (right) charged Higgs boson p_T .

Figure 5.4 also shows some expected features: the p_T of the c -quarks produced from the H^+ decays scales according to the m_{H^+} ; the p_T of the b -quarks in the event also depends significantly on m_{H^+} and becomes softer when m_{H^+} approaches m_{top} (note that this distribution does not include b -quarks produced from the SM top-quark decay); finally a limited dependence of H^+ p_T as a function of m_{H^+} is observed.

³Two more masses of 60 and 70 GeV have been added recently but not yet propagated to the analysis framework.

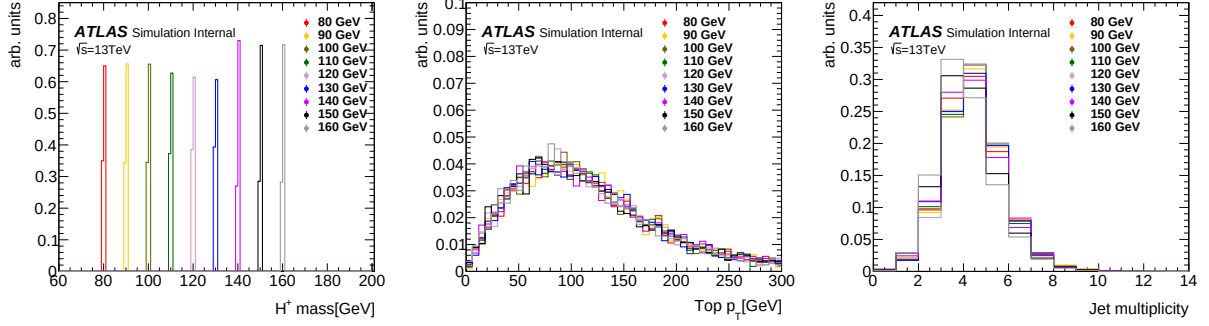


Figure 5.5: Parton level distributions of the (left) charged Higgs masses, (middle) top-quarks p_T , and (right) number of jets.

5.1.2 Background

The main background is $t\bar{t}$ +jets production, with the production of a W boson in association with jets (W +jets) and multijet events contributing to a lesser extent. Small contributions arise from single-top quark, Z +jets and diboson (WW, WZ, ZZ) production, as well as from the associated production of a vector boson V ($V = W, Z$) or a Higgs boson and a $t\bar{t}$ pair ($t\bar{t}V$ and $t\bar{t}H$). Multijet events contribute to the selected sample via the misidentification of a jet or a photon as an electron or via the presence of a non-prompt lepton (e.g. from a semileptonic b - or c -hadron decay), and the corresponding yield is estimated via data-driven methods. The rest of the background contributions are estimated from simulation and normalised to their theoretical cross sections. A few more details of each background are given below.

Depending on the characteristic features of each background, a certain generator might be better than the others to simulate such events. So different generators are used to simulate each background. Table 5.2 shows the list of backgrounds used for the analysis along with their respective generators.

Process	Generator
$t\bar{t}$	POWHEG + PYTHIA 8 [47, 205, 207, 208]
W/Z +jets	SHERPA [34]
Single-top	POWHEG + PYTHIA 8 [47, 205, 207, 208]
Diboson	SHERPA [34]
$t\bar{t}V$	MADGRAPH5_aMC@NLO + PYTHIA 8 [154, 205, 206]
$t\bar{t}H$	MADGRAPH5_aMC@NLO + PYTHIA 8 [154, 205, 206]
SM 4-tops	MADGRAPH5_aMC@NLO + PYTHIA 8 [154, 205, 206]
Multijet	data-driven

Table 5.2: Summary of the different background considered for the analysis and their respective generators.

$t\bar{t}$ +jets. The nominal sample is generated using a NLO generator. It is generated separately for “non-all hadronic” W boson decays, dilepton decays, and all-hadronic decays. The dilepton sample is a subset of the first sample. Additional samples for each of these types of W boson decays are generated with filters requiring extra b -jets, which

is important to ensure a reasonable number of simulated events passing cuts in the high b -tag multiplicity region.

The sample is normalised to the $\text{top}++2.0$ [209] theoretical cross section of 832^{+46}_{-51} pb, calculated at next-to-next-to-leading order (NNLO) in QCD that includes resummation of next-to-next-to-leading logarithmic (NNLL) soft gluon terms [210–214]. Theoretical uncertainties result from variations of the factorisation and renormalisation scales, as well as from uncertainties on the PDF and α_S . The latter two represent the largest contribution to the overall theoretical uncertainty on the cross section.

The $t\bar{t}$ sample is generated inclusively, but events are categorised depending on the flavour of partons that are matched to particle jets that do not originate from the decay of the $t\bar{t}$ system. Particle jets are reconstructed from all stable truth particles (not counting muons and neutrinos) with the anti- k_t algorithm with a radius parameter $R = 0.4$ and are required to have $p_T > 15$ GeV and $|\eta| < 2.5$. Events where at least one such particle jet is matched within $\Delta R < 0.3$ to a b -hadron with $p_T > 5$ GeV not originating from a top quark decay are labelled as $t\bar{t}+\geq 1b$ events. Similarly, events which are not already categorised as $t\bar{t}+\geq 1b$, and where at least one particle jet is matched to a charm quark not originating from a W boson decay, are labelled as $t\bar{t}+\geq 1c$ events. Events labelled as either $t\bar{t}+\geq 1b$ or $t\bar{t}+\geq 1c$ are generically referred to as $t\bar{t} + \text{HF}$ events (HF for “heavy flavour”). The remaining events are labelled as $t\bar{t} + \text{light-jet}$ events, including those with no additional jets.

$W/Z + \text{jets}$. The matrix-element calculation is performed up to two partons at NLO and up to 4 partons at LO. Both the $W + \text{jets}$ and $Z + \text{jets}$ samples are normalised to their respective inclusive NNLO theory cross section calculated with FEWZ [215]. Samples are produced for each of the $W + \text{jets}$ and $Z + \text{jets}$ categories using filters for a b -jet (Wb or $Zb + \text{jets}$), a c -jet and no b -jet (Wc or $Zc + \text{jets}$), and with a veto on b and c -jets (W or $Z + \text{light-jets}$) as well as slicing in truth level p_T of the vector boson.

Single-top. Samples of single-top quark backgrounds corresponding to the Wt -, t - and s -channel production mechanisms are generated. Overlaps between the $t\bar{t}$ and Wt final states are removed using the “diagram removal” scheme [216]. The samples are normalised to the approximate NNLO theory cross sections [217–219].

Diboson. Samples of diboson production $WW/WZ/ZZ + \text{jets}$ are generated with an NLO generator and include processes containing up to four electroweak vertices. The matrix-element includes 0 parton at NLO and up to 3 partons at LO using the same procedure as for the $W/Z + \text{jets}$. The final states simulated require one of the bosons decaying leptonically and the other boson decaying hadronically. All diboson samples are normalised to their NLO theory cross sections provided by SHERPA.

$t\bar{t}V$ and $t\bar{t}H$. Inclusive decays of the Higgs boson are assumed in the generation of the $t\bar{t}H$ sample. The $t\bar{t}V$ samples are normalised to the NLO cross section predictions [220], while the $t\bar{t}H$ sample is normalised using the NLO cross section [221–225] and the Higgs decay branching ratios calculated using HDECAY [226].

4-top-quarks. Simulated samples of four-top-quark production within the SM, within an EFT model are generated with a LO generator. The SM four-top sample is normalised to a cross section of 9.2 fb.

Multijet. Multijet events can enter the selected data sample through several production and misreconstruction mechanisms. In the electron channel, the multijet background consists of non-prompt electrons as well as misidentified photons (e.g. with a conversion into an e^+e^- pair) or jets with a high fraction of their energy deposited in the EM calorimeter. In the muon channel, the background contributed by multijet events is predominantly due to final states with non-prompt muons, such as those from semileptonic b - or c -hadron decays.

The multijet background normalisation and shape are estimated directly from data by using the “matrix method” technique [227]. 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 those where the leptons are either non-isolated or result from the misidentification of photons or jets (referred to as “fake leptons” below).

5.2 Objects definitions and event preselection

5.2.1 Objects definitions

The final state studied in this search is characterised by the presence of many different objects, so their correct reconstruction and identification are important to keep a sensitive analysis. Wherever possible, the objects used in the analysis follow the official definitions given by the collaboration, specifically from the the Top Reconstruction group [228].

Basic selections are applied to define candidates for electrons, muons and jets in the event. Also an overlap removal procedure is applied to these candidates to prevent double-counting of the objects. Some details of the object selections and of the overlap removal procedure are given below.

Primary vertex. Interaction vertices from pp collisions are reconstructed from at least two tracks with $p_T > 400$ MeV and that are consistent with originating from the beam collision region in the x - y plane. If more than one vertex is found, the hard-scatter primary vertex is taken to be the one that has the largest sum of the squared p_T of its associated tracks [229].

Leptons. Both electrons and muons are used in the analysis. Electron candidates [230–232] are reconstructed from clusters in the electromagnetic calorimeter and inner detector tracks and are required to pass the tight likelihood (**TightLH**) identification criteria with $p_T > 30$ GeV and $|\eta_{\text{cluster}}| < 2.47$. Candidates in the calorimetry transition region $1.37 < |\eta_{\text{cluster}}| < 1.52$ are excluded. In addition, electron candidates are required to pass further selections on the transverse and longitudinal impact parameters: $|z_0 \sin \theta| < 0.5$ mm and $|d_0/\sigma(d_0)| < 5$.

Muon candidates [233, 234] are reconstructed from matching tracks in the inner detector and in the muon spectrometer. Events containing one or more muon candidates that have a transverse (longitudinal) impact parameter d_0 (z_0) with respect to the primary vertex larger than 0.2 mm (1 mm) are rejected to suppress cosmic rays. Muon candidates in the remaining events are required to pass the **Medium** selection criteria with $p_T > 30$ GeV and $|\eta| < 2.5$. In addition, muon candidates are required to pass further selections on the transverse and longitudinal impact parameters: $|z_0 \sin \theta| < 0.5$ mm and $|d_0/\sigma(d_0)| < 3$. To further reduce the background from non-prompt leptons, electron

conversions and hadrons, lepton candidates are required to be isolated. A lepton isolation criterion is defined by calculating the quantity $I_R = MI_R/p_T^\ell$, where p_T^ℓ is the lepton p_T and MI_R is defined as follows (excluding the lepton's track):

$$MI_R = \sum_{\Delta R(\text{track}, \ell) < R_{\text{cut}}} p_T^{\text{trk}}, \quad (5.1)$$

where $R_{\text{cut}} = \min\{0.2 (0.3), 10 \text{ GeV}/p_T^\ell\}$ for electrons (muons). Both leptons must satisfy $MI_R/p_T^\ell < 0.06$ (`FixedCutTightTrackOnly` isolation [235]).

Jets. Candidate jets are reconstructed from three-dimensional topological energy clusters [236, 237] in the calorimeter using the anti- k_t jet algorithm [100, 238, 239] with a radius parameter of 0.4. Each topological cluster is calibrated to the electromagnetic scale response prior to jet reconstruction. The reconstructed jets are then calibrated to the particle level by the application of a jet energy scale derived from simulation and *in-situ* corrections based on $\sqrt{s} = 13 \text{ TeV}$ data [240]. After energy calibration, jets are required to have $p_T > 25 \text{ GeV}$ and $|\eta| < 2.5$. Quality criteria (*jet cleaning procedure*) are imposed to identify jets arising from non-collision sources or detector noise (using the `LooseBad` operating points) and any event containing at least one such jet is removed [162]. To reduce the contamination due to jets originating from pile-up interactions, jets with $p_T < 60 \text{ GeV}$ and $|\eta| < 2.4$ are required to have a significant fraction of any associated tracks to be compatible with originating from the primary vertex [241]. This is accomplished by requiring that the Jet Vertex Tagger (JVT) variable is larger than 0.59.

b -tagged jets. Jets containing b -hadrons are identified via the DL1 algorithm [242, 243], which uses multivariate techniques to combine information from the impact parameters of displaced tracks as well as topological properties of secondary and tertiary decay vertices reconstructed within the jet. For each jet, a value for the multivariate b -tagging discriminant is calculated. The jet is considered b -tagged if this value is above a given threshold. The one used in this search corresponds to 60% efficiency to tag a b -quark jet, with a light-jet rejection factor of ~ 1320 and a c -jet rejection factor of ~ 26 , as determined for jets with $p_T > 20 \text{ GeV}$ and $|\eta| < 2.5$ in simulated $t\bar{t}$ events. This analysis is using the recommended pseudo-continuous b -tagging flavour tagging calibrations for b - and c -jets (based on $t\bar{t}$ events) and light-jets (based on negative tags). The availability of the pseudo-continuous b -tagging calibration allows to use effectively the DL1 score, with a granularity as defined by the granularity of the calibration, for signal-to-background discrimination.

The pseudo-continuous tagging procedure allows not only to define if a jet is considered a b -jet but also further classified them according to its purity. The categories defined are loose (with an efficiency of 80%), medium (70%) and tight (50%). The advantages of using a pseudo-continuous tagging is that low purity with high statistics, and high purity with low statistics b -jet samples can be defined in the same analysis.

Missing transverse momentum. The missing transverse momentum (E_T^{miss}) is defined as the magnitude of the negative vector sum of the p_T of all selected and calibrated objects in the event, including a term to account for soft energy in the event that is not associated to any of the selected objects. This soft term is calculated from inner detector tracks matched to the selected primary vertex in the event [244, 245].

Overlap removal between leptons and jets. Overlaps between candidate objects are removed sequentially. Only “tight” leptons and jets that pass all the requirements detailed above are used. Firstly, electron candidates that lie within $\Delta R = 0.01$ of a muon candidate are removed to suppress contributions from muon bremsstrahlung. Overlaps between electron and jet candidates are resolved next, and finally, overlaps between remaining jets and muons candidates are removed.

Overlap removal between electron and jets aims to remove jets that are formed primarily from the showering of prompt electrons and electrons that are produced in the decay chains of hadrons. Since electron showers within the cone of a jet enter the measured energy of the jet, any overlap between an electron and the jet must be fully resolved. Consequently, the closest jet whose axis is within $\Delta R = 0.2$ of an electron is discarded. If the electron is within $\Delta R = 0.4$ of the axis of any jet after this initial removal, the jet is retained and the electron is removed.

The overlap removal procedure between muons and jets is designed to remove those muons that are likely to have arisen in the decay chain of hadrons and to retain the overlapping jet instead. Jets and muons may also appear in close proximity when the jet results from high- p_T muon bremsstrahlung, and in such cases the jet should be removed and the muon retained. Such jets are characterised by having very few matching inner detector tracks. Selected muons that satisfy $\Delta R(\mu, \text{jet}) < 0.04 + 10 \text{ GeV}/p_T^\mu$ are rejected if the jet has at least three tracks originating from the primary vertex; otherwise the jet is removed and the muon is kept.

5.2.2 Event preselection

Single-lepton triggers with different p_T thresholds are combined in a logical OR in order to increase the overall efficiency. The triggers with the lower p_T threshold include isolation requirements on the candidate lepton, resulting in inefficiencies at high p_T that are recovered by the triggers with higher p_T threshold.

These triggers are listed in table 5.3 for each dataset.

In 2015, the p_T thresholds are 24, 60 or 120 GeV for the electron triggers, and 20 or 50 GeV for the muon ones.

In 2016, the electron triggers are updated to tighter ID for the lowest unscaled p_T threshold single-electron trigger and a slight increase in the p_T threshold for the highest one, while the muon triggers also have tighter ID requirements and a slightly higher p_T threshold for the lowest unscaled single-muon trigger.

The electron trigger during the data taking in 2017 and 2018 was unchanged compared to 2016. For the case of the muon trigger, beside the chains present in 2016, a new HLT chain was included in logical OR with the pre-existing one, allowing to recover trigger efficiency in the Muon Spectrometer crack region at intermediate-high transverse momentum by not requiring a matched track to the muon candidate.

Events satisfying the trigger selection are required to have at least one reconstructed vertex with at least five associated tracks with $p_T > 400$ MeV, consistent with originating from the beam collision region in the x - y plane. If more than one vertex is found, the hard-scatter primary vertex is taken.

Events are required to have exactly one reconstructed electron or muon and ≥ 4 jets satisfying the quality and kinematic criteria discussed in section 5.2.1. At least two of the four jets are required to be tagged as originating from b -hadrons. DL1 tagger with a

Dataset	Single-lepton triggers
2015	HLT_e24_lhmedium_L1EM20VH HLT_e60_lhmedium HLT_e120_lhloose HLT_mu20_iloose_L1MU15 HLT_mu50
2016	HLT_e26_lhtight_nod0_ivarloose HLT_e60_lhmedium_nod0 HLT_e140_lhloose_nod0 HLT_mu26_ivarmedium HLT_mu50
2017 & 2018	HLT_e26_lhtight_nod0_ivarloose HLT_e60_lhmedium_nod0 HLT_e140_lhloose_nod0 HLT_mu26_ivarmedium HLT_mu50 HLT_mu60_0eta105_msonly

Table 5.3: Summary of the single-lepton triggers used in the analysis for each data-taking period.

60% WP is used⁴. The events are required to fire a single-lepton trigger, moreover, the selected reconstructed leptons are required to match a trigger object with $\Delta R < 0.15$.

Since the background from multijet production is expected to be sufficiently small in the ≥ 2 b -tags region, which is the focus of this analysis, no requirements on E_T^{miss} or transverse mass of the lepton and E_T^{miss} (m_T^W)⁵ are applied. The above requirements are referred to as the “preselection” and are summarised in table 5.4. In the following, events satisfying either the electron or muon selections are combined and treated as a single analysis channel.

Preselection requirements	
Trigger	Single-lepton trigger
Leptons	=1 isolated e or μ
Jets	≥ 4 jets
b -tagging	≥ 2 b -tagged jets (DL1@60%WP)

Table 5.4: Summary of preselection requirements (see text for details).

After the event preselection, events are divided in multiple analysis regions, depending on the number of jets and b -jets, in order to disentangle more clearly different background components, this procedure is referred to as categorisation.

⁴Tight cut at 60% for b -tagging is based on the experience from the previous publication, and it aims to suppress $t\bar{t} \rightarrow WbWb \rightarrow \ell\nu bcsb$ background.

⁵ $m_T^W = \sqrt{2p_T^\ell E_T^{\text{miss}}(1 - \cos \Delta\phi)}$, where p_T^ℓ is the transverse momentum (energy) of the muon (electron) and $\Delta\phi$ is the azimuthal angle separation between the lepton and the direction of the missing transverse momentum.

Further discussion on the optimisation of the analysis regions definition is given in section 5.4 when introducing the analysis strategy.

5.3 Data to Monte Carlo comparison

In order to validate the modelling of the main backgrounds by the simulation, detailed comparisons between data and MC are performed. Basic kinematic variables at the preselection level are shown in figure 5.6 for the control region and figure 5.7 for one of the main signal regions. While figures 5.8 and 5.9 are dominated by $t\bar{t}$ +light and $t\bar{t}+b$ background events.

Comparison between other variables and for different regions can be found in the appendix D of the internal note [203].

It can be seen from figure 5.6 that there is a clear mis-modelling for jets and b -jets multiplicity, as well as for the jet and lepton p_T 's (probably due to a mis-modelling of the top p_T). This is a known feature that it will be discussed in section 5.5.

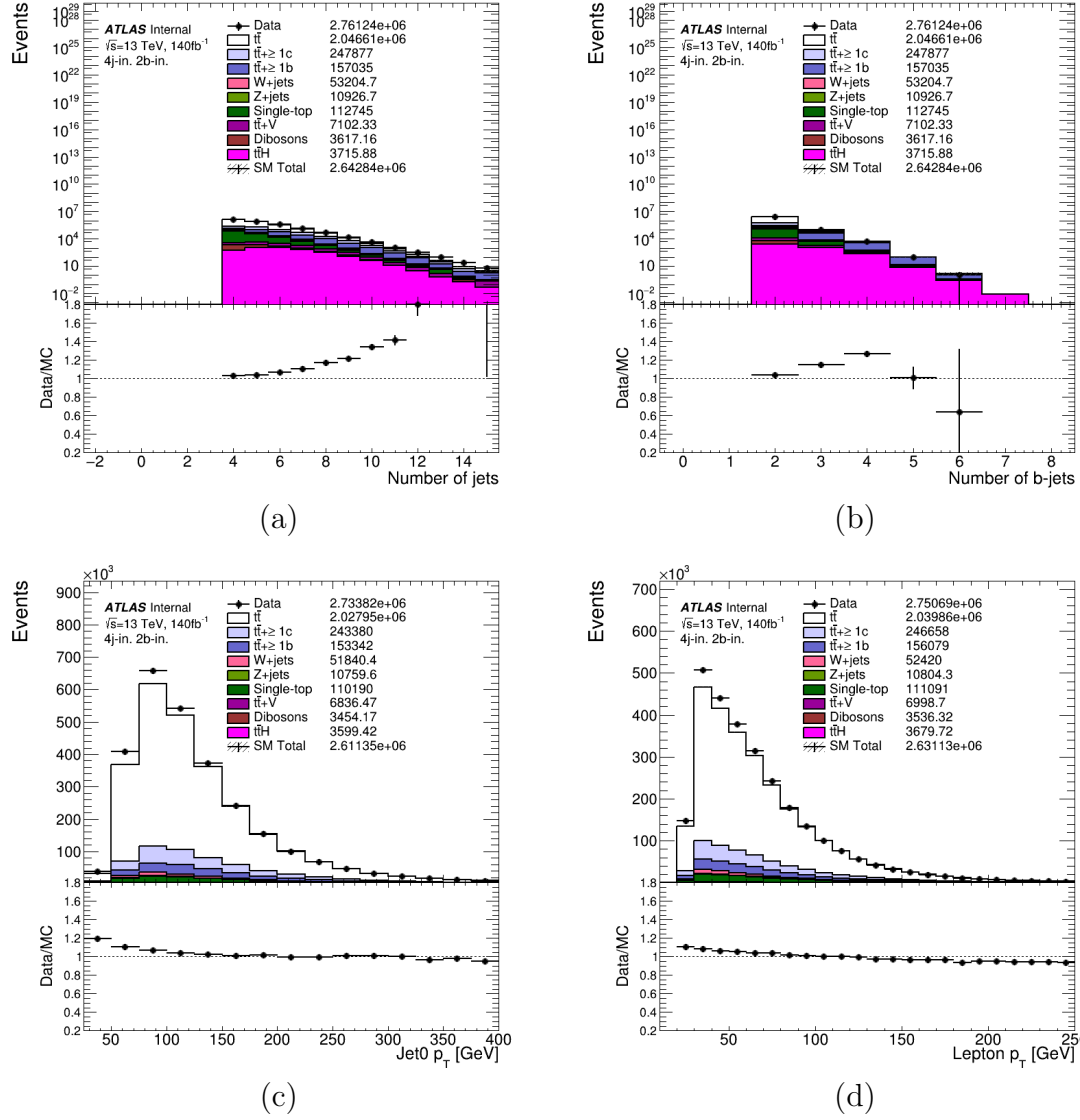


Figure 5.6: Comparison between data and prediction for the combined $e+jets$ and $\mu+jets$ channels in a region with at least 4 jets and at least 2 of them b -tagged (4jin-2bin), considered a control region for the analysis. The kinematic variables displayed are: (a) number of jets, (b) number of b -jets, (c) leading jet p_T and (d) leading lepton p_T . The background prediction is pre-fit. Only statistical uncertainties are being shown. Underflow and overflow bins are included respectively in the first and last bins.

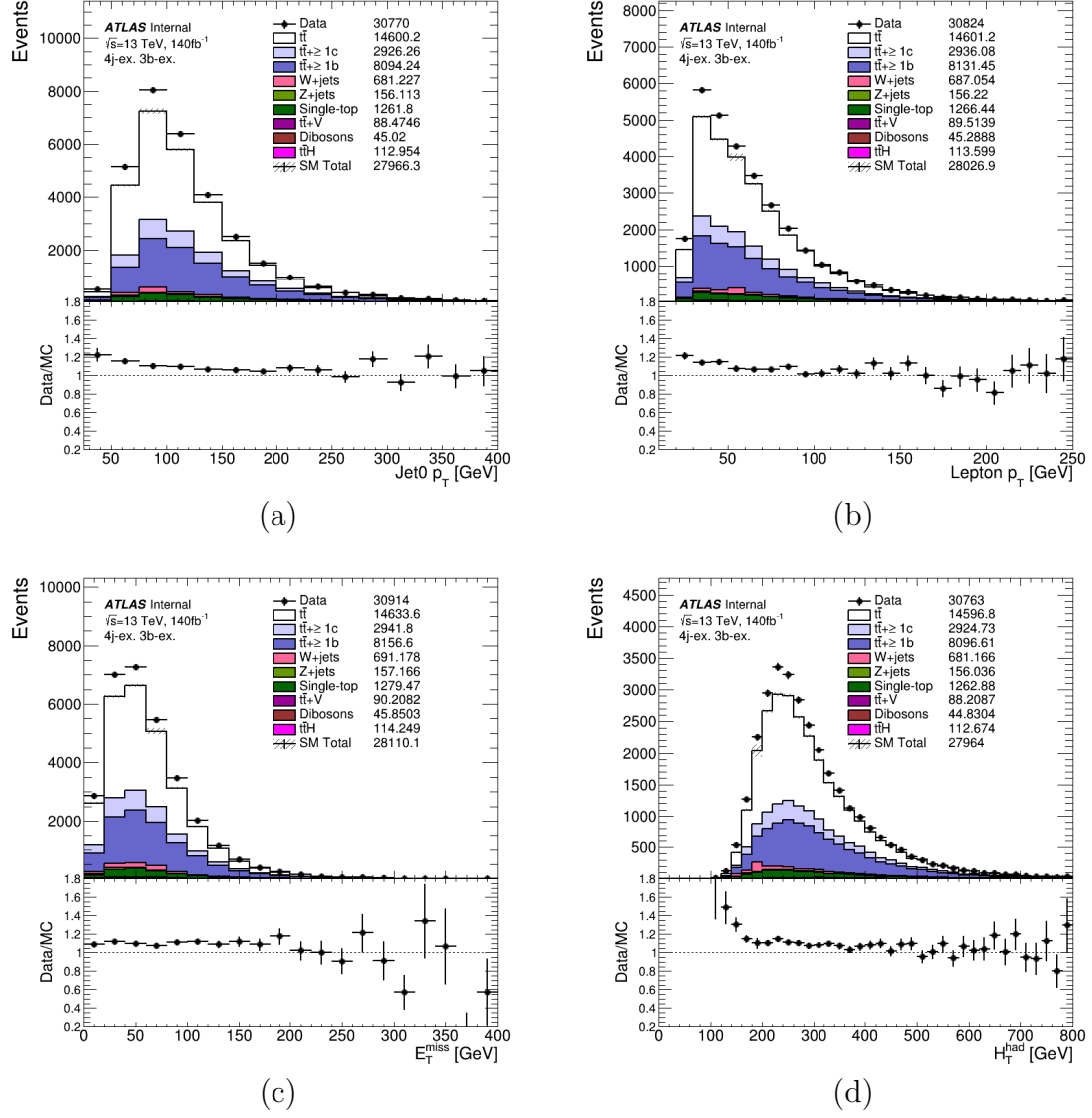


Figure 5.7: Comparison between data and prediction for the combined e +jets and μ +jets channels in a region with exactly 4 jets and 3 b -jets (4jex-3bex), considered a signal region for the analysis. The kinematic variables displayed are: (a) leading jet p_T , (b) leading lepton p_T , (c) missing transverse energy and (d) H_T^{had} . The background prediction is pre-fit. Only statistical uncertainties are being shown. Underflow and overflow bins are included respectively in the first and last bins.

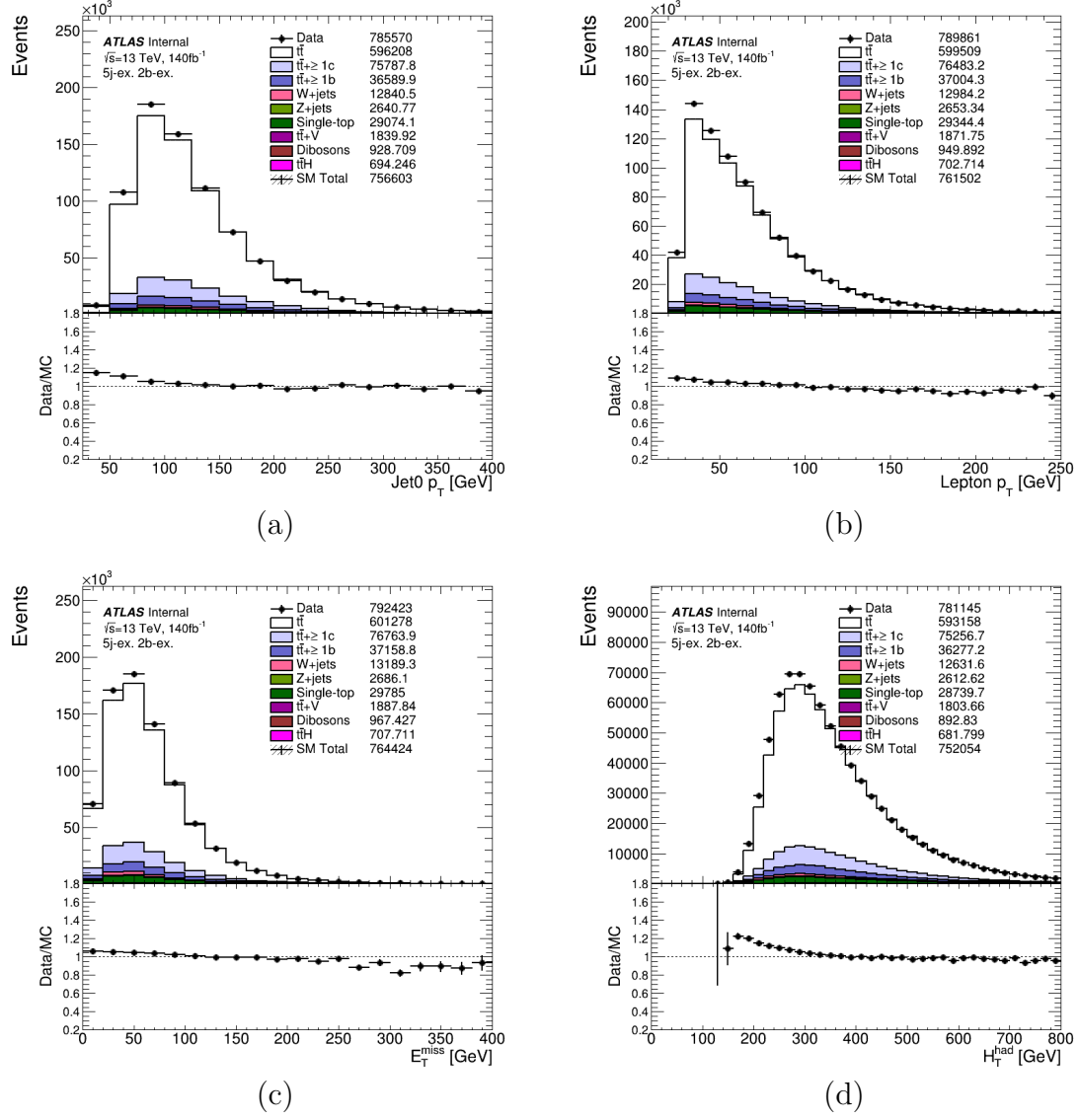


Figure 5.8: Comparison between data and prediction for the combined e +jets and μ +jets channels in a region with exactly 5 jets and 2 b -jets (5jex-2bex), dominated by $t\bar{t}$ +light events. The kinematic variables displayed are: (a) leading jet p_T , (b) leading lepton p_T , (c) missing transverse energy and (d) H_T^{had} . The background prediction is pre-fit. Only statistical uncertainties are being shown. Underflow and overflow bins are included respectively in the first and last bins.

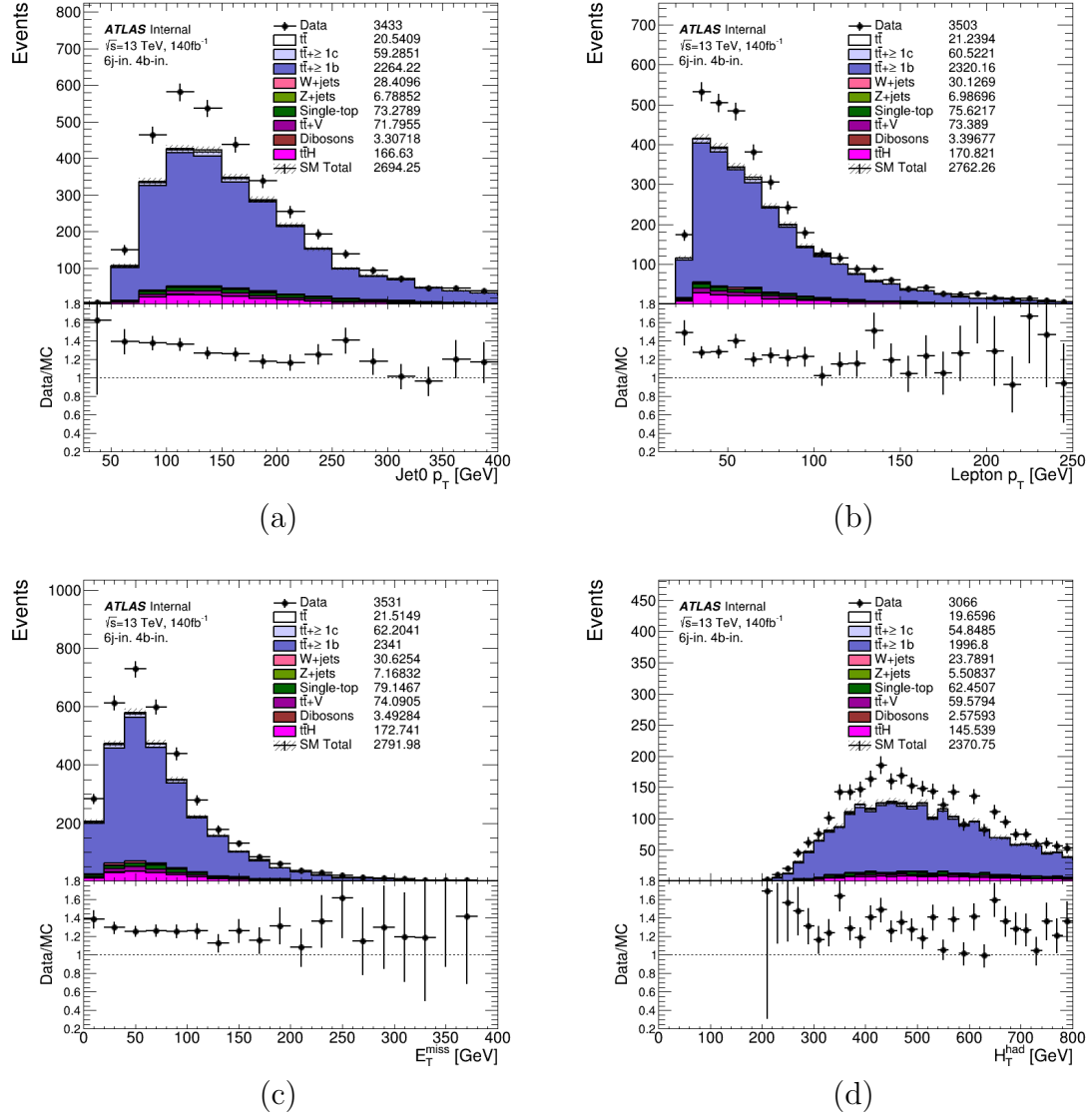


Figure 5.9: Comparison between data and prediction for the combined e +jets and μ +jets channels in a region with at least 6 jets and at least 4 of them b -tagged (6jin-4bin), dominated by $t\bar{t} + b$ events. The kinematic variables displayed are: (a) leading jet p_T , (b) leading lepton p_T , (c) missing transverse energy and (d) H_T^{had} . The background prediction is pre-fit. Only statistical uncertainties are being shown. Underflow and overflow bins are included respectively in the first and last bins.

5.4 Analysis strategy

5.4.1 Categorisation

Since the search focus on the $t\bar{t} \rightarrow WbH^+b$ process, with $W \rightarrow \ell\nu$ and $H^+ \rightarrow c\bar{b}$, the signal is expected to have at least four jets and high b -tag multiplicity. As shown in figure 5.10a, the jet multiplicity distribution is similar between signal and the $t\bar{t} \rightarrow WbWb$ background. On the other hand, a requirement on the b -tag multiplicity can be effectively exploited to suppress background, as illustrated in figure 5.10b. The usage of the 60% b -tagging working point is characterised by a low mistag rate from charm and light jets, hence improving the search sensitivity on these channels.

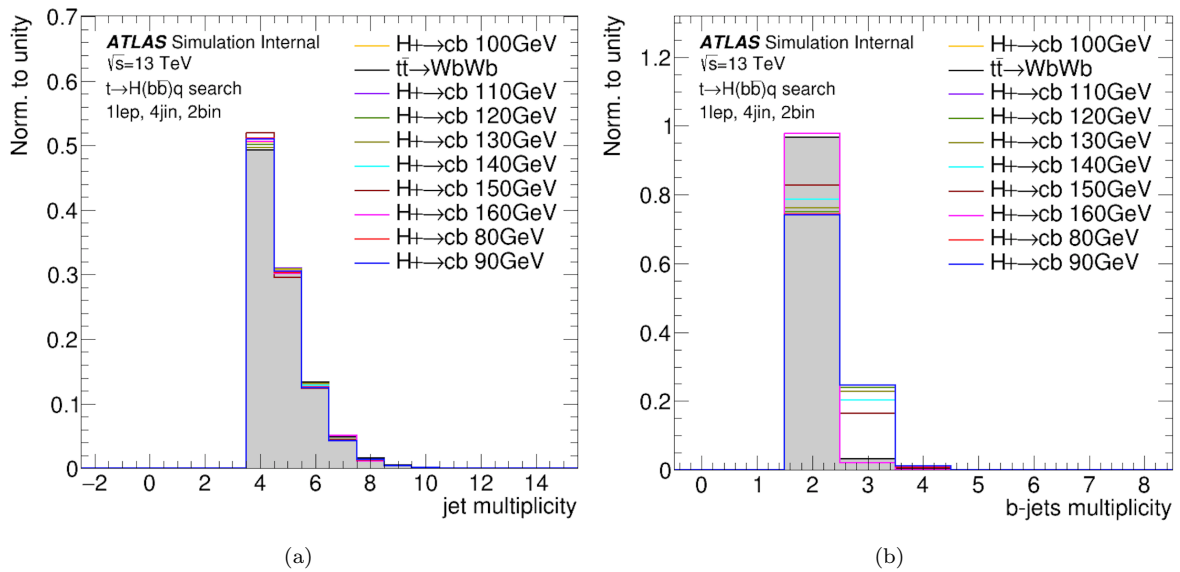


Figure 5.10: Comparison of the shape of (5.10a) the jet multiplicity and (5.10b) the b -tag multiplicity distributions between total background and $t\bar{t} \rightarrow WbH^+b$ signal events satisfying the preselection requirements.

In order to optimise the sensitivity of the search, the selected events are categorised in different channels depending on the number of jets (4, 5 and ≥ 6) and on the number of b -tagged jets (2, 3 and ≥ 4). Therefore, the total number of analysis regions considered in this search are nine:

- regions with exactly two b -jets (4jex-2bex, 5jex-2bex, 6jin-2bex)⁷,
- regions with exactly three b -jets (4jex-3bex, 5jex-3bex, 6jin-3bex),
- regions with at least four b -jets (4jex-4bex, 5jex-4bin, 6jex-4bin).

In the case of the 2bex regions, which have significantly lower signal-to-background ratio (S/B) than the 3bex regions, an additional cut is made in order to minimise strong constraints/pulls on systematic uncertainties related to $t\bar{t}$ +light jets modelling and/or jet

⁷The “ex” suffix comes from exclusive and it refers to the strict requirement over the number of jets or b -jets; while “in” is for inclusive and it refers to the more flexible requirement of *at least* a certain number of jets or b -jets.

energy scale/resolution. In regions with exactly two b -jets it is required the presence of a third *loose* b -jet tagged at with the DL1 algorithm with 70% working point efficiency. This cut was optimised based on S/B .

More distributions comparing signal and background shapes for the various analysis regions can be found in appendix C of the internal note [203].

Figure 5.11 summaries the analysis regions definitions and the motivation to used each.

Nj Nb 			
	2b-ex, 1b-70% (exactly two b -tagged jets + one loose b -tagged jet)	3b-ex (exactly three b -tagged jets)	4b-in (at least four b -tagged jets)
4j-ex (exactly four jets)	4j-ex, 2b-ex, 1b-70% (pull the $t\bar{t}$ +light background)	4j-ex, 3b-ex (main signal region)	4j-ex, 4b-in ($t\bar{t}$ + b background control and large S/B region)
5j-ex (exactly five jets)	5j-ex, 2b-ex, 1b-70% (pull the $t\bar{t}$ +light background, one bin)	5j-ex, 3b-ex (main signal region)	5j-ex, 4b-in ($t\bar{t}$ + b background control and large S/B region)
6j-in (at least six jets)	6j-in, 2b-ex, 1b-70% (pull the $t\bar{t}$ +light background)	6j-in, 3b-ex (shape correction for the NN discriminant in background dominated region)	6j-ex, 4b-in ($t\bar{t}$ + b background control)

Figure 5.11: Summary of the analysis regions along with information about their usage and definition. Regions in green are used for $t\bar{t}$ +light background control, and the ones in orange for $t\bar{t} + b$ background control. Regions in red are the candidates to contain signal events.

Apart from these nine regions, some other complementary regions are defined (e.g. 4jin-2bin) and used for inclusive validation of MC predictions of the background, also called control regions.

Considering the different b -tag multiplicities is particularly useful to isolate regions with different signal-to-background ratio, while at the same time calibrating the $t\bar{t}$ +jets background prediction and constraining the related systematic uncertainties. In particular, significant insights can be gained on the heavy-flavour content of the $t\bar{t}$ +jets sample, which varies strongly as a function of the b -tag multiplicity, as shown in figure 5.12: e.g. events with exactly 2 b -tags are dominated by $t\bar{t}$ +light jets, while event with ≥ 4 b -tags are dominated by $t\bar{t} + b\bar{b}$, with intermediate compositions found in events with exactly 3 b -tags. Due to the large $t\bar{t}$ +light jets background in the regions with exactly 2 b -tags, and the low signal acceptance in the region with ≥ 4 b -tags, the regions with exactly 3 b -tags are considered the main signal regions for this analysis. This is illustrated in figure 5.13.

Another motivation for the splitting of channels in the jet multiplicity ($=4$ jets, $=5$ jets and ≥ 6 jets) is the fact that at high b -tag multiplicity the $t\bar{t}$ +jets background typically has higher jet multiplicity than the signal because additional heavy flavour jets (from $t\bar{t} + b\bar{b}$ and $t\bar{t} + c\bar{c}$) are necessary in order to have so many b -tags.

The predicted yields for a signal benchmark ($m_{H^+}=110$ GeV) and the various backgrounds are shown in figure 5.14. A table with more detailed information on the yields

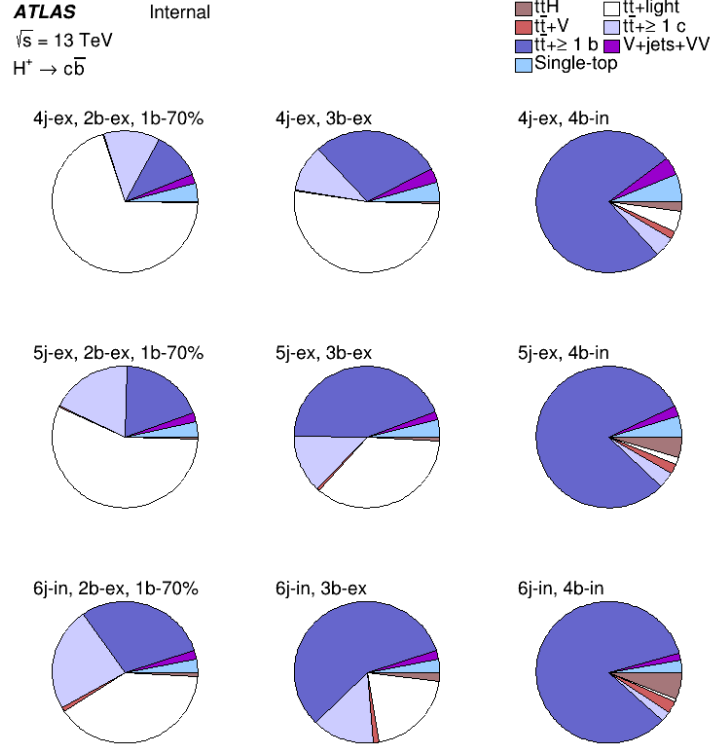


Figure 5.12: Fractional contributions of the various backgrounds to the total background prediction in each of the analysis regions considered.

can be found in appendix C.1.

Once the analysis regions are determined, a discriminating variable based on a neural network classifier is defined and a profile-likelihood fit is performed to this variable in each of the multiple regions. Details about the discriminating variable are given in section 5.4.2, and the fit preliminary results can be seen in section 5.7.

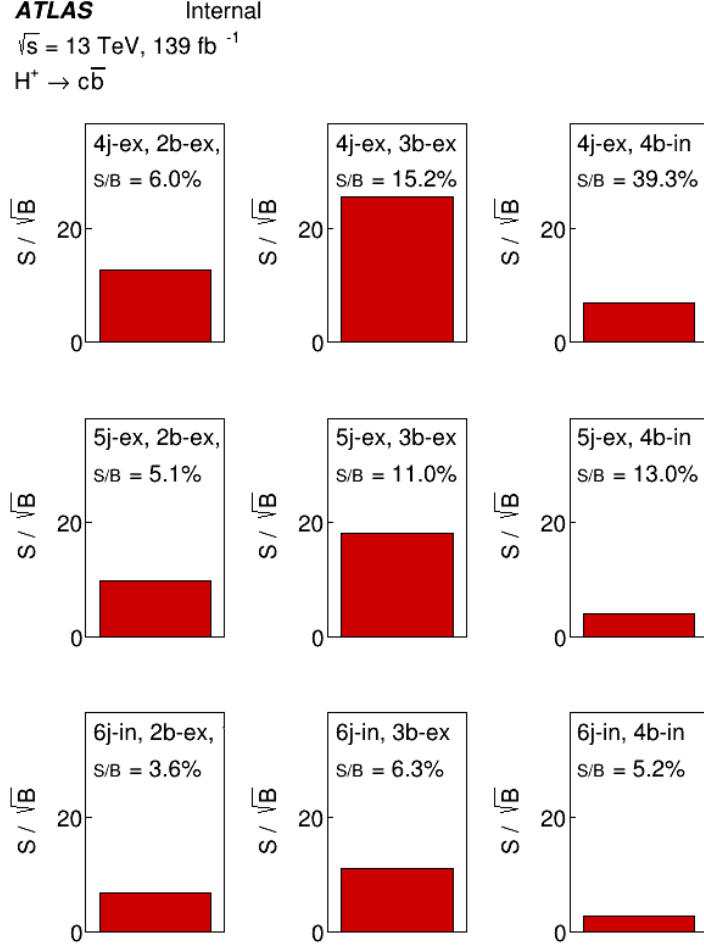


Figure 5.13: $S/\sqrt{B}$ (assuming an integrated luminosity of 139 fb^{-1}) and S/B in each of the analysis regions considered, where S and B represent the expected yields for the $t\bar{t} \rightarrow WbH^+b$ signal with $\mathcal{B}(H^+ \rightarrow c\bar{b}) = 1.0$ and the total SM background, respectively. Here the signal mass is taken to be $m_{H^+} = 110 \text{ GeV}$.

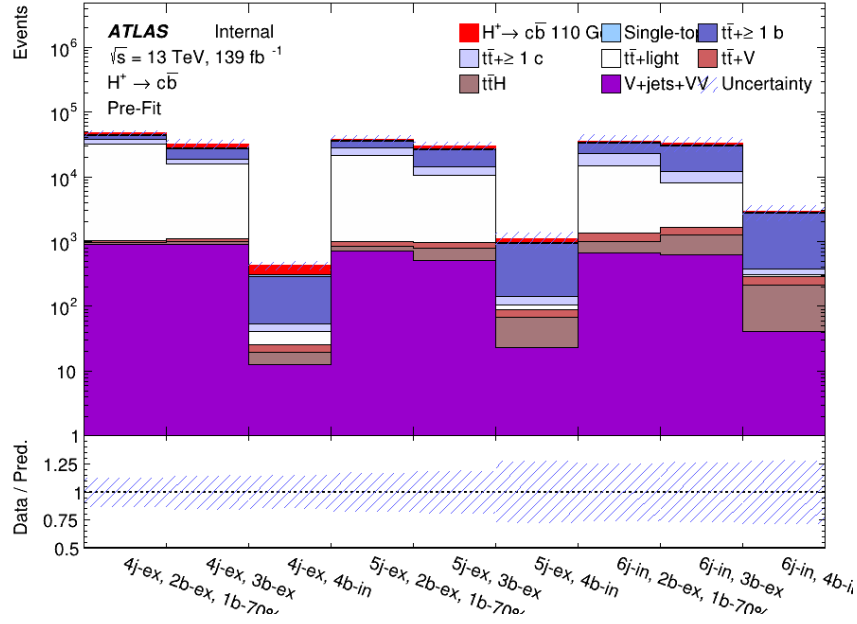


Figure 5.14: Comparison between the background and signal prediction for the yields in each of the analysis channels considered. Backgrounds are normalised to their nominal cross sections. The expected $t\bar{t} \rightarrow WbH^+b$ signal for the $m_{H^+}=110$ GeV mass point is normalised to $\mathcal{B}(H^+ \rightarrow c\bar{b}) = 1.0$. The dashed area represents the total uncertainty on the background.

5.4.2 Discriminating variable

The large number of b -tagged jets in the final state causes ambiguities in the calculation of a kinematic variable to discriminate signal from background events. For this reason, a likelihood discriminant was developed in the Run 1 search [200] and further improved for the Run 2 analysis [202].

While this approach has been shown to provide competitive sensitivity for the FCNC search, it is difficult to extend it to multiple signal hypothesis as needed for the H^+ signal which incorporates multiple masses.

For this reason a new discriminant has been developed which incorporates a training parametrised as a function of a signal label (such as m_{H^+}) thus retaining high performance for all signal benchmarks as discussed in section 5.4.2.3. The classifier is based on a feed-forward neural network (NN) build from the Keras framework [246], running on top of Theano [247].

The following sections describe the definition of the neural network structure, input features to the training, data manipulation, and initial optimisation results. The current NN discriminant is not yet fully optimised but the preliminary results look very promising.

5.4.2.1 Neural network structure

The neural network setup is based on a feed-forward architecture featuring a fully connected variable number of hidden layers following an initial input layer which collects all training features.

Feed-forward neural networks, also called multilayer perceptrons (MLPs), map an input $\mathbf{x}$ to a category y defining a mapping $y = f(\mathbf{x}; \theta)$ and learning the value of the parameters θ that result in the best solution for a given problem. These models are called feed-forward because information flows through the function being evaluated from $\mathbf{x}$, through the intermediate computations used to define f , and finally to the output y .

Feed-forward neural networks are typically represented by composing together many different functions. For example, let's consider the case of three functions f_1 , f_2 , and f_3 connected in a chain, to form $f(x) = f_3(f_2(f_1(\mathbf{x})))$. These chain structures are the most commonly used structures of neural networks. In this case, f_1 is called the first layer of the network, f_2 is called the second layer, and so on. The final layer of a feed-forward network is called the output layer.

The training data specifies directly what the output layer must do at each point $\mathbf{x}$, it must produce a value that is close to y . The learning algorithm must decide how to use the other layers to produce the desired output, but the training data do not say what each individual layer should do. Instead, the learning algorithm must decide how to use these layers to best implement an approximation of the function f . Since the training data does not show the desired output for each of these layers, they are called hidden layers.

Each hidden layer of the network is typically vector valued. The dimensionality of these hidden layers determines the width of the model. Each element of the vector may be interpreted as playing a role analogous to a neuron. Rather than thinking of the layer as representing a single vector-to-vector function, the layer can be think as consisting of many units or nodes that act in parallel, each representing a vector-to-scalar function. In this sense, each unit resembles a neuron.

In each hidden layer a variable number of nodes incorporating a leaky-rectified-linear-unit functions (LeakyReLU), as activation function, is introduced. The LeakyReLU func-

tion are defined as $n(x) = \alpha x$ if $x < 0$ or x if $x \geq 0$ with α set to a common small number for all neurons. The definition of the activation functions has been optimised in an early version of the NN. The choice of using LeakyReLU is found to have all advantages of ReLU activations (fast convergence of the stochastic gradient descent, simplicity) while solving “dying ReLU” problems [248]. It was checked that this configuration leads to the best analysis performance.

The output layer is a sigmoid function, $g(x) = (1 + e^{-x})^{-1}$, which collects the NN score for the considered classes. In this case two classes are considered, one for the signals and another for the background. It was checked that the NN performance does not depend on the assumed activation function for the output layer while the use of a sigmoid function naturally provides a NN discriminant defined in the standard range $[0,1]$.

Batch normalisation [249] is applied before each activation layer. Batch normalisation alleviates the problem of properly initialising neural networks by explicitly forcing the activations throughout a network to take on a unit gaussian distribution at the beginning of the training. The core observation is that this is possible because normalisation is a simple differentiable operation.

The Adam optimiser method is used [250]. It consists of an efficient stochastic optimisation that only requires first-order gradients with little memory requirement. The method computes individual adaptive learning rates for different parameters from estimates of first and second moments of the gradients. Binary cross entropy is used as loss function.

In order to minimise the NN overtraining a “dropout” [251] probability of 0.5 is introduced during the training. The dropout is an effective regularisation technique that is implemented by only keeping a neuron active with some probability, or setting it to zero otherwise.

The analysis started with a configuration of the NN structure that has overcome several rounds of fine tuning over the past year, with the goal of building an optimised NN discriminant for this analysis. As it will be explained in section 5.4.2.3, a subset of the neural network parameters is considered for systematic optimisation for each round: the number of layers, number of neurons, learning rate and batch-size. They are treated as hyper-parameters and adjusted to maximise the performance of the NN.

An illustration of the NN structure is displayed in figure 5.15.

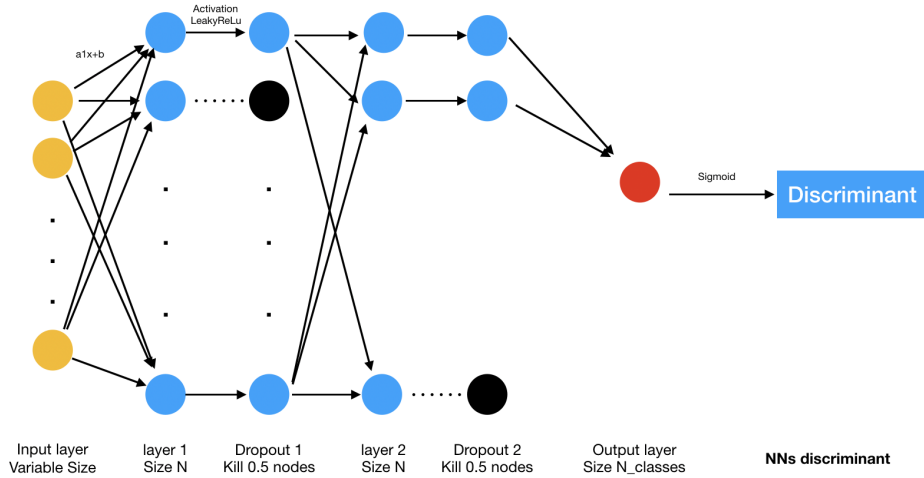


Figure 5.15: Illustration of the neural network structure.

5.4.2.2 Input features to the training

The training is based on low level input features which can be used in full generality without relying on signal-specific optimisation. The used input features are:

- four-momentum of the first five leading jets (ordered by b -tagging score): several checks have been performed to define this set of training features, including re-parametrisation of the four-momenta, re-definition of the jets ordering, using additional jets (first six leading) or fewer jets (first four leading),
- “discrete” b -tagging score for the third, fourth and fifth jets (ordered by b -tagging score): “discrete” b -tagging weight with granularity corresponding to available granularity of the pseudo-continuous b -tagging calibration,
- lepton four-momenta and missing transverse energy.

While simplifying the analysis strategy and the definition of a suitable discriminant for multiple signal benchmarks, the performance of the training based on low-level training features was found to be consistent with “signal-dependent” training based on several invariant mass combinations using H^+ signals as benchmark.

5.4.2.3 Data manipulation and optimisation

The main signal regions feature exactly three b -jets and four or five jets. In order to obtain an efficient classifier in regions with three b -jets, the NN is trained for a selection requiring at least four jets, with exactly three b -tagged jets (4jin-3bex region) for all H^+ mass points. Other alternatives have been studied in the past with an initial version of the NN. For example a training of a NN in 4jex-3bex was performed and compared to a training with the requirement of at least four jet and exactly three b -tagged jets, the latter

provided a better signal-to-background separation (as evaluated in a validation sample) in all jet multiplicity regions: 3% improvement in 4jex-3bex, 27% improvement in 5jex-3bex, 50% improvement in 6jin-3bex. Additionally a neural network has been trained in a more inclusive region having at least four jets of which at least two must be b -tagged. This configuration results in a loss of separation which ranges from about 40% to 10% depending on the signal benchmark.

The use of the NN is combined with a novel structure which incorporates physics parameters of interest, for example the charged Higgs boson mass as features for the training [252], leading to a so-called parametrised NN classifier. Parametrised NN classifiers provide smooth interpolation across physics parameters and improve the performance of isolated classifiers (see figure 5.16).

The technical implementation is based on introducing a pseudo-mass feature in the background sample used for the training. This is a discrete variable assuming values between 80 to 160 GeV in step of 10 GeV as available for the $t\bar{t} \rightarrow WbH^+b$ signal benchmarks. The distribution of the pseudo-mass is obtained by looking at signal rates per mass point after the event selection as needed for defining the training sample.

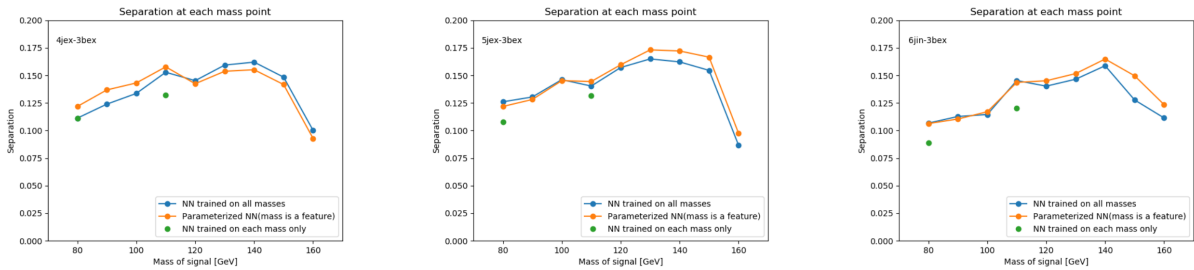


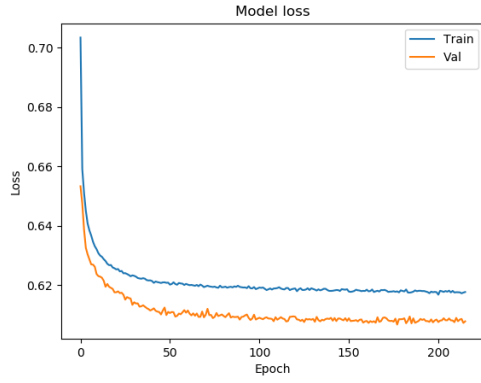
Figure 5.16: Separation as a function of H^+ mass for three different training configurations: NN trained with all masses in blue, NN trained on each mass separately in green and NN trained using the parametrised mass in orange.

After the event selection, the data on the 4jin-3bex region is then divided in three orthogonal sets [248]:

- Training set: used for training the NN discriminant. 50% of events are used at this step.
- Testing set: used for the final analysis. 20% of events are kept for this part.
- Validation set: used for hyper-parameter optimisation. 30% of the events are used.

The training is performed by means of the gradient descent method. It includes an early stopping criterion which is based on the model loss variation as a function of the training epochs. This is monitored during the training process in the validation sample. Figure 5.17 (a) shows the model loss as a function of the training epochs for both training and validation sample.

The NN model is optimised by measuring the performance in the validation sample. The optimisation process is based on a grid scan of multiple hyper-parameter configurations. The best configuration is obtained by the setting that provides the largest ROC integral in the validation sample. The best hyper-parameter configuration is shown in figure 5.17 (b).



(a)

Options	Value
Number of input variables	28
Number of hidden layer	2
Number of nodes	100
Optimizer	adam
learning rate	0.001
Batch size	1028
Dorput	0.5
activation	leakyrelu
activation for output	sigmoid
loss function	binary_crossentropy
epoch	300
patience	30
loss	0.608(0.605)
accuracy	0.661(0.664)
ROC Integral	0.728

(b)

Figure 5.17: (a) Loss as a function of the number of training epochs. The blue solid line shows the loss in the training sample, while the orange solid line displays the loss for the validation sample. (b) Best hyper-parameter set according to the optimisation process.

An almost finalised version of the NN discriminant is used for the results presented in this thesis. Nevertheless, there are some more studies undergoing at the moment that would help defining the ultimate version of the NN. A brief description of them is given in section 5.4.2.4.

Figure 5.18 shows the obtained discriminant for a set of H^+ mass points (80, 110 and 140 GeV) in three signal regions, (4jex, 3bex), (5jex, 3bex), (6jex, 3bex). Regions with different flavour tagging content have limited impact on the analysis sensitivity and are not shown here. The figures show the NN discriminant in the training and testing samples.

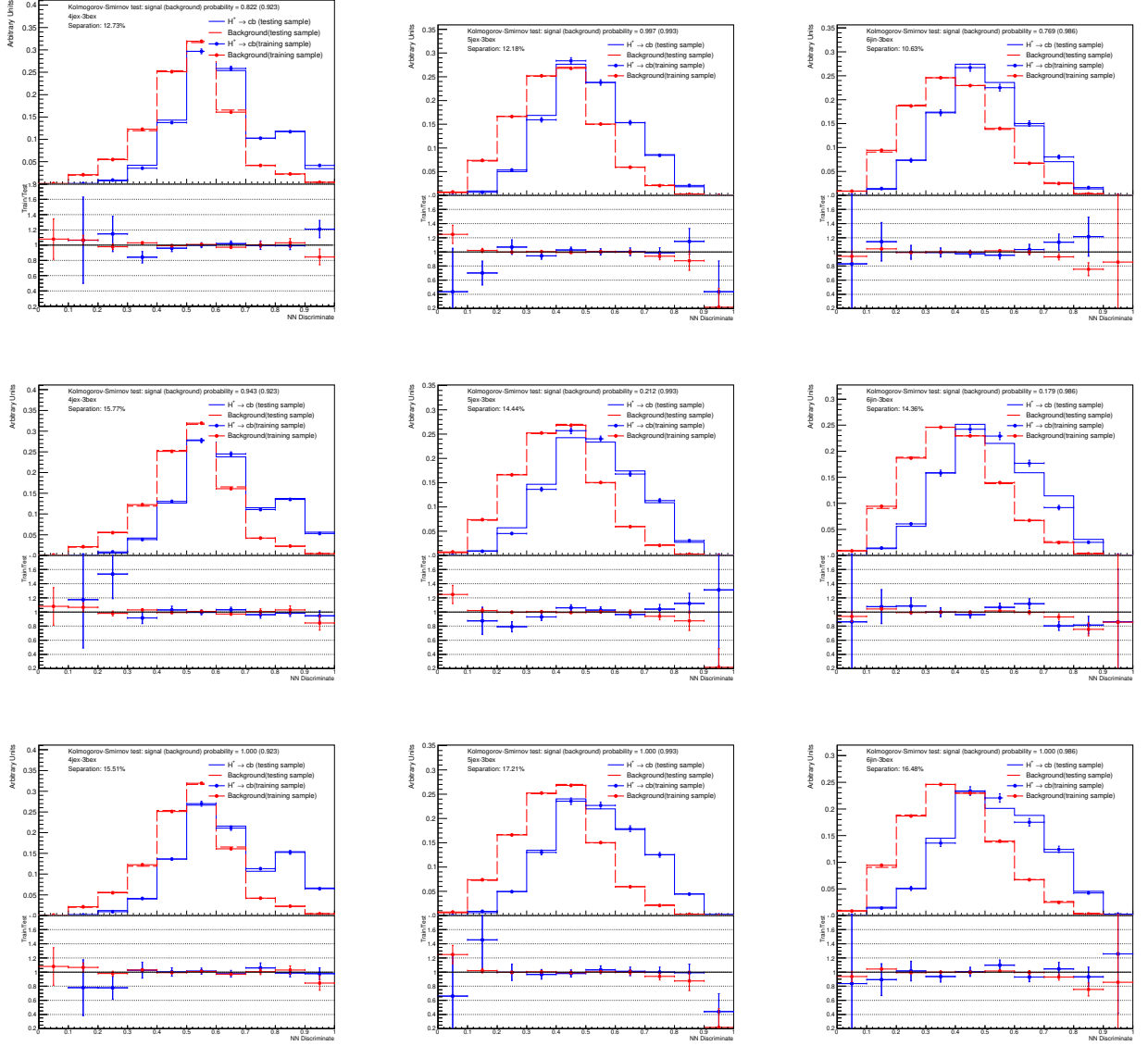


Figure 5.18: Comparison of the shape of the NN discriminant distribution between the signals H^+ (blue lines) and the $t\bar{t}$ background (red lines), in the 3bex regions. Three H^+ mass points are shown: $m_{H^+} = 80$ GeV (top row), $m_{H^+} = 110$ GeV (middle row) and $m_{H^+} = 140$ GeV (bottom row). Also shown is the “separation” between signal and background computed with `TMVA::Tools::GetSeparation`. Underflow and overflow bins are included respectively in the first and last bins.

5.4.2.4 Further studies

The version of the NN discriminant used for the results shown in this thesis already presents a level of separation between signal and background for the whole signal mass range that improves the sensitivity with respect to the previous version of the analysis. Even though, a few more studies are still undergoing to test if the separation could be improved a bit more. Some of these studies and preliminary results are shown in this section, but they have not been propagated to the analysis yet.

Cross-training. In order to improve the accuracy of the discriminants, increasing

the available statistics used in the training, the cross-training [253] method could be used. Diagram in figure 5.19 illustrates the workflow of the method. The main idea of cross training consists of redefining the training/testing/validation sets three times. Each time their role is swapped, resulting in three NN models which can be applied to the full analysis samples, thus making use of the full MC statistics. While this method is implemented and tested it has not yet been propagated to the results presented in this thesis.

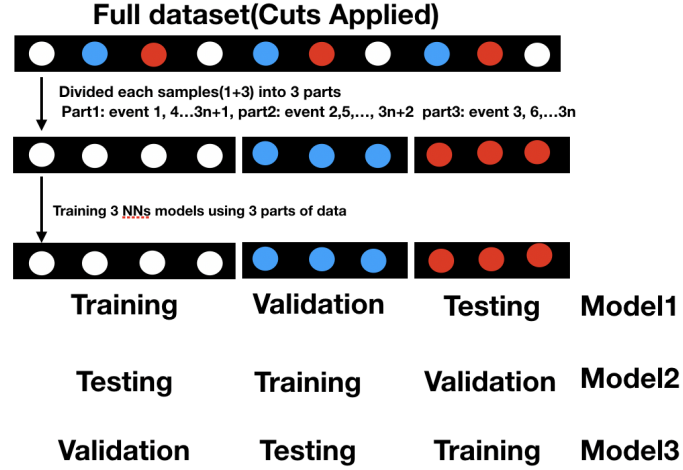


Figure 5.19: Illustration of cross-training method.

Input parameters. The current setting of the NN uses low level variables as inputs, but adding some high level variables for H^+ could be test to understand if high level kinematics are able to learned from the low level inputs already used with the current NN setting. For example, adding the invariant mass distribution between jets and b -jets ($m_{j,b}$) as input parameter for the NN training. This already shows an improvement in the separation with respect to the current NN training configuration, as seen in figure 5.20 (b).

On top of these options, finer tuning on the hyper-parameter setting is taking place. And also alternative configurations of the NN are being tested, such as the usage of an alternative regularizer (for example L2, MaxNorm + Dropout) or replacing the grid scan on the hyper-parameters for a random scan, which at first glance shows an improvement on the separation as shown in figure 5.21.

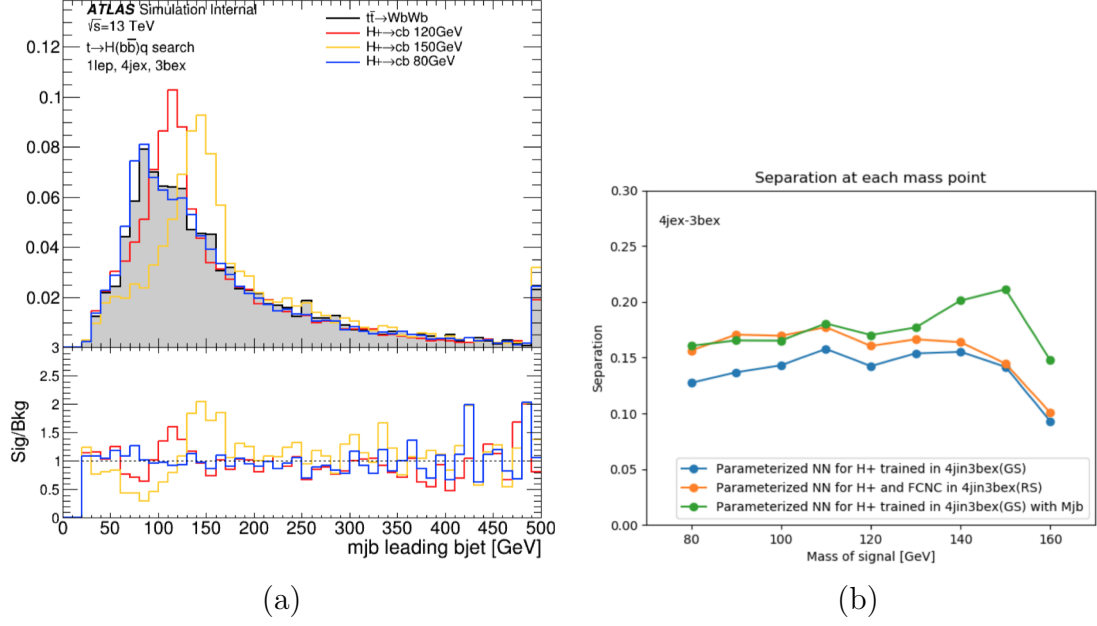


Figure 5.20: (a) Invariant mass distribution between jets and b -jets for $t\bar{t} \rightarrow WbWb$ background and three H^+ signal masses: 80, 120 and 150 GeV in the 4jex-3bex region. (b) Separation as a function of H^+ mass for different training configurations: in blue the NN trained with the current configuration, in green the NN trained adding $m_{j,b}$ as feature.

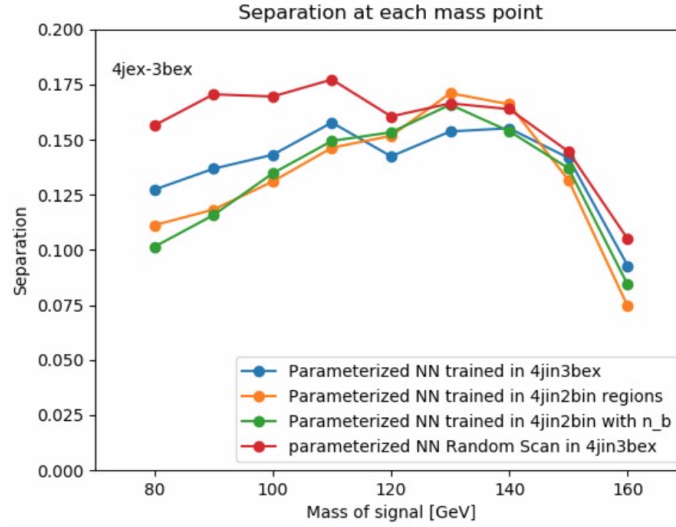


Figure 5.21: Separation as a function of H^+ mass for different training configurations: in blue the NN trained with the current configuration including the grid scan on the hyper-parameter, and in red the NN trained using the random scan on them.

5.4.2.5 Discriminant binning

The binning of the NN discriminants is broadly optimised simultaneously for all signals. The method is based on the implementation available in the software framework [254]. The main idea is to define the binning in an iterative manner based on the variable:

$$Z = Z_b \frac{n_b}{N_b} + Z_s \frac{n_s}{N_s} \quad (5.2)$$

where “s” and “b” refers to “signal” and “background”. The two input parameters of the algorithm are Z_b and Z_s , and their sum is taken as the total number of bins. In order to define each bin, a boundary is obtained from the condition: $Z \geq 1$. The variable n_X ($X=s,b$) is defined as

$$n_X = \sum_{i=a}^b n_X^i \quad (5.3)$$

and N_X ($X=s,b$) is

$$N_X = \sum_{i=1}^{N_{bins}} n_X^i \quad (5.4)$$

As an example, for $Z_b = N_{bins}$ and $Z_s = 0$, the corresponding binning will have $n_b = N_b$ in each bin, that is the binning will be constructed in a way that makes the background flat in the investigated NN discriminant. For this search $Z_b = N_{bins}/2$ and $Z_s = N_{bins}/2$ is used in all regions with at least two bins. In regions with exactly three b -jets (4jex-3bex, 5jex-3bex, 6jin-3bex) ten bins in total are used, in regions with at least four b -jets (4jex-4bex, 5jex-4bin, 6jex-4bin) two bins are used, and in regions with exactly two b -jets (4jex-2bex, 5jex-2bex, 6jin-2bex) a single bin is used.

The binning definition is a function of both the signal yields and the NN discriminant. In order to avoid defining a signal dependent binning, upon inspection of the NN discriminant, all signals are summed up and the combined signal is used for deriving the binning. The analysis performance with the binning derived in such way was compared to the expected performance of signal-specific binning and the observed degradation in performance is observed to be less 1% across all signal benchmarks.

A summary of the used analysis regions along with their binning is given in figure [5.22](#).

Nb Nj			
	2b-ex, 1b-70% (exactly two b-tagged jets + one loose b-tagged jet)	3b-ex (exactly three b-tagged jets)	4b-in (at least four b-tagged jets)
4j-ex (exactly four jets)	4j-ex, 2b-ex, 1b-70% (one bin)	4j-ex, 3b-ex (10 bins)	4j-ex, 4b-in (2 bins)
5j-ex (exactly five jets)	5j-ex, 2b-ex, 1b-70% (one bin)	5j-ex, 3b-ex (10 bins)	5j-ex, 4b-in (2 bins)
6j-in (at least six jets)	6j-in, 2b-ex, 1b-70% (one bin)	6j-in, 3b-ex (10 bins)	6j-ex, 4b-in (2 bins)

Region for NN training

Figure 5.22: Summary of the analysis regions along with information about their binning and the NN training.

5.5 Systematic uncertainties

Several sources of systematic uncertainties are considered that can affect the normalisation of signal and background, as well as the shape of their corresponding final discriminant distributions. Individual sources of systematic uncertainties are considered uncorrelated. Correlations of a given systematic uncertainty are maintained across processes and channels. Table 5.5 presents a list of all systematic uncertainties considered in the analysis and indicates whether they are taken to be normalisation-only (N), or to affect both shape and normalisation (SN). Figures illustrating the effect of systematic uncertainties on the shape of the final discriminating variable can be found in appendix E of the internal note [203].

The following sections describe each of the systematic uncertainties considered, focusing only on the ones that have been already propagated into the analysis.

Systematic uncertainty	Type	Components
Luminosity	N	1
Pileup reweighting	SN	1
Reconstructed Objects		
Electron trigger+reco+ID+isolation	SN	5
Electron energy scale+resolution	SN	2
Muon trigger+reco+ID+isolation	SN	6
Muon momentum scale+resolution	SN	3
Jet vertex tagger	SN	1
Jet energy scale ^(*)	SN	N/A
Jet energy resolution ^(*)	SN	N/A
Missing transverse momentum	SN	3
<i>b</i> -tagging efficiency	SN	44
<i>c</i> -tagging efficiency	SN	14
Light-jet tagging efficiency	SN	19
Background Model		
$t\bar{t}$ cross section	N	1
$t\bar{t} + \geq 1c$: normalisation	N	1
$t\bar{t} + \geq 1b$: normalisation	N (free floating)	1
$t\bar{t} + \geq 1b$: NLO Shape ^(*)	SN	N/A
$t\bar{t}$ modelling: residual NLO generator	SN	3
$t\bar{t}$ modelling: residual Radiation	SN	3
$t\bar{t}$ modelling: residual parton shower+hadronisation	SN	3
<i>V</i> +jets normalisation	N	3
Single top cross-section	N	1
Single top model	SN	7
Diboson normalisation	N	3
$t\bar{t}V$ cross section	N	1
$t\bar{t}H$ cross section	N	1
Multijet normalisation ^(**)	N	N/A
Signal Model		
$t\bar{t}$ cross section ^(**)	N	1
$t\bar{t}$ modelling: residual NLO generator ^(**)	SN	1
$t\bar{t}$ modelling: residual Radiation ^(**)	SN	1
$t\bar{t}$ modelling: residual parton shower+hadronisation ^(**)	SN	1

Table 5.5: List of systematic uncertainties considered. An “N” means that the uncertainty is taken as normalisation-only for all processes and channels affected, whereas “SN” means that the uncertainty is taken on both shape and normalisation. Some of the systematic uncertainties are split into several components for a more accurate treatment. For those systematics marked with ^(*) it means that they have not been yet properly propagated to this version of the analysis, while the ones marked with ^(**) have not yet been included in the analysis.

5.5.1 Luminosity

The uncertainty on the integrated luminosity is 2.1%, affecting the overall normalisation of all processes estimated from the simulation. It is derived, following a methodology similar to that detailed in refs. [255], from a preliminary calibration of the luminosity scale using x - y beam-separation scans performed for different data taking periods.

5.5.2 Pileup reweighting

A variation in the pileup reweighting of MC is included to cover the uncertainty on the ratio between the predicted and measured inelastic cross-section in the fiducial volume defined by $M_X > 13$ GeV, where M_X is the mass of the non-diffractive hadronic system [256]. For more information see ref. [257].

5.5.3 Reconstructed objects

Leptons. Uncertainties associated with leptons arise from the trigger, reconstruction, identification, and isolation, as well as the lepton momentum scale and resolution [230, 231, 233]. The reconstruction, identification and isolation efficiency of electrons and muons, as well as the efficiency of the trigger used to record the events, differ slightly between data and simulation. Scale factors are derived using tag-and-probe techniques on $Z \rightarrow \ell^+\ell^-$ ($\ell = e, \mu$) data and simulated samples, and are applied to the simulation to correct for differences. The effect of these uncertainties is propagated as corrections to the event weight.

Additional sources of uncertainty originated from the corrections applied to adjust the lepton momentum scale and resolution in the simulation to match those in data are applied. They are measured using reconstructed distributions of the $Z \rightarrow \ell^+\ell^-$ and $J/\psi \rightarrow \ell^+\ell^-$ masses, as well as the measured E/p in $W \rightarrow e\nu$ events, where E and p are the electron energy and momentum, as measured by the calorimeter and the tracker respectively. To evaluate the effect of momentum scale uncertainties, the event selection is redone with the lepton momentum varied by $\pm 1\sigma$. For the momentum resolution uncertainties the event selection is redone with the lepton momentum smeared.

The combined effect of all these uncertainties results in an overall normalisation uncertainty on the signal and background of approximately 1%.

Missing transverse momentum. The E_T^{miss} reconstruction is affected by uncertainties associated with leptons and jet energy scales and resolutions, which are propagated to E_T^{miss} and thus are included under the corresponding per-object uncertainty category. Additional small uncertainties associated with the modelling of the underlying event, in particular its impact on the p_T scale and resolution of unclustered energy, are also taken into account.

Heavy- and light-flavour tagging. Efficiencies to tag jets from b - and c -quarks in the simulation are corrected to match the efficiencies in data by p_T -dependent factors, whereas the light-jet efficiency is scaled by p_T - and η -dependent factors. The b -tagging calibration used can be found in ref. [258]. Uncertainties on these scale factors (SF) include a total of forty-four independent sources affecting b -jets and fourteen sources affecting c -jets. Each of these uncertainties has different jet p_T dependence. Nineteen uncertainties are considered for the light-jets tagging, which depend on the jet p_T and η regions. Few

examples of their impact are shown in figure 5.23. These uncertainties are taken to be correlated among the three jet flavours. Finally, τ -jets are assigned the c -jet SF.

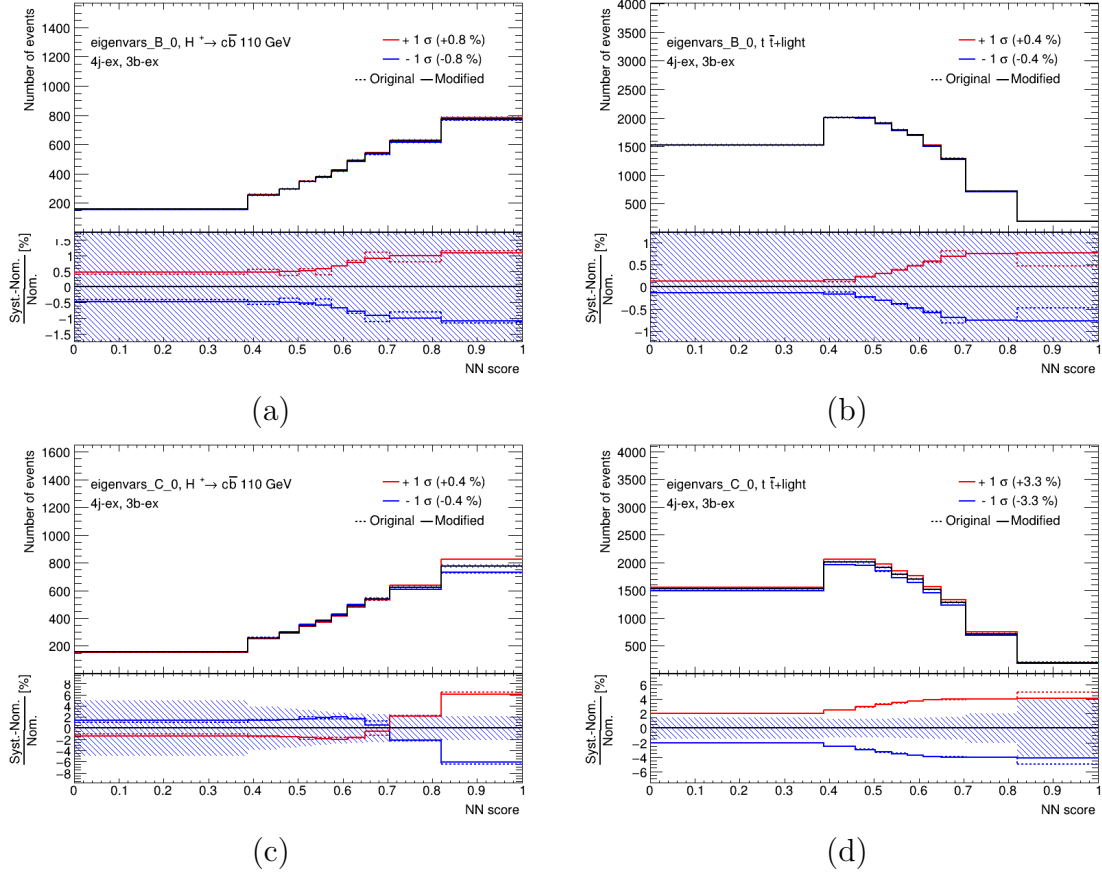


Figure 5.23: Shape-dependent systematic uncertainty for one of the b -jets uncertainties (eigenvars_B.0) and one of the c -jets uncertainties (eigenvars_C.0) in the 4jex-3bex region. Samples: (a) (c) H^+ with $m_{H^+}=110$ GeV, and (b) (d) $t\bar{t}$ +light. In the figures, “Original” refers to the raw systematic uncertainty whereas “Modified” corresponds to the actual systematic uncertainty used in the statistical analysis, resulting after the application of a smoothing algorithm.

5.5.4 Background modelling

$t\bar{t}$ background. A number of systematic uncertainties affecting the modelling of the $t\bar{t}$ +jets background are considered, summarised in table 5.6. An uncertainty of $\pm 6\%$ is assumed for the inclusive $t\bar{t}$ NNLO+NNLL production cross-section [209], including effects from varying the factorisation (μ_F) and renormalisation (μ_R) scales, the PDF, α_S , and the top quark mass. An uncertainty associated with the choice of NLO generator is derived by comparing two alternative predictions, POWHEG PYTHIA 8 with a prediction from SHERPA, as it can be seen in figure 5.24.

An uncertainty due to the choice of parton shower (see figure 5.25) and hadronisation model is derived by comparing the prediction from POWHEG interfaced either to PYTHIA 8 or Herwig7. Additionally, the uncertainty on modelling initial (ISR) and final state radiation (FSR) is assessed with two alternative Powheg +Pythia 8 samples: the sample with radiation increased has the renormalisation and factorisation scales decreased

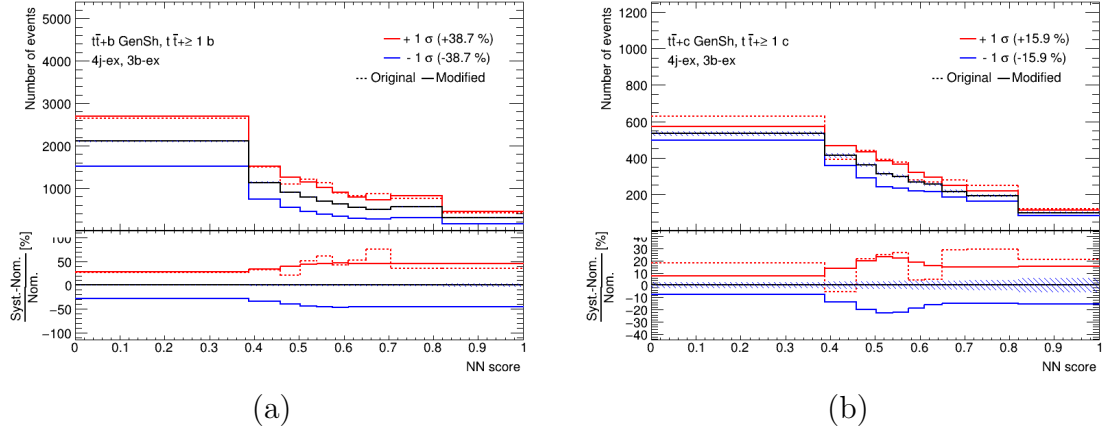


Figure 5.24: Shape-dependent systematic uncertainty from the choice generator in the 4jex-3bex region. Samples: (a) $t\bar{t} + b\bar{b}$ and (b) $t\bar{t} + c\bar{c}$. In the figures, ‘Original’ refers to the raw systematic uncertainty whereas ‘Modified’ corresponds to the actual systematic uncertainty used in the statistical analysis, resulting after the application of a smoothing algorithm.

by a factor of two, the h_{damp} ⁸ parameter doubled, and the A14 eigentune parameter Var3c increased, while the sample with radiation decreased has the scales increased by a factor of two and the A14 Var3c parameter decreased [259].

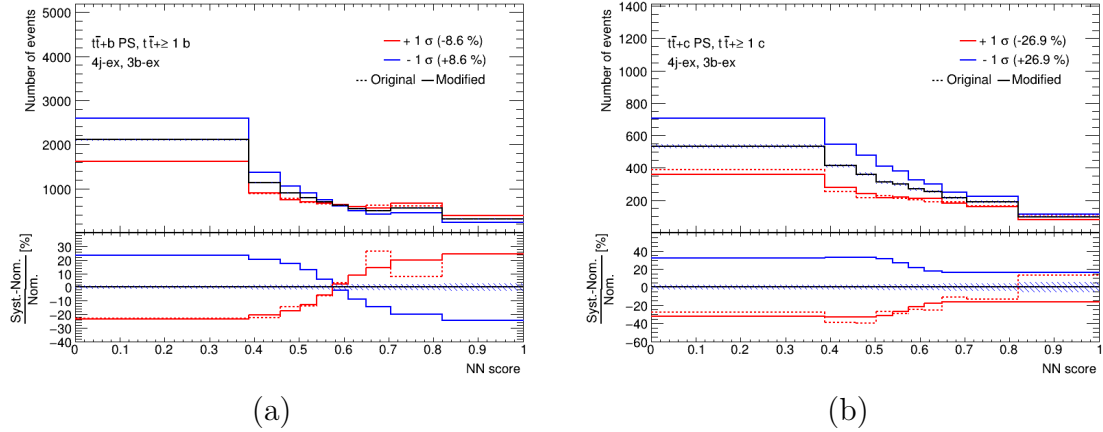


Figure 5.25: Shape-dependent systematic uncertainty from the parton shower choice in the 4jex-3bex region. Samples: (a) $t\bar{t} + b\bar{b}$ and (b) $t\bar{t} + c\bar{c}$. In the figures, ‘Original’ refers to the raw systematic uncertainty whereas ‘Modified’ corresponds to the actual systematic uncertainty used in the statistical analysis, resulting after the application of a smoothing algorithm.

Since the diagrams that contribute to $t\bar{t} + \geq 1b$, $t\bar{t} + \geq 1c$, and $t\bar{t} + \text{light-jets}$ production are different and the uncertainties may affect these processes in different regions in different ways, all uncertainties on $t\bar{t} + \text{jets}$ background modelling, except the uncertainty on the inclusive cross-section, are considered to be uncorrelated among $t\bar{t} + \geq 1b$, $t\bar{t} + \geq 1c$ and $t\bar{t} + \text{light-jets}$.

The normalisation of $t\bar{t} + \geq 1b$ is allowed to float freely in the fit, with no prior uncertainty applied. In the case of the $t\bar{t} + \geq 1c$ normalisation, since the fit to the data is unable

⁸The main effect of the h_{damp} setting is to regulate the high- p_T emission against which the $t\bar{t}$ system recoils.

Systematic source	How evaluated	$t\bar{t}$ categories
$t\bar{t}$ cross-section	+5.5%/−6.1%	All, correlated
NLO generator	POWHEG +PYTHIA 8 vs.SHERPA	All, uncorrelated
Radiation	Variations of μ_R , μ_F , h_{damp} , A14/Var3c parameters	All, uncorrelated
PS & hadronisation	POWHEG + PYTHIA 8 vs. POWHEG +Herwig7	All, uncorrelated

Table 5.6: A summary of the systematic uncertainties on the $t\bar{t}$ +jets modelling. For the $t\bar{t}+ \geq 1b$ background, the inclusive $t\bar{t}$ sample is reweighted to a NLO $t\bar{t}+ \geq 1b$ prediction. NLO generator and radiation uncertainties affect the inclusive sample.

to precisely determine it and the analysis has very limited sensitivity to its uncertainty, a normalisation uncertainty of 50% is assumed.

The shape of these distributions, and the relative normalisation of the $t\bar{t}+ \geq 1b$ and $t\bar{t}+ \geq 1c$ sub-components, are constrained by the uncertainties described above.

W/Z +jets. Uncertainties affecting the normalisation of the V +jets background are estimated for the sum of W +jets and Z +jets, and separately for V +light-jets, $V+ \geq 1c$ +jets, and $V+ \geq 1b$ +jets subprocesses. Agreement between data and total background prediction in the different analysis regions considered, but requiring exactly 0 b -tagged jets, which are dominated by V +light-jets, is found to be within approximately 30%, which is taken to be the total normalisation uncertainty correlated across all V +jets subprocesses. Since SHERPA has been found to underestimate V +heavy-flavour by about a factor of 1.3 [260], additional 30% normalisation uncertainties are assumed for $V+ \geq 1c$ +jets and $V+ \geq 1b$ +jets subprocesses, considered uncorrelated between them.

Other simulated background. Uncertainties affecting the modelling of the single-top-quark background include a +5%/−4% uncertainty on the total cross section estimated as a weighted average of the theoretical uncertainties on t -, Wt - and s -channel production [217–219]. Additional uncertainties associated with the choice of the generator are evaluated by comparing POWHEG +PYTHIA 8 to MADGRAPH5_aMC@NLO +PYTHIA 8, an uncertainty on the parton-shower model is estimated by comparing POWHEG +PYTHIA 8 to POWHEG +Herwig7. These uncertainties are treated as uncorrelated among single-top production processes, as well as with the corresponding uncertainties in the $t\bar{t}$ +jets background. Finally, an additional systematic uncertainty on the Wt -channel process concerning the separation between $t\bar{t}$ and Wt at NLO [261] is assessed by comparing the nominal sample, which uses the so-called “diagram subtraction” scheme, with an alternative sample using the “diagram removal” scheme.

Uncertainties on the diboson background normalisation include 5% from the NLO theory cross sections [262], as well as an additional 24% normalisation uncertainty added in quadrature for each additional inclusive jet-multiplicity bin, based on a comparison among different algorithms for merging LO matrix elements and parton showers [263] (assuming that already two jets come from the W/Z decay, as in $WW/WZ \rightarrow \ell\nu jj$). Therefore, the total uncertainty would be $5\% \oplus \sqrt{N-2} \times 24\%$, where N is the desired jet multiplicity, i.e. 34%, 42%, and 48%, for events with exactly 4 jets, 5 jets, and ≥ 6 jets, respectively. Recent comparisons between data and SHERPA for $WZ(\rightarrow \ell\nu\ell\ell)+ \geq 4$ jets show agreement within the experimental uncertainty of approximately 40% [264], which further justifies the above uncertainty.

Uncertainties on the $t\bar{t}V$ and $t\bar{t}H$ cross sections are 15% and $+10\%/ -13\%$ respectively, from the uncertainties on their respective NLO theoretical cross sections [220, 265, 266].

5.6 Statistical analysis

The NN discriminant distributions from each of the regions considered are combined to test for the presence of a signal. A single bin is used in the 2b regions, ten bins in the 3b regions, and two bins in the $\geq 4b$ regions. The statistical analysis is based on a binned likelihood function $\mathcal{L}(\mu, \theta)$ constructed as a product of Poisson probability terms over all bins considered in the analysis. This function depends on the signal strength parameter μ , a multiplicative factor for the branching ratio $t \rightarrow H^+b$ (normalised to a reference branching ratio $\mathcal{B}_{\text{ref}}(t \rightarrow H^+b) = 0.5$), and θ , a set of nuisance parameters that encode the effect of systematic uncertainties on the signal and background expectations and are implemented in the likelihood function as Gaussian or log-normal priors. The relationship between μ and the corresponding $\mathcal{B}(t \rightarrow H^+b)$ signal events is:

$$\mu = \frac{\mathcal{B}(t \rightarrow H^+b)(1 - \mathcal{B}(t \rightarrow H^+b))}{\mathcal{B}_{\text{ref}}(t \rightarrow H^+b)(1 - \mathcal{B}_{\text{ref}}(t \rightarrow H^+b))}. \quad (5.5)$$

For a given μ value, the SM $t\bar{t} \rightarrow WbWb$ background contribution should in principle be scaled accordingly in order to preserve the inclusive $t\bar{t}$ cross section. The corresponding multiplicative factor would be $(1 - \mathcal{B}(t \rightarrow H^+b))^2$, with $\mathcal{B}(t \rightarrow H^+b)$ being a function of μ as can be derived from equation 5.5:

$$\mathcal{B}(t \rightarrow H^+b) = \frac{1 - \sqrt{1 - 4\mathcal{B}_{\text{ref}}(t \rightarrow H^+b)(1 - \mathcal{B}_{\text{ref}}(t \rightarrow H^+b))\mu}}{2}. \quad (5.6)$$

Please note that the $1 + \sqrt{}$ solution is not correct since for $\mu = 0$ it must be satisfied that $\mathcal{B}(t \rightarrow H^+b) = 0$. Since the values of $\mathcal{B}(t \rightarrow H^+b)$ this analysis is sensitive to are well below 1%, such small correction to the $t\bar{t} \rightarrow WbWb$ background normalisation is neglected as it is much smaller than the systematic uncertainties on this background.

Therefore, the total number of expected events in a given bin depends on μ and θ . The nuisance parameters θ adjust the expectations for signal and background according to the corresponding systematic uncertainties, and their fitted values correspond to the deviations from the nominal expectations that globally provide the best fit to the data. This procedure allows a reduction of the impact of systematic uncertainties on the search sensitivity by taking advantage of the highly populated background-dominated channels included in the likelihood fit. It requires a good understanding of the systematic effects affecting the shapes of the discriminant distributions. Detailed validation studies of the fitting procedure have been performed using the simulation. To verify the improved background prediction, fits are performed under the background-only hypothesis. Statistical uncertainties in each bin of the discriminant distributions are also taken into account by dedicated parameters in the fit, referred to as “ γ factors”. In order to speed up the fit, systematic uncertainties that have very small effects on normalisation or shape are pruned, per process and analysis channel. The pruning algorithm removes systematic uncertainties that have a $\leq 0.2\%$ impact on normalisation or those that cause a negligibly small impact on the shape of the final discriminant (all bins are within 0.2% of the nominal shape).

The test statistic q_μ is defined as the profile likelihood ratio: $q_\mu = -2\ln(\mathcal{L}(\mu, \hat{\theta}_\mu)/\mathcal{L}(\hat{\mu}, \hat{\theta}))$, where $\hat{\mu}$ and $\hat{\theta}$ are the values of the parameters that maximise the likelihood function (with the constraint $0 \leq \hat{\mu} \leq \mu$), and $\hat{\theta}_\mu$ are the values of the nuisance parameters that maximise the likelihood function for a given value of μ .

The test statistic q_μ is implemented in the TREXFITTER package [267, 268] and is used to measure the compatibility of the observed data with the background-only hypothesis (i.e. the discovery test) setting $\mu = 0$ in the profile likelihood ratio: $q_0 = -2\ln(\mathcal{L}(0, \hat{\theta}_0)/\mathcal{L}(\hat{\mu}, \hat{\theta}))$. The p -value (referred to as p_0) representing the compatibility of the data with the background-only hypothesis is estimated by integrating the distribution of q_0 from background-only pseudo-experiments, approximated using the asymptotic formulae given in ref. [269, 270], above the observed value of q_0 . Some model dependence exists in the estimation of the p_0 -value, as a given signal scenario needs to be assumed in the calculation of the denominator of q_μ , even if the overall signal normalisation is left floating and fitted to data. The observed p_0 -value is checked for each explored signal scenario.

In the absence of any significant excess above the background expectation, upper limits on μ , and thus on $\mathcal{B}(t \rightarrow H^+b)$ via equation 5.6, for each of the signal scenarios considered are derived by using q_μ in the CL_s method [271, 272]. For a given signal scenario, values of $\mathcal{B}(t \rightarrow H^+b)$ yielding CL_s < 0.05, where CL_s is computed using the asymptotic approximation [269], are excluded at $\geq 95\%$ CL.

The likelihood function is built out of individual likelihood terms for different background components. Each likelihood function is defined based in input histograms of the discriminant. A smoothing algorithm, based on a ROOT implementation, is applied before a histogram is translated into a likelihood function as needed in cases where the input histograms suffer from large statistical fluctuations.

Once unblinded, fits are performed to data under the signal-plus-background hypothesis, where the signal strength parameter, μ , is the parameter of interest in the fit and is allowed to float freely, but is required to be the same in all fitted regions.

In order to study the expected behavior of the fit, fits are also performed to the “Asimov dataset”, defined as the sum of the total expected background, although for some tests (e.g. the calibration of the signal strength parameter μ), simulated signal assuming a given branching ratio can also be included on the Asimov dataset. Normalisation of all backgrounds is determined from the fit simultaneously with the μ . Contributions from $t\bar{t}$, W/Z +jets production, single top, diboson, $t\bar{t}H$ and $t\bar{t}V$ backgrounds are constrained by the uncertainties of the respective theoretical calculations, the uncertainty on the luminosity, and the data themselves. Statistical uncertainties in each bin of the discriminant distributions are taken into account by dedicated parameters in the fit.

The following blinding procedure is adopted: in each analysis channel, those bins of the NN discriminant distribution with a signal-to-background ratio (S/B) greater than 5%, assuming $\mathcal{B}(t \rightarrow H^+b) = 0.5$ (a value excluded by ref. [273]), are removed. This removes the bins of the NN discriminant distribution above ~ 0.5 for the 4jex-3bex region, 0.47 for the 5jex-3bex region, and above 0.54 for the 6jin-3bex region. Given the large observed S/B in the 4jex-4bin and 5jex-4bin regions, these are fully blinded, while the remaining regions are fully unblinded. The same blinding cuts are applied for all considered signal benchmarks. The procedure is illustrated in figure 5.27.

An summary of the blinding strategy for the fit regions is given in figure 5.26.

Nb Nj				
		2b-ex, 1b-70% (exactly two b-tagged jets + one loose b-tagged jet)	3b-ex (exactly three b-tagged jets)	4b-in (at least four b-tagged jets)
4j-ex (exactly four jets)		4j-ex, 2b-ex, 1b-70% (pull the ttbar+light background, one bin)	4j-ex, 3b-ex (main signal region, 10 bins) Last 7 bins blinded	4j-ex, 4b-in (ttbar+b background control and large S/B region, 2 bins)
5j-ex (exactly five jets)		5j-ex, 2b-ex, 1b-70% (pull the ttbar+light background, one bin)	5j-ex, 3b-ex (main signal region, 10 bins) Last 5 bins blinded	5j-ex, 4b-in (ttbar+b background control and large S/B region, 2 bins)
6j-in (at least six jets)		6j-in, 2b-ex, 1b-70% (pull the ttbar+light background, one bin)	6j-in, 3b-ex (shape correction for the NN discriminant in background dominated region, 10 bins) Last 3 bins blinded	6j-ex, 4b-in (ttbar+b background contro, 2 bins)
		Fully unblinded	Fully unblinded	Fully blinded

Figure 5.26: Summary of the fit regions along with information about their usage in the fit model and the blinding strategy.

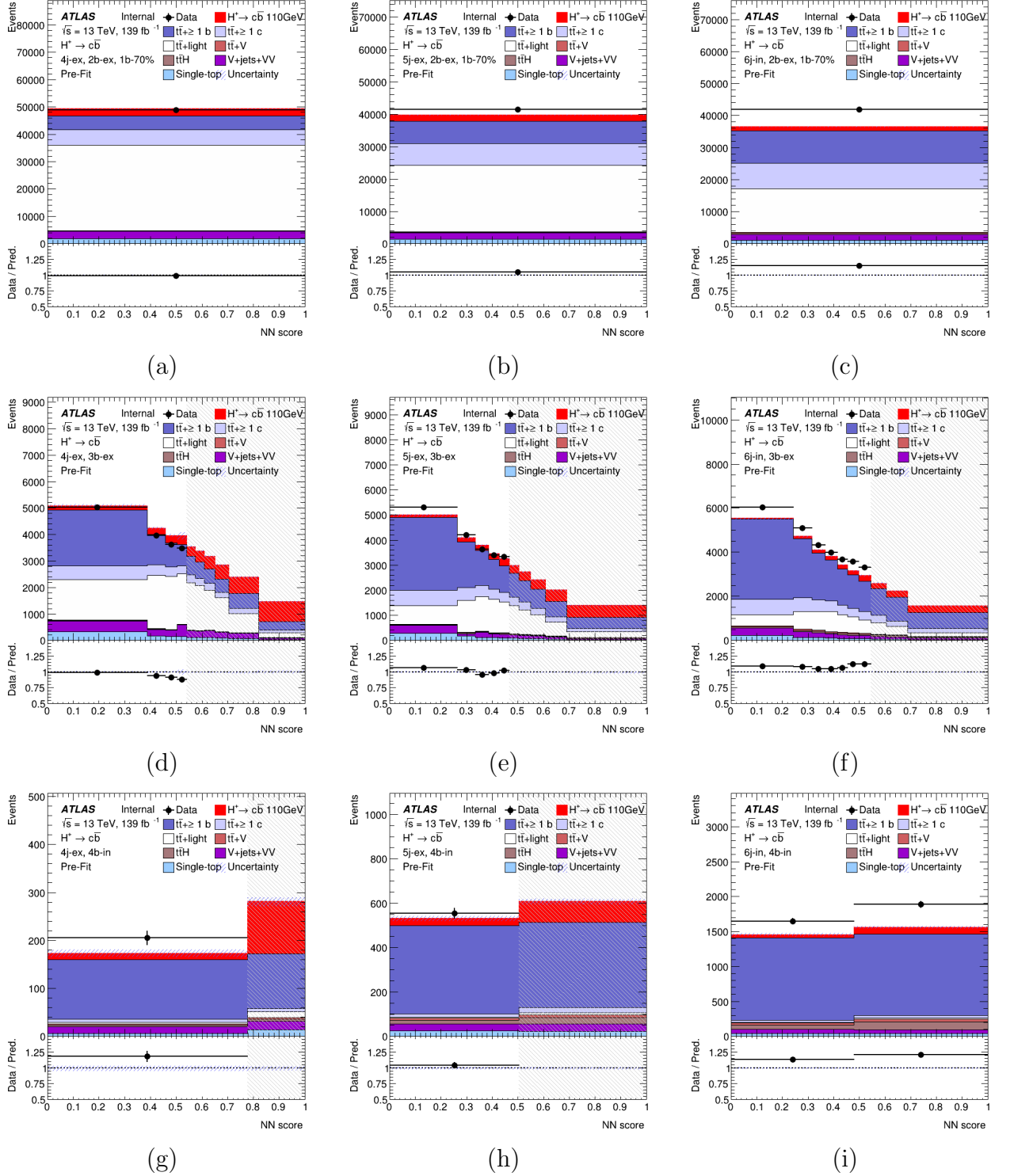


Figure 5.27: Comparison of the NN discriminant distribution between the blinded data and prediction before the fit to data (“Pre-fit”) in each of the regions considered in the analysis: (a) (4j, 2b), (b) (5j, 2b), (c) ($\geq 6j$, 2b), (d) (4j, 3b), (e) (5j, 3b), (f) ($\geq 6j$, 3b), (g) (4j, $\geq 4b$), (h) (5j, $\geq 4b$), and (i) ($\geq 6j$, $\geq 4b$). Contributions from the different background sources are shown in different colours. The expected H^+b signal (solid red) corresponding to $\mathcal{B}(t \rightarrow H^+b) = 1.0$ is also shown, added on top of the background prediction. The bottom panel displays the ratio of data to the total prediction (“Pred”), which includes the signal plus the SM background. The dashed area represents the total uncertainty on the background. In the case of the pre-fit background uncertainty, the normalisation uncertainty on the $tt + \geq 1b$ background is not included. Dashed vertical areas represent the blinded bins resulting from the blinding procedure.

5.7 Preliminary results

5.7.1 Fits to Asimov dataset

As already discussed, a pruning algorithm is applied to remove nuisance parameters that are expected to have a negligible impact on the fit result. A summary of the pruned nuisance parameters is provided in appendix C.2. Similar pruning pattern is observed across all signal benchmarks.

Figure 5.28 displays the fitted nuisance parameters to the unblinded Asimov dataset (defined as the sum of expected background, assuming an integrated luminosity of 139 fb^{-1}) under the background-only hypothesis. For each nuisance parameter, the fitted value represents the preferred shift with respect to the nominal prediction in units of its prior uncertainty, whereas the fitted error represents the post-fit uncertainty in units of the prior uncertainty. Therefore, a fitted value close to 0 and a fitted error close to 1 indicates that the data does not have enough statistical power to induce a pull in the nuisance parameter and reduce the original uncertainty. The exception is the $t\bar{t} + \geq 1b$ normalisation parameter, which is taken as a free-floating parameter and thus the fitted value in the Asimov dataset is expected to be 1. Its post-fit value, determined with about 8% precision, is also presented in figure 5.28. As can be appreciated, a number of nuisance parameters are expected to be overconstrained, in particular several large uncertainties related to $t\bar{t}$ +jets modelling (such as $t\bar{t} + \geq 1c$ normalisation, generator and parton shower uncertainties on $t\bar{t} + \geq 1b$ and $t\bar{t}$ +light-jets), as well as the leading eigenvectors for b -tagging, c -tagging, and light-jet tagging (referred to section 5.5). The analysis of the NN discriminant variable across several analysis regions, split by jet and b -tag multiplicities, allows the fit disentangling the effect of these different uncertainties. The corresponding expected correlation matrix for the fitted nuisance parameters can be found in figure 5.28. In general correlations are small, although there are several nuisance parameters correlated at the level of 40–70%, which is not unexpected as several of them have large uncertainties that cause similar changes in the background prediction. This is the case in particular for the $t\bar{t}$ +jets generator and PS & hadronisation uncertainties.

The γ factors, describing the per-bin statistical uncertainties, are also shown in figure 5.28.

A comparison of the distribution of expected yields per analysis region before and after the fit can be found in figure 5.29. Figures 5.30, 5.31 and 5.32 show the comparison of the expected NN distribution in each of the regions considered, both pre- and post-fit to Asimov data.

As a result of the fit, the large uncertainty in the background prediction pre-fit is significantly reduced, which should result in a large increase in the search sensitivity. This can be easily explained: in regions with large data statistics, uncertainties cannot vary independently if the total background prediction is to remain consistent with the data, so the associated nuisance parameters become anti-correlated. As a result, in those regions the post-fit background uncertainty becomes as small as the data statistical uncertainty itself (which is exactly what is expected). This is why it is so important to have a sophisticated systematic model, so that those constraints and/or anti-correlations can confidently be ported into the signal region.

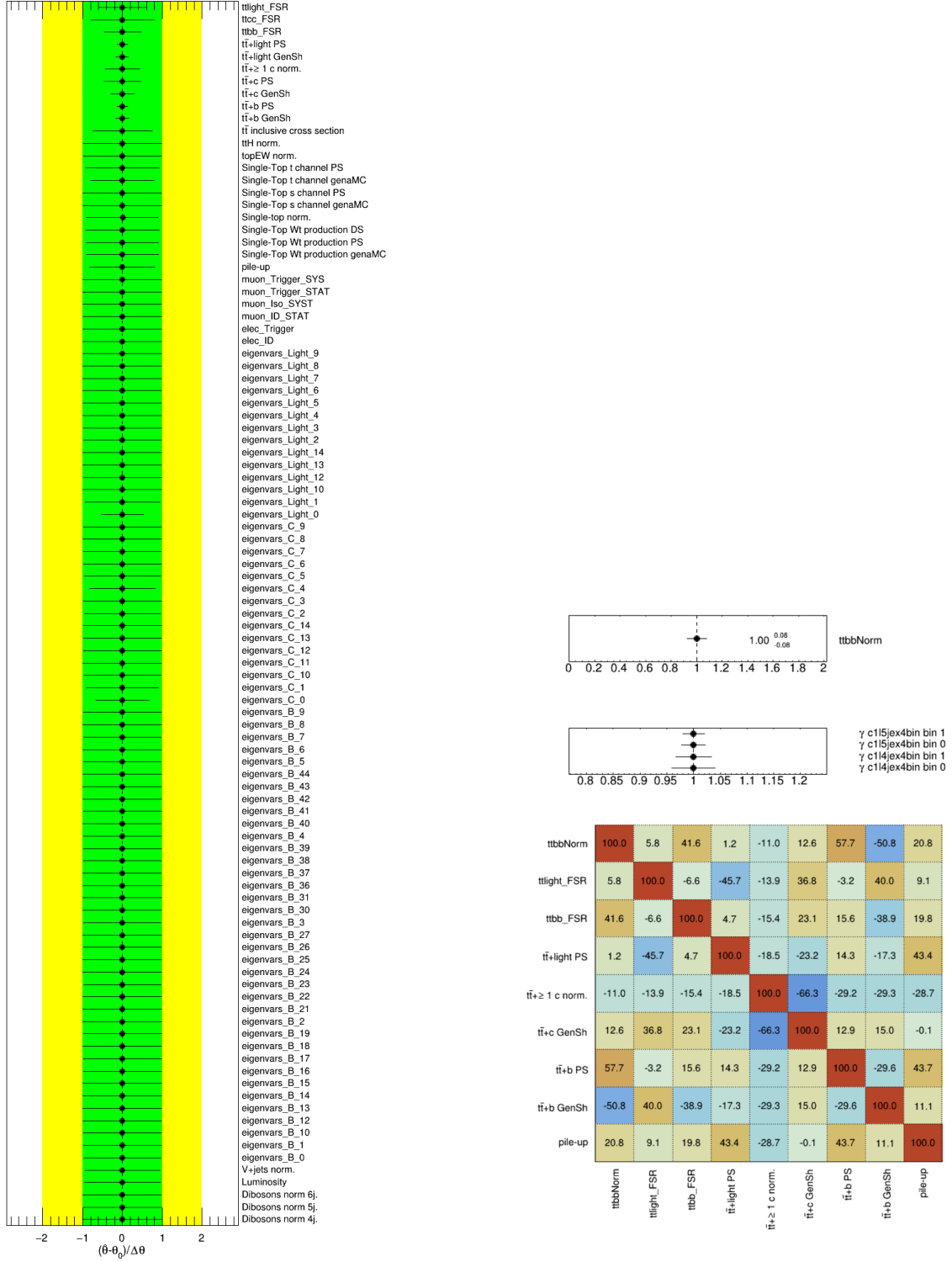


Figure 5.28: Expected fitted nuisance parameters (on the left), normalisation factors (top right), γ factors (middle right) and correlation matrix corresponding to the fit (bottom right) to the unblinded Asimov dataset under the background-only hypothesis for the H^+b signal with $m_{H^+} = 110\text{GeV}$. Only nuisance parameters with a correlation coefficient of at least 20% with any other parameter are displayed.

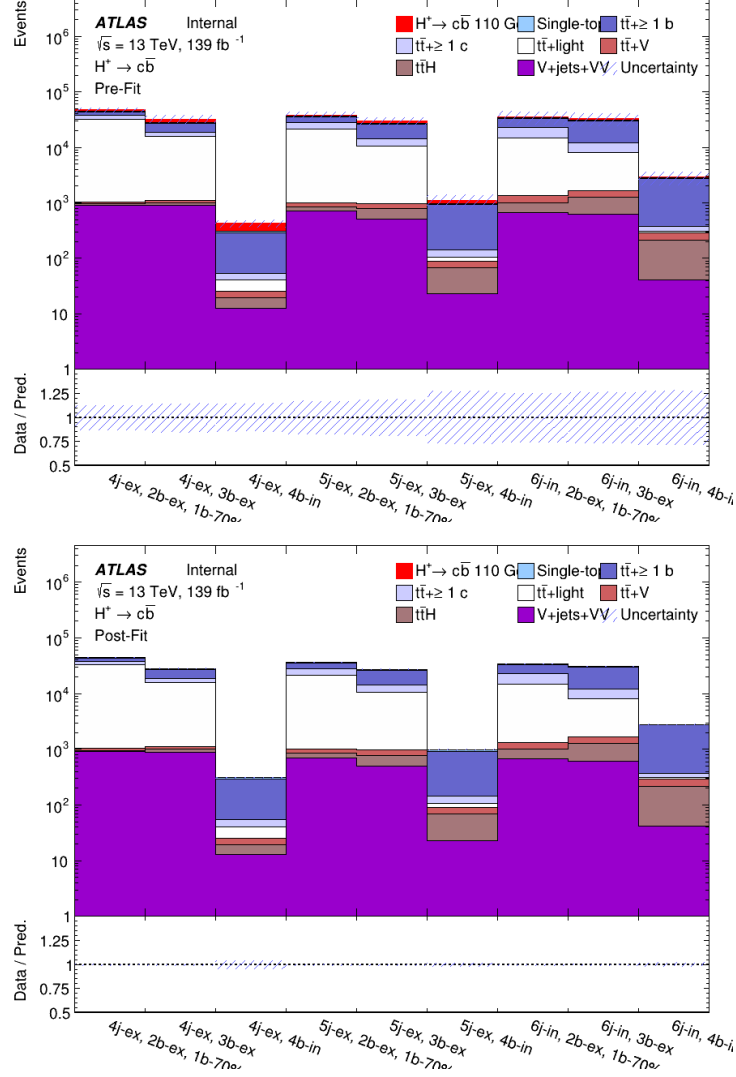


Figure 5.29: Comparison between Asimov data and prediction of the yields per analysis region (a) before and (b) after the fit to Asimov data under the background-only hypothesis. In the case of the pre-fit figure, the expected signal from $t \rightarrow H^+ b$ with $m_{H^+} = 110 \text{ GeV}$ (solid red) corresponding to $\mathcal{B}(t \rightarrow H^+ b) = 0.5$ is also shown, added on top of the background prediction. The bottom panel displays the ratio of data to the total prediction (“Pred”), which for the pre-fit plots includes the signal plus the SM background, whereas for the post-fit plots includes only the SM background. The dashed area represents the total uncertainty on the background. In the case of the pre-fit background uncertainty, the normalisation uncertainty on the $t\bar{t} + \geq 1b$ background is not included.

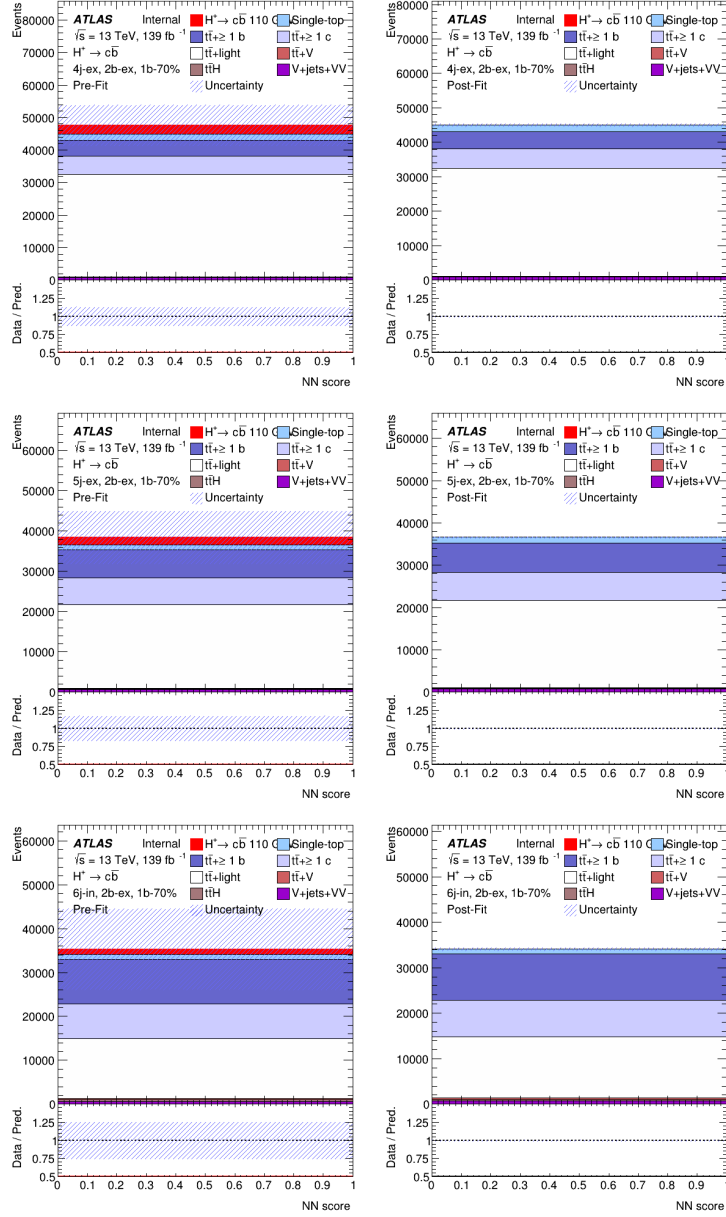


Figure 5.30: Comparison between the Asimov data and prediction for the NN distribution in the 2b regions, before and after performing the fit to Asimov data (“Pre-fit” and “Post-fit”, respectively) under the background-only hypothesis. Shown are the (4j, 2b) region (a) pre-fit and (b) post-fit, the (5j, 2b) region (c) pre-fit and (d) post-fit, and the ($\geq 6j$, 2b) region (e) pre-fit and (f) post-fit. In the pre-fit figures the expected signal from $t \rightarrow H^+b$ with $m_{H^+} = 110\text{GeV}$ (solid red) corresponding to $\mathcal{B}(t \rightarrow H^+b) = 0.5$ is also shown, added on top of the background prediction. The bottom panel displays the ratio of data to the total prediction (“Pred”), which for the pre-fit plots includes the signal plus the SM background, whereas for the post-fit plots includes only the SM background. The dashed area represents the total uncertainty on the background. In the case of the pre-fit background uncertainty, the normalisation uncertainty on the $t\bar{t} + \geq 1b$ background is not included. Underflow and overflow bins are included respectively in the first and last bins.

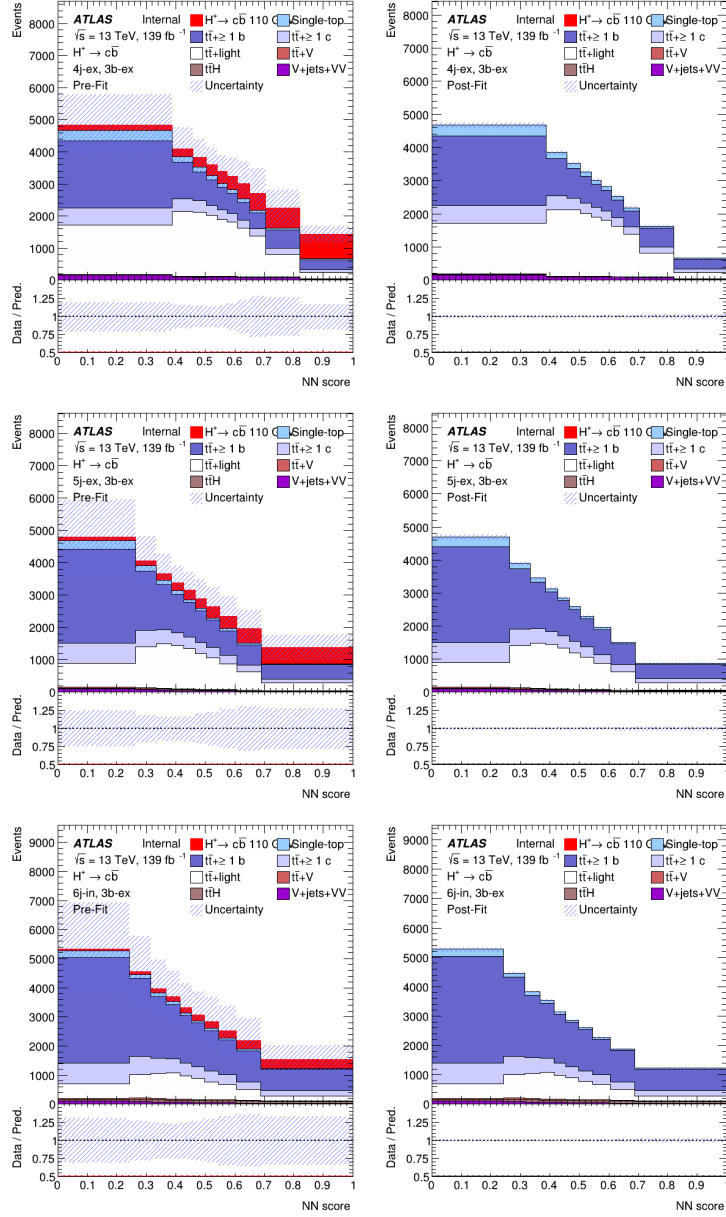


Figure 5.31: Comparison between the Asimov data and prediction for the NN distribution in the 3b regions, before and after performing the fit to Asimov data (“Pre-fit” and “Post-fit”, respectively) under the background-only hypothesis. Shown are the (4j, 3b) region (a) pre-fit and (b) post-fit, the (5j, 3b) region (c) pre-fit and (d) post-fit, and the ($\geq 6j$, 3b) region (e) pre-fit and (f) post-fit. In the pre-fit figures the expected signal from $t \rightarrow H^+b$ with $m_{H^+}=110\text{GeV}$ (solid red) corresponding to $\mathcal{B}(t \rightarrow H^+b) = 0.5$ is also shown, added on top of the background prediction. The bottom panel displays the ratio of data to the total prediction (“Pred”), which for the pre-fit plots includes the signal plus the SM background, whereas for the post-fit plots includes only the SM background. The dashed area represents the total uncertainty on the background. In the case of the pre-fit background uncertainty, the normalisation uncertainty on the $t\bar{t} + \geq 1b$ background is not included. Underflow and overflow bins are included respectively in the first and last bins.

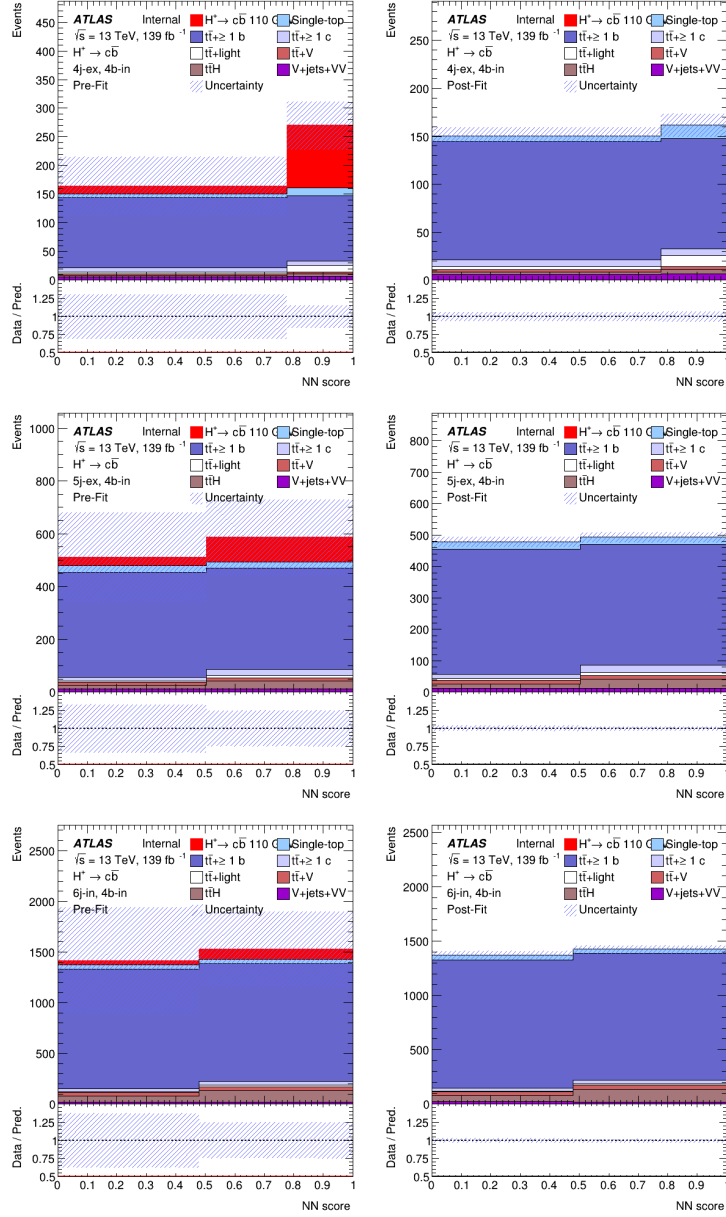


Figure 5.32: Comparison between the Asimov data and prediction for the NN distribution in the $\geq 4b$ regions, before and after performing the fit to Asimov data (“Pre-fit” and “Post-fit”, respectively) under the background-only hypothesis. Shown are the (4j, $\geq 4b$) region (a) pre-fit and (b) post-fit, the (5j, $\geq 4b$) region (c) pre-fit and (d) post-fit, and the ($\geq 6j$, $\geq 4b$) region (e) pre-fit and (f) post-fit. In the pre-fit figures the expected signal from $t \rightarrow H^+b$ with $m_{H^+}=110\text{GeV}$ (solid red) corresponding to $\mathcal{B}(t \rightarrow H^+b) = 0.5$ is also shown, added on top of the background prediction. The bottom panel displays the ratio of data to the total prediction (“Pred”), which for the pre-fit plots includes the signal plus the SM background, whereas for the post-fit plots includes only the SM background. The dashed area represents the total uncertainty on the background. In the case of the pre-fit background uncertainty, the normalisation uncertainty on the $t\bar{t} + \geq 1b$ background is not included. Underflow and overflow bins are included respectively in the first and last bins.

5.7.2 Fits to blinded data

Prior to removal of the blinding cuts, a simultaneous fit is performed to the NN distributions in the analysis regions, as discussed in section 5.6, in order to be able to scrutinise the fitted nuisance parameters and verify that any pulls or over-constraints are as expected.

A summary of the pruned nuisance parameters is provided in appendix C.2.

Figure 5.33 displays the fitted nuisance parameters to the blinded data under the background-only hypothesis, showing only few pulls or constraints. Constraints are in general consistent with those found in the Asimov fit. The pull on the charm tagging NP (“btag C EV0”) is consistent with improving the agreement with the $t\bar{t}$ -based charm tagging calibration. Figure 5.33 also shows the fitted value of the free-floating $t\bar{t} + \geq 1b$ normalisation parameter, which is found to be 1.21 ± 0.15 . The corresponding correlation matrix for the fitted nuisance parameters is also shown, presenting a limited number of nuisance parameters with significant correlations. Nuisance parameter constraints and correlations are in general consistent with those found in the Asimov fit.

The γ factors, describing the per-bin statistical uncertainties, have all value below 0.2%, thus they are pruned away.

A comparison of the distribution of observed and expected yields per analysis region, before and after the fit, can be found in figure 5.34. Figures 5.35, 5.36 and 5.37 show the comparison of the expected NN distribution in each of the regions considered, both pre- and post-fit to blinded data.

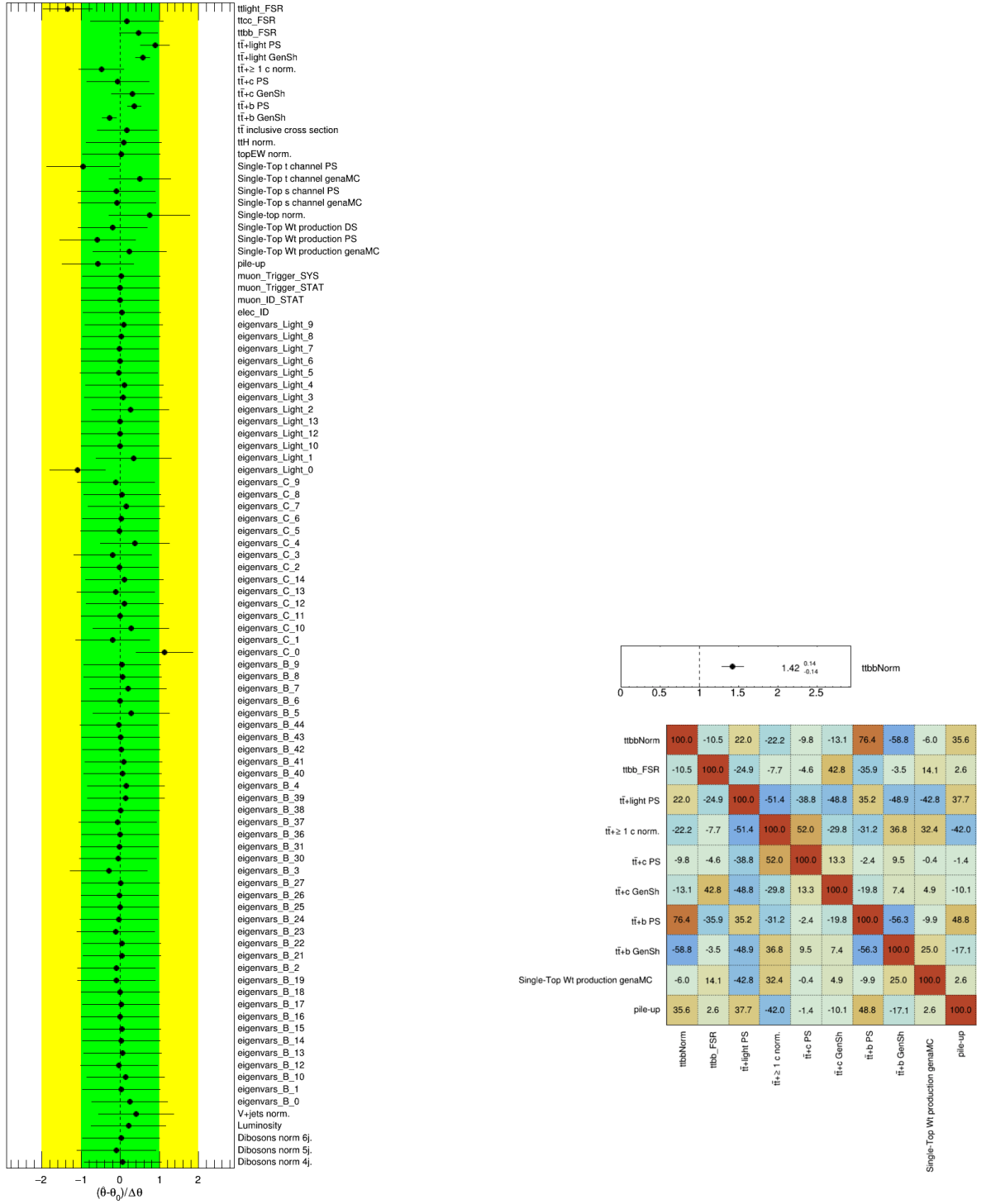


Figure 5.33: Expected fitted nuisance parameters (on the left), normalisation factors (top right) and correlation matrix corresponding to the fit (bottom right) to the blinded data under the background-only hypothesis.

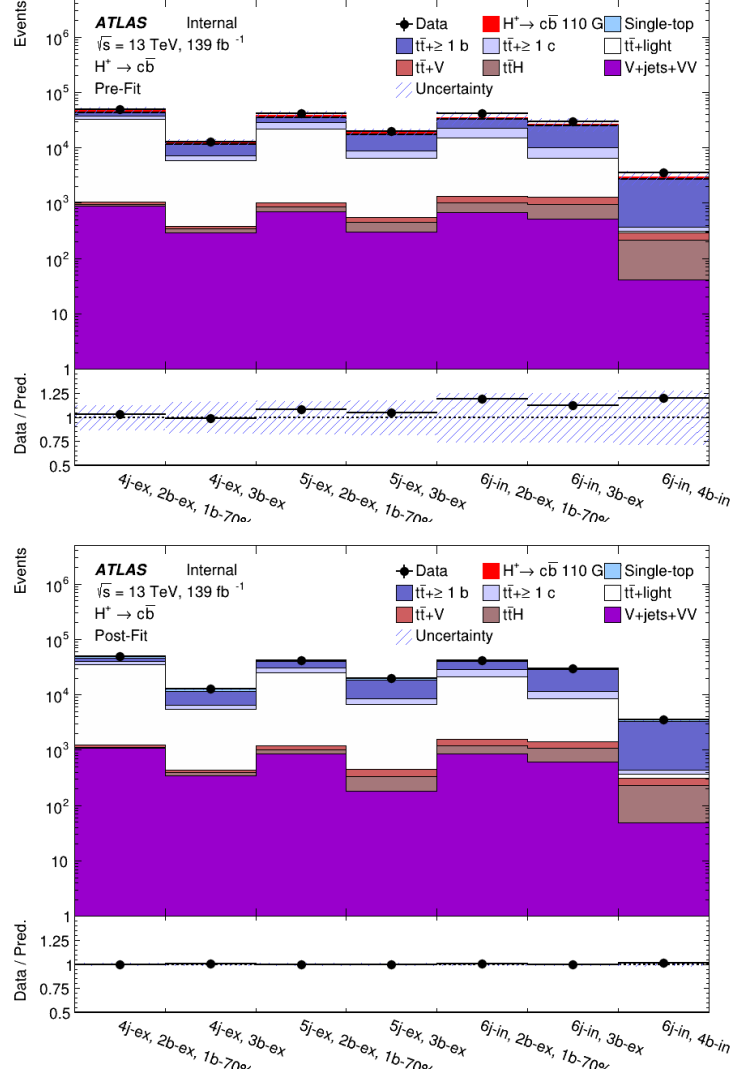


Figure 5.34: Comparison between blinded data and prediction of the yields per analysis region (a) before and (b) after the fit to Asimov data under the background-only hypothesis. In the case of the pre-fit figure, the expected signal from $t \rightarrow H^+ b$ with $m_{H^+} = 110 \text{ GeV}$ (solid red) corresponding to $\mathcal{B}(t \rightarrow H^+ b) = 0.5$ is also shown, added on top of the background prediction. The bottom panel displays the ratio of data to the total prediction (“Pred”), which for the pre-fit plots includes the signal plus the SM background, whereas for the post-fit plots includes only the SM background. The dashed area represents the total uncertainty on the background. In the case of the pre-fit background uncertainty, the normalisation uncertainty on the $t\bar{t} + \geq 1b$ background is not included.

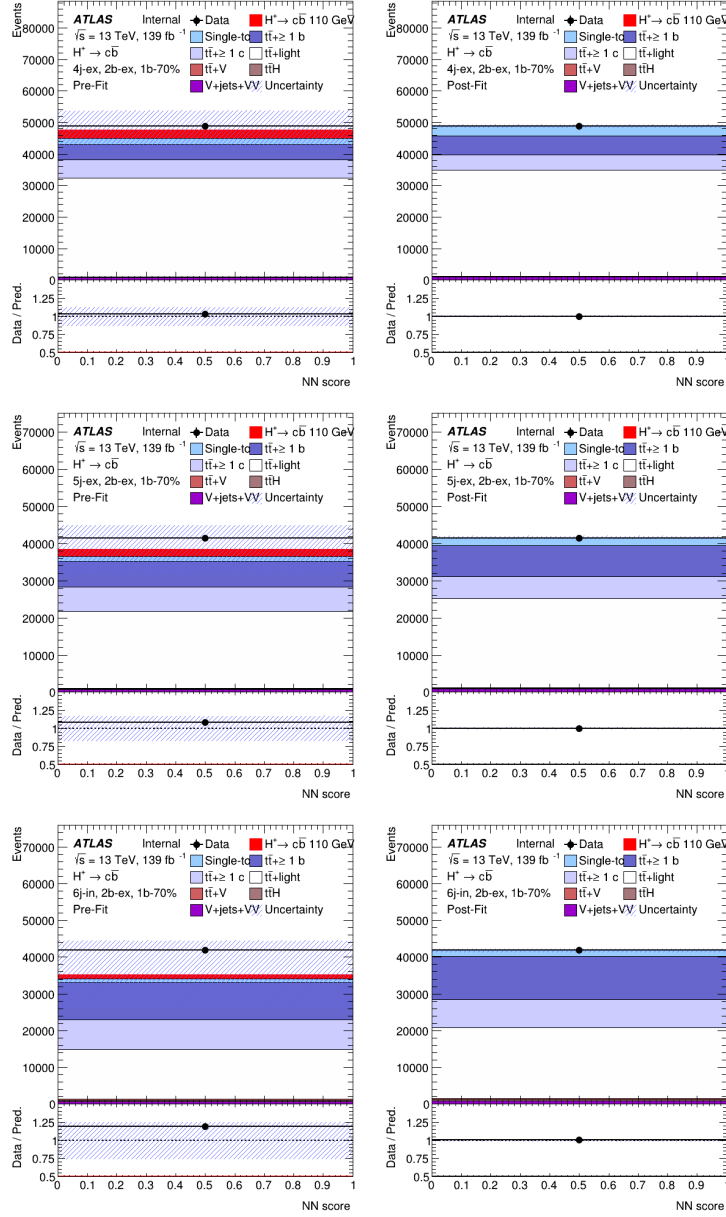


Figure 5.35: Comparison between the blinded data and prediction for the NN distribution in the 2b regions, before and after performing the fit to Asimov data (“Pre-fit” and “Post-fit”, respectively) under the background-only hypothesis. Shown are the (4j, 2b) region (a) pre-fit and (b) post-fit, the (5j, 2b) region (c) pre-fit and (d) post-fit, and the ($\geq 6j$, 2b) region (e) pre-fit and (f) post-fit. In the pre-fit figures the expected signal from $t \rightarrow H^+b$ with $m_{H^+} = 110\text{ GeV}$ (solid red) corresponding to $\mathcal{B}(t \rightarrow H^+b) = 0.5$ is also shown, added on top of the background prediction. The bottom panel displays the ratio of data to the total prediction (“Pred”), which for the pre-fit plots includes the signal plus the SM background, whereas for the post-fit plots includes only the SM background. The dashed area represents the total uncertainty on the background. In the case of the pre-fit background uncertainty, the normalisation uncertainty on the $tt + \geq 1b$ background is not included. Underflow and overflow bins are included respectively in the first and last bins.

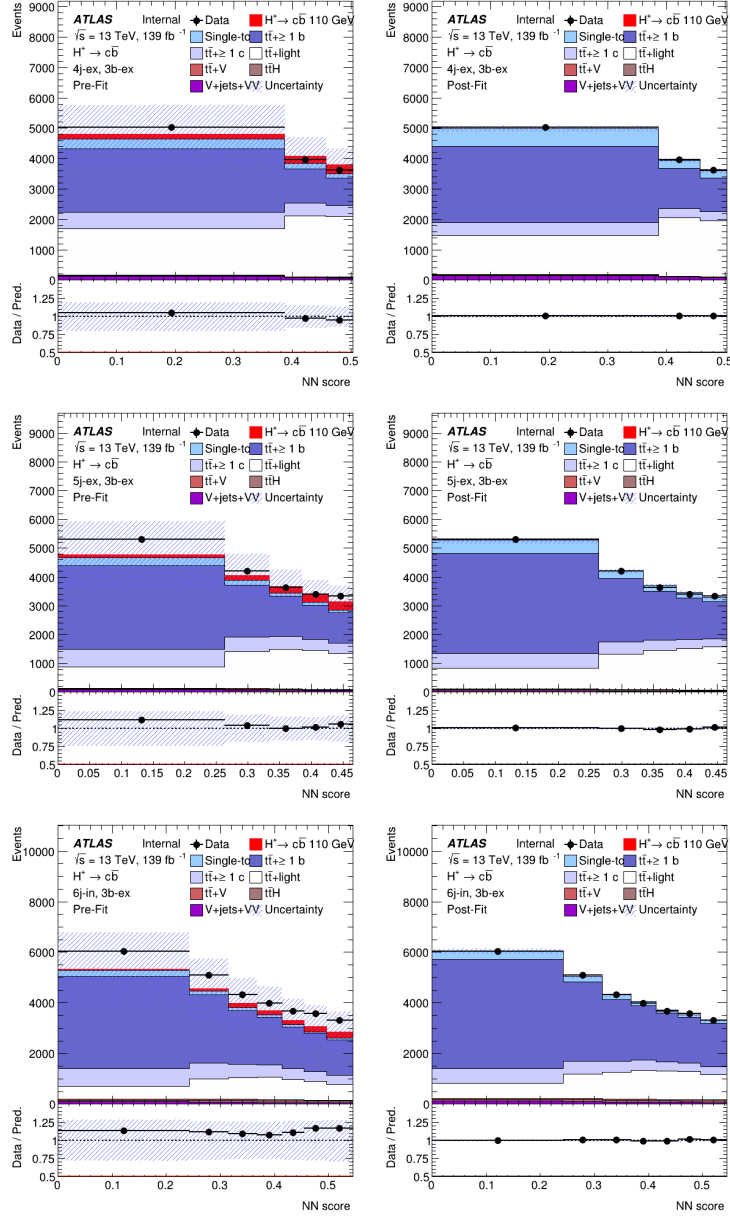


Figure 5.36: Comparison between the blinded data and prediction for the NN distribution in the 3b regions, before and after performing the fit to Asimov data (“Pre-fit” and “Post-fit”, respectively) under the background-only hypothesis. Shown are the (4j, 3b) region (a) pre-fit and (b) post-fit, the (5j, 3b) region (c) pre-fit and (d) post-fit, and the ($\geq 6j$, 3b) region (e) pre-fit and (f) post-fit. In the pre-fit figures the expected signal from $t \rightarrow H^+b$ with $m_{H^+} = 110\text{GeV}$ (solid red) corresponding to $\mathcal{B}(t \rightarrow H^+b) = 0.5$ is also shown, added on top of the background prediction. The bottom panel displays the ratio of data to the total prediction (“Pred”), which for the pre-fit plots includes the signal plus the SM background, whereas for the post-fit plots includes only the SM background. The dashed area represents the total uncertainty on the background. In the case of the pre-fit background uncertainty, the normalisation uncertainty on the $tt + \geq 1b$ background is not included. Underflow and overflow bins are included respectively in the first and last bins.

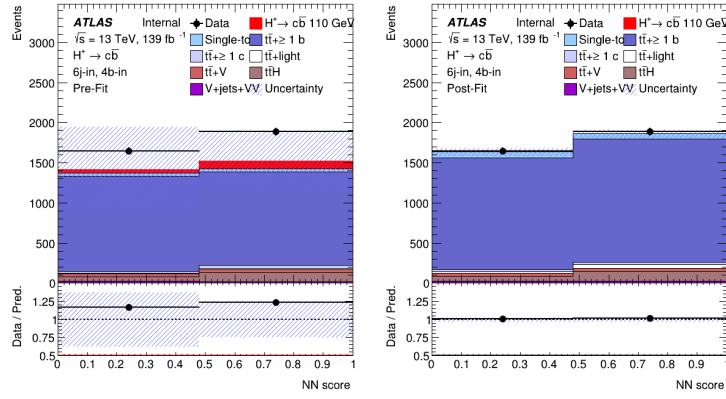


Figure 5.37: Comparison between the blinded data and prediction for the NN distribution in the $\geq 4b$ regions, before and after performing the fit to Asimov data (“Pre-fit” and “Post-fit”, respectively) under the background-only hypothesis. Shown are the (6j, $\geq 4b$) region (a) pre-fit and (b) post-fit. In the pre-fit figures the expected signal from $t \rightarrow H^+b$ with $m_{H^+}=110\text{GeV}$ (solid red) corresponding to $\mathcal{B}(t \rightarrow H^+b) = 0.5$ is also shown, added on top of the background prediction. The bottom panel displays the ratio of data to the total prediction (“Pred”), which for the pre-fit plots includes the signal plus the SM background, whereas for the post-fit plots includes only the SM background. The dashed area represents the total uncertainty on the background. In the case of the pre-fit background uncertainty, the normalisation uncertainty on the $t\bar{t} + \geq 1b$ background is not included. Underflow and overflow bins are included respectively in the first and last bins.

5.7.3 Upper limits

The median expected limits using the background from the Asimov dataset range between about $\mathcal{B}(t \rightarrow H^+b) < 0.065\%$ to $\mathcal{B}(t \rightarrow H^+b) < 0.14\%$ at 95% CL depending on the assumed mass for the charged Higgs boson, m_{H^+} . As expected from signal acceptance loss and limited signal-to-background separation, the exclusion limits become weaker as m_{H^+} approaches the top quark mass. The expected exclusion limits as a function of m_{H^+} are shown in figure 5.38. These expected exclusion limits show already a major improvement compared the best results available from literature [198].

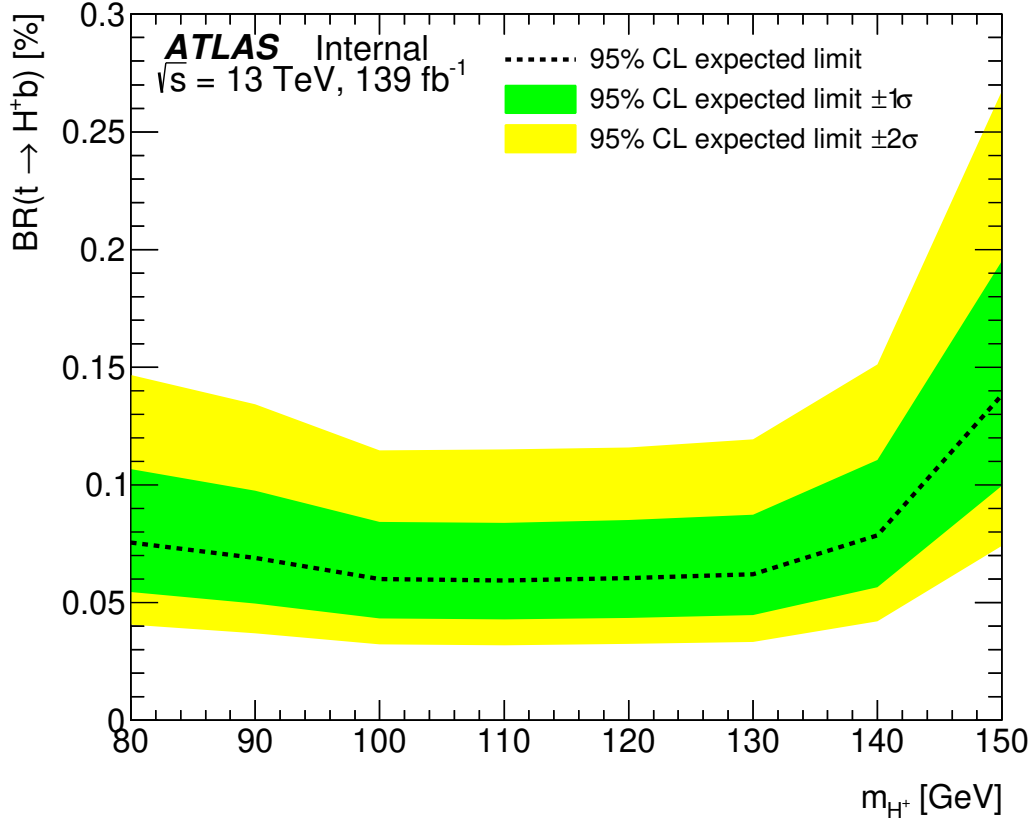


Figure 5.38: Upper limits at the 95% confidence level (CL) on the branching fraction $\mathcal{B}(t \rightarrow H^+b)$, assuming $\mathcal{B}(H^+ \rightarrow cb) = 1.0$, for the combined μ +jets and e +jets channels. The mean expected limit is shown as a black dashed line and the green/yellow bands indicate the 68/95% confidence intervals for the expected limits.

Conclusions

This thesis was carried out within the ATLAS experiment at the LHC complex and it involves a performance development and two searches for new physics.

The first of these three studies describes a novel in-situ method to calibrate jets of different sizes. The energetic pp collisions produced by the LHC yield final states that are predominantly characterised by jets, which have a fundamental role in the different searches and precision measurements. An accurate calibration is thus needed to correct the full four-momenta of each jet. Up to this day, ATLAS has fully-calibrated jets with $R = 0.4$ radius only. The complex calibration procedure is based on a chain of different corrections, first a set of MC-based corrections is applied and then an in-situ correction that measures and corrects the difference in jet response between data and MC simulations. However, it would be possible to use jets with different radii than the standard $R = 0.4$, for instance $R = 0.2$ and $R = 0.6$. These objects are interesting for many analysis since they present characteristics that make them more accurate than the standard ones for certain analysis and interpretations. But unfortunately, these R -scan jets are not fully-calibrated from scratch. So other methods are implemented instead that make benefit of the already fully-calibrated $R = 0.4$ jets to calibrate the ones with smaller and bigger sizes. Chapter 3 of this thesis introduces a new technique to derive an in-situ calibration for R -scan jets based on the fully-calibrated $R = 0.4$ ones.

A description of the MC-based corrections applied to R -scan jets and how they differ from the standard ones is shown, along with some results to illustrate their effects on the jets four-momenta. Then the in-situ “direct matching method” is presented. This technique compares the p_T of an R -scan jet against a fully-calibrated $R = 0.4$ jet (called reference), by geometrically matching an R -scan to a reference jet. Two different topologies are used to derive the in-situ calibrations: dijets and $Z(\mu\mu)$ +jets, in order to cover a wide jet p_T range. These two calibrations are finally statistically combined into a single one. The basic idea is that the ratio between the two jets p_T is computed for data and MC separately, and then an average value is taken from a fit to a gaussian distribution. From the data MC ratio of these average values, a correction factor is determined in terms of p_T and η . Details of the procedure and the results on each topology are given along the chapter. Then, a closure test is performed to verify the correctness of the derived calibration. Finally, the systematic uncertainties are studied to assess their impact on the calibration and they are added to the final results.

The calibrations for $R = 0.2$ and $R = 0.6$ jets presented are derived in MC simulation and in pp collisions collected by the ATLAS detector at a centre-of-mass energy of $\sqrt{s}=13$ TeV during the 2015 and 2016 data taking periods of Run 2.

Afterwards, two searches for Beyond Standard Model (BSM) physics targeting different final states and employing different analysis strategies are described.

The first one is a search for resolved dijet resonances produced in association with a

photon. It is a search for a Dark Matter candidate in a scenario where a dark matter mediator particle interacts with Standard Model particles. A leptophobic axial-vector mediator Z' particle is used as a benchmark model. ATLAS has carried out many dijet searches targeting different and complementary phase space regions. This search focus on the low-mass resonances. Since these are limited by the prescaled triggers used to reduce the high rate of the large multi-jet background, a different approach is needed to reach low mass sectors. This analysis considers the production of a high- p_T initial-state radiation (ISR) object, a photon, against which the new particle recoils. The ISR photon is used for triggering, allowing the resonance to be reconstructed from jets with lower transverse momentum.

Thus the final state is characterised by the presence of two jets and a photon. The signal significance for certain scenarios can be further improved by requiring both jets to be tagged as b -jets. Besides, two different triggers are implemented in order to go lower in mass but not compromising the sensitivity. A single-photon trigger that extends the search below ~ 300 GeV, and a multi-object trigger (combined) that increases the sensitivity where both options are available. So four channels are analysed: the two jet inclusive and the two b -tagged jets, each for both trigger options.

Optimisation studies have been carried out to determine the best event selection, which includes the selection of an accurate signal-background discriminating variable, and the optimal b -tagging configuration that gives the highest sensitivity.

The analysis searches for a localised excess scanning a smoothly falling background distribution, which must be properly fit. In order to achieve the most accurate fit, several studies are performed over non-sensitive samples: MC simulations and a fraction of the data collected during 2015-2017 which has already gave a null-result in a previous version of this same analysis. Given the complexity of the background a sliding window fit (SWiFt) is used, which consists of a background estimation method which looks for localised excesses by sliding over the data spectrum of a given half-width in small, overlapping windows. Several studies were performed to determine the optimal window size and to verify how robust this method was in the presence of signal. All details are given in chapter 4.

Also, a comprehensive study over the systematic uncertainties and their impact on the analysis has been done. Finally, the invariant mass distribution was analysed using a bayesian approach. The search uses $76.6\text{--}79.8\text{ fb}^{-1}$ of LHC pp collisions collected by ATLAS at a centre-of-mass-energy of 13 TeV during 2015-2017 period. Since no evidence of new physics was observed, upper limits at 95% CL were set on the possible number of events from resonant new physics processes on the cross-section times acceptance for new phenomena signal, and a limit on the cross-section times acceptance times efficiency times branching ratio which can be applied to any model which would be approximated by a gaussian signal shape. These limits extend the current ATLAS constraints on dijet resonances to the mass range between 225 and 1100 GeV that was unexplored before, and it was published in [5].

The second analysis is a search for a top-quark decay to a charged Higgs boson and a b -quark. In the BSM context, the existence of an extended Higgs sector is a common prediction in many scenarios. For example models with multiple Higgs doublets, where extended Higgs sectors typically feature additional electrically neutral or charged Higgs bosons. This analysis focus in the scenario where the charged Higgs boson (H^+) is lighter than the top quark, hence it can be produced in rare $t \rightarrow H^+b$ decays. In this mass regime the charged Higgs boson will predominantly decay in a charm quark and a bottom

quark, $H^+ \rightarrow cb$, in a charm quark and a strange quark, $H^+ \rightarrow cs$ or in a tau lepton and a tau neutrino $H^+ \rightarrow \tau\nu$. This search targets the $H^+ \rightarrow c\bar{b}$ decay, where some of these models present higher expected branching ratios.

The analysis searches for top quark pair events in which one top quark decays to Wb , with the W boson decaying leptonically, and the other top quark decays to H^+b . The search is based on pp collisions at $\sqrt{s}=13$ TeV recorded between 2015 and 2018 with the ATLAS detector and uses an integrated luminosity of 139 fb^{-1} . Data are analysed in the lepton-plus-jets final state, characterised by an isolated electron or muon and at least four jets plus missing transverse energy. The search exploits the high multiplicity of b -quark jets characteristic of signal events, and defines several analysis regions based on the number of jets and b -jets. This categorisation procedure increases the sensitivity of the search, and helps disentangle more clearly the different background components, which is useful to further constraint/pull the related systematic uncertainties. Afterwards, a profile-likelihood fit is performed over these regions. Signal-to-background discrimination is achieved by means of a neural network classifier which incorporates kinematic and jets flavour information. The neural network is trained simultaneously on all signal benchmarks with a signal label as training feature. A detail description is given in chapter 5.

Finally, the discriminant distributions from each of the regions are combined to test for the presence of signal. A test statistic involving profile likelihood ratios was defined for this, which takes into account the effect of the different systematic uncertainties. The test was performed over Asimov and blinded data under the background-only-hypothesis. Due to some constraints and throwbacks that we have experienced along the working process, data could not be unblinded by the time this thesis was written. So all the results shown in chapter 5 are preliminar. When the time comes, datasets from 2015 to 2018 will be used resulting in a total integrated luminosity of 138.9 fb^{-1} . We expect to get the final results by mid-year. So for now, only expected 95% CL upper limits were placed on $t \rightarrow H^+b$ branching ratio as a function of the mass of the charged Higgs boson, ranging between 80 to 160 GeV, assuming $\mathcal{B}(H^+ \rightarrow c\bar{b}) = 1.0$.

Appendix A

In-situ calibration for R -scan jets

A.1 Statistical combination for the in-situ calibration for R -scan jets

Given the consistency of the calibration results obtained in the dijet and Z +jet topologies from section 3.2.3 as shown in figures 3.12, the two sets of calibration results can be statistically combined into a single calibration, to reduce the uncertainty and to maximise the domain of the jet calibration.

The statistical combination of calibration results is based on the JES in situ combination method described in ref.[274]. It allows combining an arbitrary number of p_T -dependent calibrations, correctly propagating all the uncertainties and correlations, while minimising the bias and the overall uncertainty. The steps of this p_T -dependent combination are:

1. Interpolate the input data to a common, fine binning.
2. Average the contributions of the different measurements to each bin, weighting each measurement based on the full variance, i.e., considering statistical and systematic uncertainties.
As expected, the relative contribution from the Z +jet topology dominates at low p_T , while for $p_T \gtrsim 100$ GeV the dijet topology takes over.
3. Propagate statistical and systematic uncertainties by repeating the above steps for a large number of pseudo-experiments, drawn according to the known uncertainties and correlations of the inputs.
4. In cases where a measurement deviates significantly ($\chi^2/n_{\text{d.o.f.}} > 1$) from the average, rescale the uncertainties to larger values so that $\chi^2/n_{\text{d.o.f.}} = 1$ is obtained per construction.
5. Smooth the resulting calibration factor distributions as a function of (p_T, η) using a sliding window Gaussian smearing, to reduce the impact of statistical bin-to-bin fluctuations.

The combination method from ref.[274] described above is defined as a function of p_T . To adapt it to the p_T - and η dependent R -scan in situ JES calibrations, additional steps are required before the ones listed above:

1. The distributions of the relative impact of the systematic variations are rebinned in η to match the finer η binning of the nominal calibration. This is done by splitting the bins, but keeping the values unchanged.
2. The distributions of the relative impact of the systematic variations are extended at low and high p_T to match the p_T range of the nominal calibration. This is done through freezing, i.e., by assigning the relative impact of the lowest (highest) p_T bin with known impacts to each p_T bin below (above) the lowest (highest) bin, separately in each η bin.

After multiplexing the inputs into the 60 fine η bins, the two contributions from Z +jet and dijet samples are then combined using the standard p_T -dependent combination from ref [274]. This combination is performed separately for each of the 60 η bins in the inputs.

To consistently treat the additional η dependence of the calibration factors, the combined result needs further post-processing:

1. The 60 p_T independent calibrations for the 60 η bins are concatenated into a single (p_T, η) dependent distribution.
2. The concatenated distribution is smoothed by folding it with a two-dimensional Gaussian distribution. A detailed description of the parametrization of this smoothing is given in the appendix A.1.1;
3. The smoothed distribution is frozen, meaning it is extended by filling with the last derived calibration value such that the calibrated domain is a rectangle in η, p_T space.

The resulting combined calibration is compared to the input calibrations using dijet and Z +jet topologies for representative η bins in figure A.1, along with the respective uncertainties. The combined results are found to be consistent with the input calibrations. The central values of the combined calibration factors remain within a few percent of unity. The resulting uncertainties on the combined result, as propagated from the inputs, are typically within a fraction of a percent in the bulk of the distribution, increasing to a couple of percent towards low and high p_T . The uncertainties are discussed in detail in appendix A.1.2.

The final combined calibration as a function of (p_T, η) is shown in figure A.2.

The results discussed in here as well as in appendices A.1.2 and A.1.1 were arrived at using the `rscaninsitucombi` package [275].

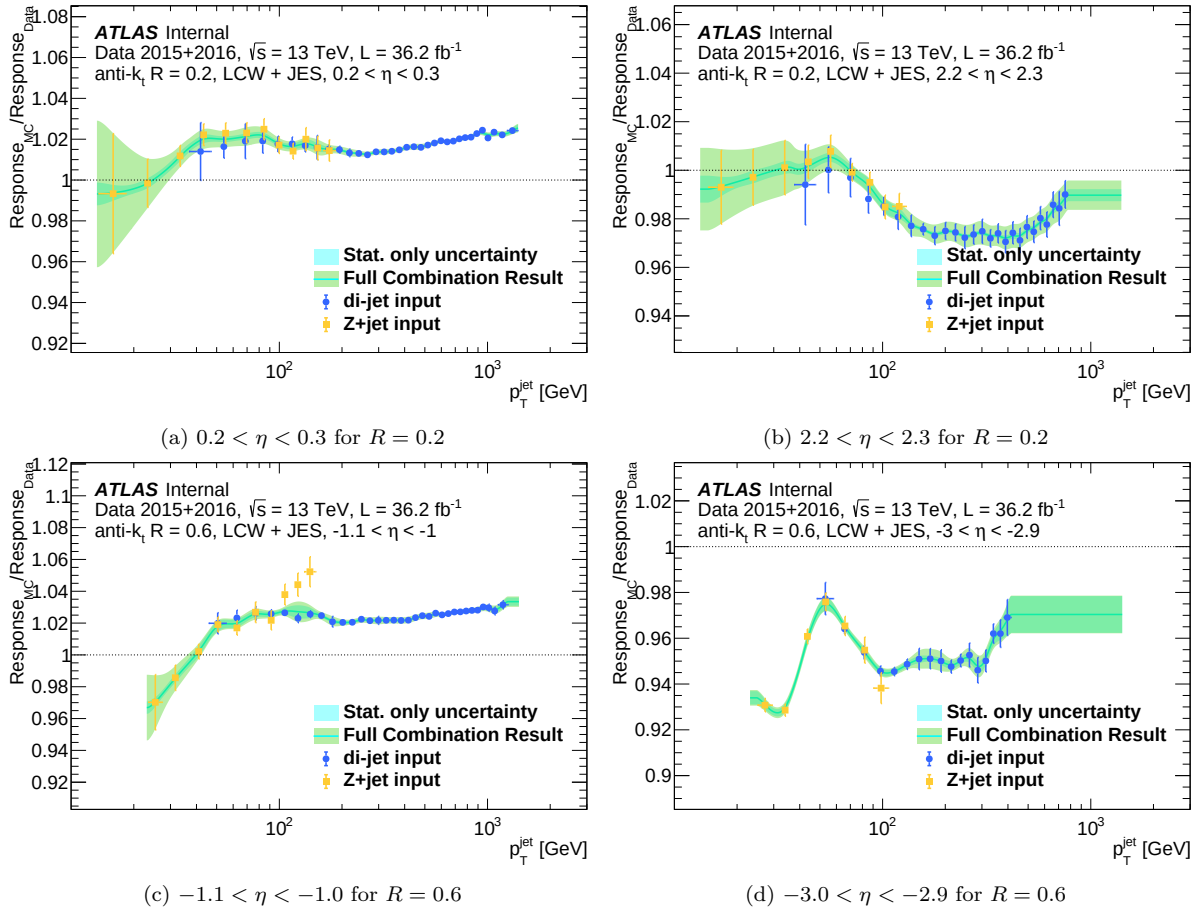


Figure A.1: Combined in situ calibration compared to individual inputs, for $R = 0.2$ and $R = 0.6$ R -scan jets, in selected η bins.

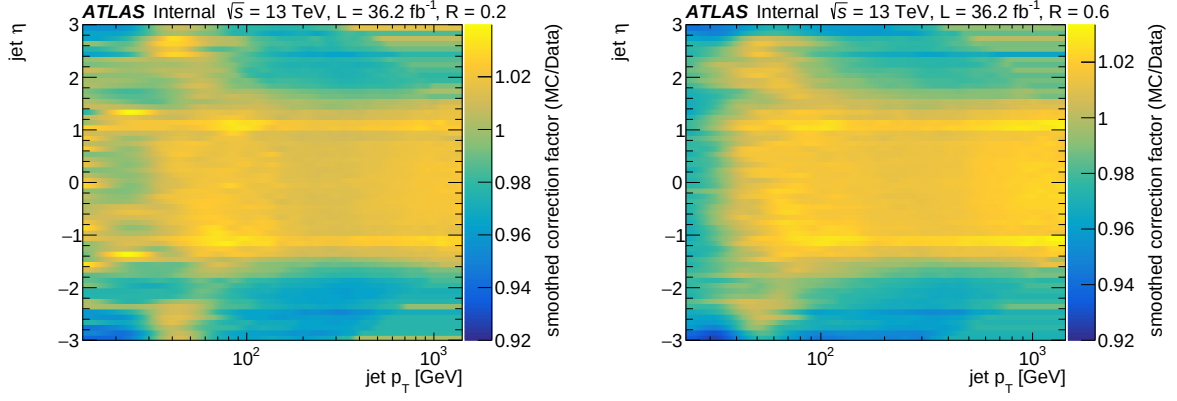


Figure A.2: Smoothed combined insitu calibration for $R = 0.2$ and $R = 0.6$ R -scan jets.

A.1.1 Smoothing kernel optimization for the statistical combination

The two-dimensional smoothing of the statistical combination result in η and p_T is implemented through folding the output distribution with a kernel¹

$$f_{\text{kernel}}(p_T^0, p_T^1, \eta^0, \eta^1) \propto e^{-\Lambda(p_T^0, p_T^1, \eta^0, \eta^1)^2/2}, \quad (\text{A.1})$$

where (p_T^0, η^0) is the point being smoothed, and (p_T^1, η^1) is the point integrated out in the folding, and the rescaled η, p_T distance $\Lambda(p_T^0, p_T^1, \eta^0, \eta^1)$ is defined by

$$\Lambda(p_T^0, p_T^1, \eta^0, \eta^1)^2 = \left(\frac{\Delta p_T}{p_T^0 \times \sigma_{p_T}} \right)^2 + \left(\frac{\Delta \eta}{\sigma_\eta} \right)^2, \quad (\text{A.2})$$

where $\Delta p_T = p_T^0 - p_T^1$ and $\Delta \eta = \eta^0 - \eta^1$.

The kernel sizes σ_{p_T} and σ_η are free parameters of the smoothing, which control the strength of the smoothing. σ_{p_T} is dimensionless, since the p_T -only distance Δp_T is rescaled by the p_T of the point being smoothed. Locally (i.e. for any given point being smoothed) the smoothing kernel appears like a gaussian with widths $\sigma_{p_T} \times p_T^0$, σ_η . The size of the kernel in the p_T dimension scales with the p_T of the point being smoothed, fixing the relative width of the kernel. This is appropriate because the calibration spans several orders of magnitude in p_T .

To better be able to judge the size of the effect of a smoothing kernel choice, it is useful to consider the local significance of the smoothed- w.r.t. the not-smoothed distribution

$$\chi(p_T, \eta) = \frac{|\text{residual}(p_T, \eta)|}{\text{stat. uncertainty}(p_T, \eta)} = \frac{|\text{smoothed}(p_T, \eta) - \text{original}(p_T, \eta)|}{\text{stat. uncertainty}(p_T, \eta)}, \quad (\text{A.3})$$

The use of the statistical uncertainty in the significance definition is motivated by the idea that the smoothing procedure aims to reduce statistical fluctuations of the combined calibration result. Shape changes compatible with known nuisance parameters should instead be fitted to account for their likelihoods. In general, larger values of σ_{p_T} (σ_η) more strongly smooth the distribution along the p_T (η) axis.

¹normalised such that the integral of the kernel over the smoothed domain is unity

To choose the size of the smoothing kernel to use for smoothing the statistical combination result, a wide range of kernel sizes is scanned, and the smoothing strength evaluated. The smoothing strength is evaluated using the target function

$$f_{\text{target}} = \left(1 - \frac{\chi^2}{n_{\text{d.o.f.}}}\right)^2 + \left(1 - \frac{n_{\text{d.o.f.}}}{\chi^2}\right)^2, \quad (\text{A.4})$$

where χ^2 is the squared sum of the residual distribution over all points, and $n_{\text{d.o.f.}}$ is the number of points. This target function is constructed to have a root where $\chi^2 = n_{\text{d.o.f.}}$, which for large values of $n_{\text{d.o.f.}}$ indicates that the observed residual matches the variance expected for $n_{\text{d.o.f.}}$ independent normal-distributed random variables. The motivation for the smoothing is to reduce the effect of expected random fluctuations on the calibration curve, so $f_{\text{target}} = 0$ indicates that the smoothing is neither too strong nor too weak. The target function is used for this, instead of just $\chi^2/n_{\text{d.o.f.}}$ directly, because the target function maps too weak smoothing and too strong smoothing to similar values in $(0, \infty)$, whereas $\chi^2/n_{\text{d.o.f.}}$ maps too weak smoothing to $[0, 1)$, but too strong smoothing to $(1, \infty)$.

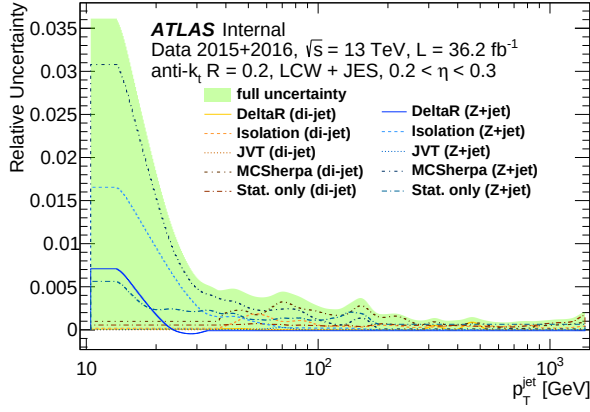
The optimal relative kernel size in p_T is $\sigma_{p_T} = 0.045$ for both jet calibrations studied. The optimal kernel size in η is $\sigma_\eta = 0.035$ for $R = 0.2$ R -scan jets, but $\sigma_\eta = 0.03$ for $R = 0.6$ R -scan jets.

A.1.2 Uncertainties after statistical combination

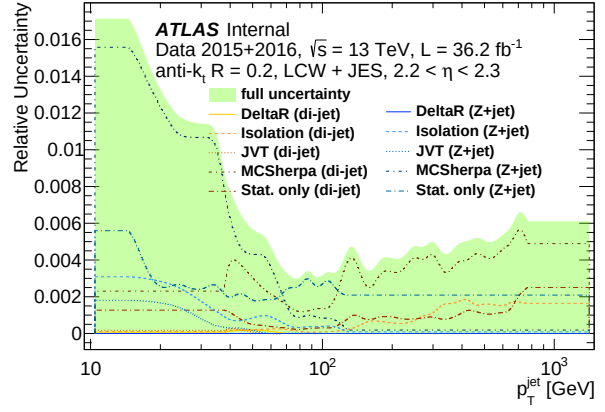
The uncertainties on the final in-situ calibrations are propagated as described in appendix A.1. The 2D processing steps applied to the nominal calibration (concatenation to 2D, smoothing, freezing to rectangular domain) are applied to the systematic uncertainties as well, in the same way as is done for the nominal calibration.

For the statistical uncertainties, two output variants are prepared. In one, the per bin statistical uncertainties are simply read out and saved as separate nuisance parameters. In the other, the per-bin statistical uncertainties of Z +jet and dijet are quadratically summed into one global statistical uncertainty component due to the Z +jet samples, and another one due to the dijet samples. These two sums are then smoothed and frozen in the same way as the nominal calibration and systematic variation impact distributions are.

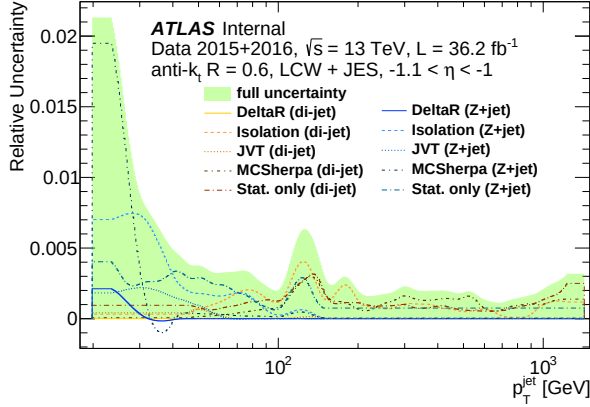
The impact of all uncertainties on the calibration, and their contribution to the full uncertainty on the calibration, are shown in figure A.3 for selected η bins and for both R -scan jets. The full combined uncertainty on the calibration is shown in figure A.4.



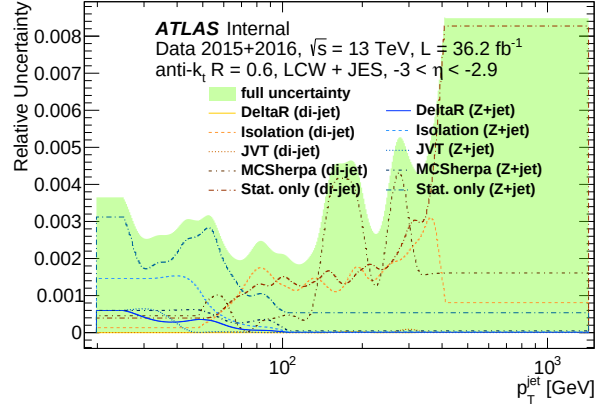
(a) $0.2 < \eta < 0.3$ for $R = 0.2$



(b) $2.2 < \eta < 2.3$ for $R = 0.2$



(c) $-1.1 < \eta < -1.0$ for $R = 0.6$



(d) $-3.0 < \eta < -2.9$ for $R = 0.6$

Figure A.3: Uncertainties affecting the combined calibration (lines), and their quadratic sum (filled area), for $R = 0.2$ and $R = 0.6$ anti- k_t jets, in selected η bins. The individual contributions are smoothed and frozen prior to their inclusion in the quadratic sum.

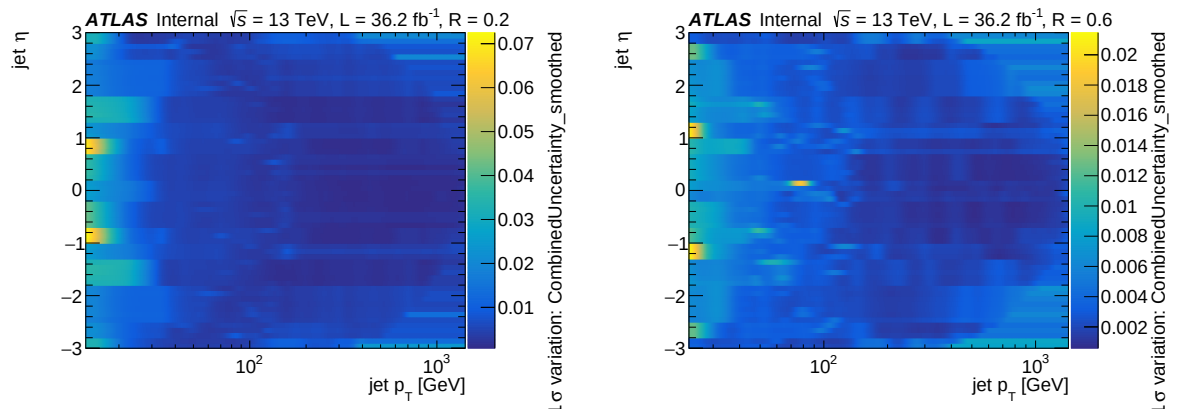


Figure A.4: Full uncertainty on the combined insitu calibration for $R = 0.2$ and $R = 0.6$ anti- k_t jets.

Appendix B

Search for resolved dijet resonances produced in association with a photon

B.1 Event selection: cutflows

Cutflows for the different samples after the final event selection is applied (see section 4.2.4) are shown next. Table B.1 shows these values for data samples, while B.2 shows the MC values. In tables B.3 and B.4 these values are shown for two samples of simulated Z' generated with different masses. In each case the initial number of events is shown along with the remaining number of events after each particular selection for the single-photon and the combined trigger selection and the two selections.

Criterion	Single photon trigger		Combined trigger	
	Events remaining	% remaining	Events remaining	% remaining
Trigger	202639180	–	76850212	–
Cleaning	202302890	100%	76743740	100%
$n_{jets} \geq 2$	193205510	96%	75005508	98%
$n_\gamma \geq 1$	44098255	23%	37211972	50%
Lead γ p_T	11575203	26%	22090737	59%
Lead jet p_T	11575203	100%	20837871	94%
Sublead jet p_T	11575203	100%	13013218	62%
$ y^* < 0.75$	7369609	64%	8031090	62%
Minimum m_{jj}	2522549	34%	1520114	19%
b -tagging	15557	0.62%	9015	0.59%

Table B.1: Selections placed on the data samples after pre-selection requirements and the numbers of events that satisfy each successive requirement. The percentages of remaining events are calculated relative to the previous line. The initial number of events for the combined trigger is smaller than for the single-photon trigger because no combined trigger existed for the portion of the data collected in 2015.

Criterion	Single photon trigger		Combined trigger	
	Events remaining	% remaining	Events remaining	% remaining
Trigger	233150 ± 120	–	310130 ± 220	–
Cleaning	232940 ± 120	100%	309820 ± 220	100%
$n_{jets} \geq 2$	174280 ± 110	75%	297140 ± 210	96%
$n_\gamma \geq 1$	135008 ± 91	77%	255080 ± 190	86%
Lead γ p_T	98202 ± 48	73%	176590 ± 130	69%
Lead jet p_T	98202 ± 48	100%	166010 ± 120	94%
Sublead jet p_T	98202 ± 48	100%	102350 ± 100	62%
$ y^* < 0.75$	59955 ± 35	61%	60290 ± 74	59%
Minimum m_{jj}	19741 ± 17	33%	11149 ± 31	18%
b -tagging	106.0 ± 1.9	0.54%	56.6 ± 2.6	0.51%

Table B.2: Selections placed on the samples of simulated background events after pre-selection requirements and the numbers of events that satisfy each successive requirement. Uncertainties reported are statistical uncertainties only. The percentages of remaining events are calculated relative to the previous line. The samples consist of multijet + γ processes, simulated as described in 4.1, with the total event yield normalised to 1 fb^{-1} of integrated luminosity.

Criterion	Single photon trigger		Combined trigger	
	Events remaining	% remaining	Events remaining	% remaining
Trigger	222.8 ± 2.4	–	322.5 ± 2.9	–
Cleaning	222.6 ± 2.4	100%	322.3 ± 2.9	100%
$n_{jets} \geq 2$	207.1 ± 2.3	93%	313.4 ± 2.8	97%
$n_\gamma \geq 1$	176.7 ± 2.1	85%	289.6 ± 2.7	92%
Lead γ p_T	143.8 ± 1.9	81%	284.2 ± 2.7	98%
Lead jet p_T	143.8 ± 1.9	100%	280.1 ± 2.7	99%
Sublead jet p_T	143.8 ± 1.9	100%	219.3 ± 2.4	78%
$ y^* < 0.75$	108.4 ± 1.7	75%	177.3 ± 2.1	81%
Minimum m_{jj}	81.5 ± 1.4	75%	5.83 ± 0.39	3.3%
b -tagging	7.01 ± 0.41	8.6%	0.048 ± 0.034	0.82%

Table B.3: Selections placed on the samples of simulated Z' events where $m_{Z'} = 250 \text{ GeV}$ and $g_q = 0.2$, after pre-selections are applied. Also shown are the numbers of events that satisfy each successive requirement. Uncertainties reported are statistical uncertainties only. The percentages of remaining events are calculated relative to the previous line.

Criterion	Single photon trigger		Combined trigger	
	Events remaining	% remaining	Events remaining	% remaining
Trigger	68.22 ± 0.65	–	101.10 ± 0.79	–
Cleaning	68.17 ± 0.65	100%	101.01 ± 0.79	100%
$n_{jets} \geq 2$	66.36 ± 0.64	97%	99.75 ± 0.79	99%
$n_\gamma \geq 1$	56.32 ± 0.59	85%	90.88 ± 0.75	91%
Lead γ p_T	46.48 ± 0.54	83%	88.60 ± 0.74	97%
Lead jet p_T	46.48 ± 0.54	100%	88.42 ± 0.74	100%
Sublead jet p_T	46.48 ± 0.54	100%	83.80 ± 0.72	95%
$ y^* < 0.75$	31.55 ± 0.44	68%	58.50 ± 0.60	70%
Minimum m_{jj}	29.19 ± 0.43	93%	49.57 ± 0.56	85%
b -tagging	2.43 ± 0.12	8.3%	4.52 ± 0.16	9.1%

Table B.4: Selections placed on the samples of simulated Z' events where $m_{Z'} = 550 \text{ GeV}$ and $g_q = 0.2$, after pre-selection requirements are applied. Also shown are the numbers of events that satisfy each successive requirement. Uncertainties reported are statistical uncertainties only. The percentages of remaining events are calculated relative to the previous line.

B.2 Kinematic checks

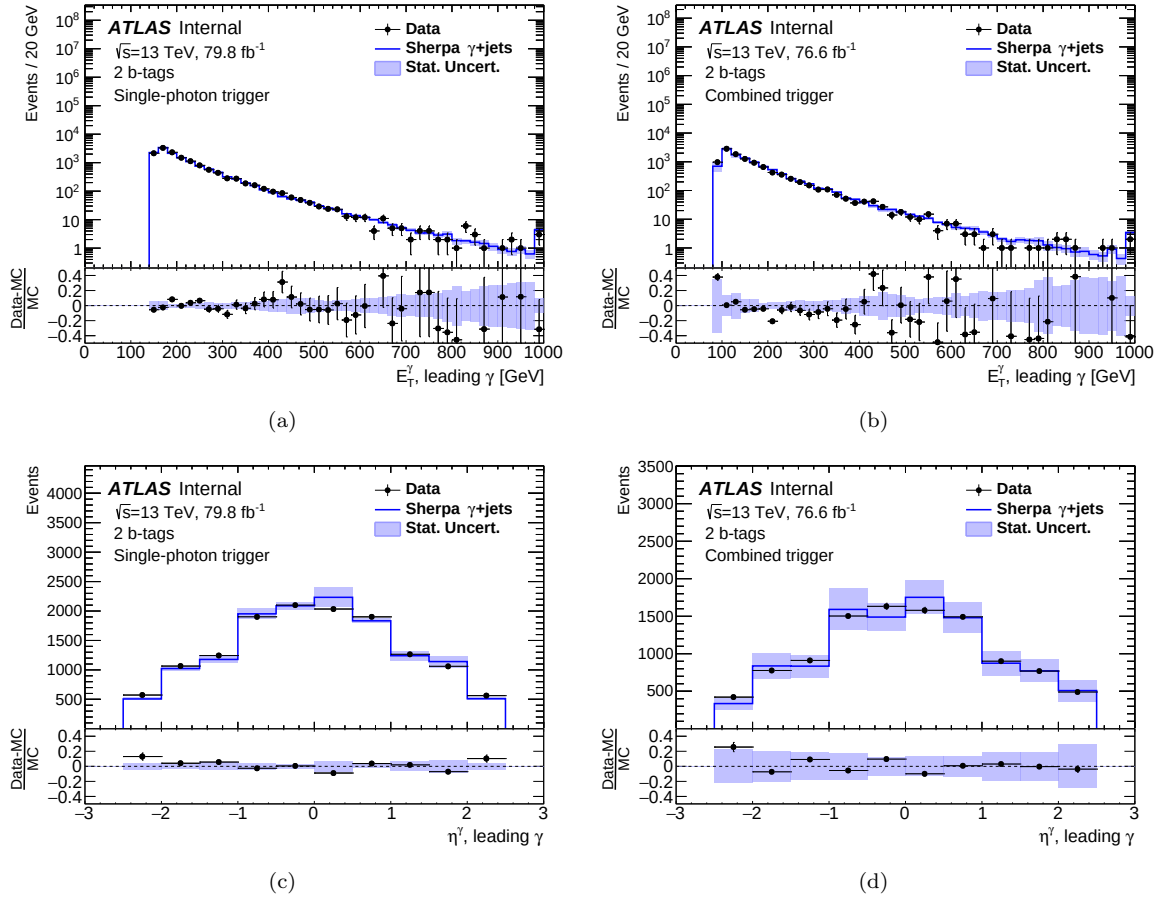


Figure B.1: Comparisons of data to MC for the photon p_T and η distributions of the 2 b -tagged categories. Figs.(a) and (c) show the single-photon-trigger data while (b) and (d) show the combined-trigger data.

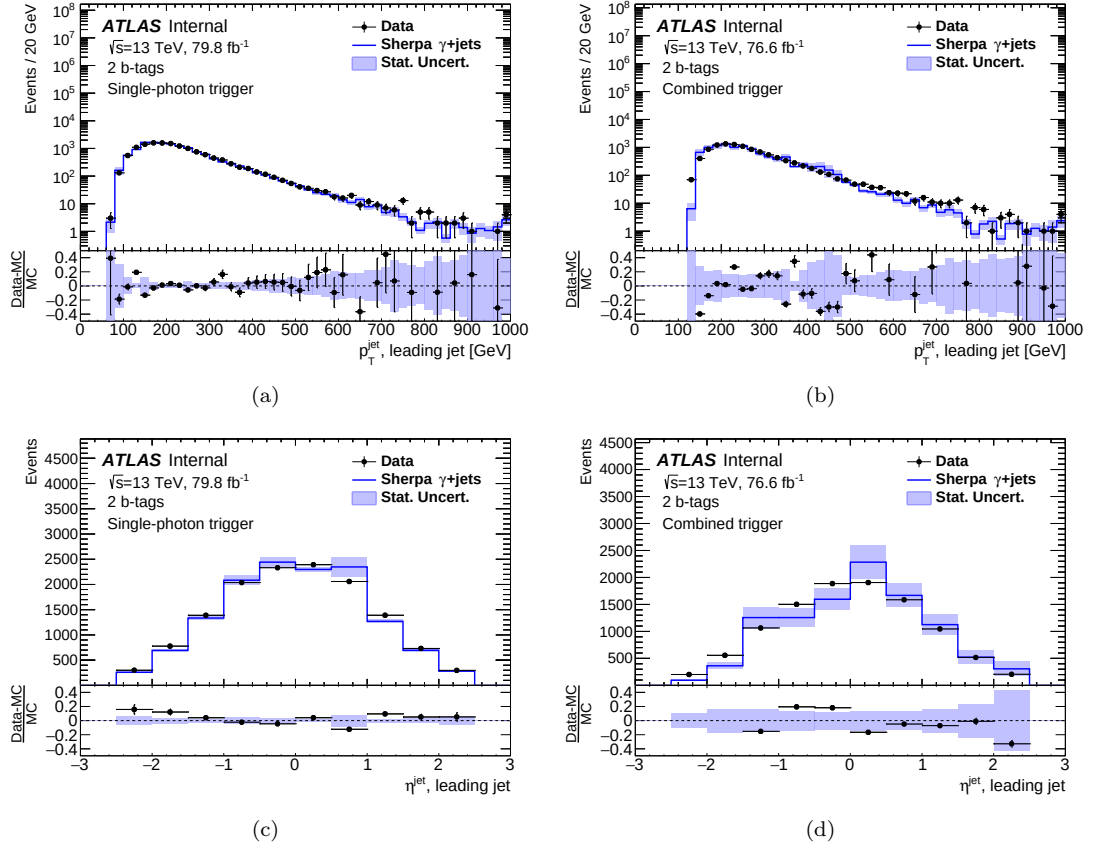


Figure B.2: Comparisons of data to MC for the distributions of p_T and η of the highest- p_T jet in the 2 b -tagged categories. Figs.(a) and (c) use the single-photon trigger while (b) and (d) use the combined trigger.

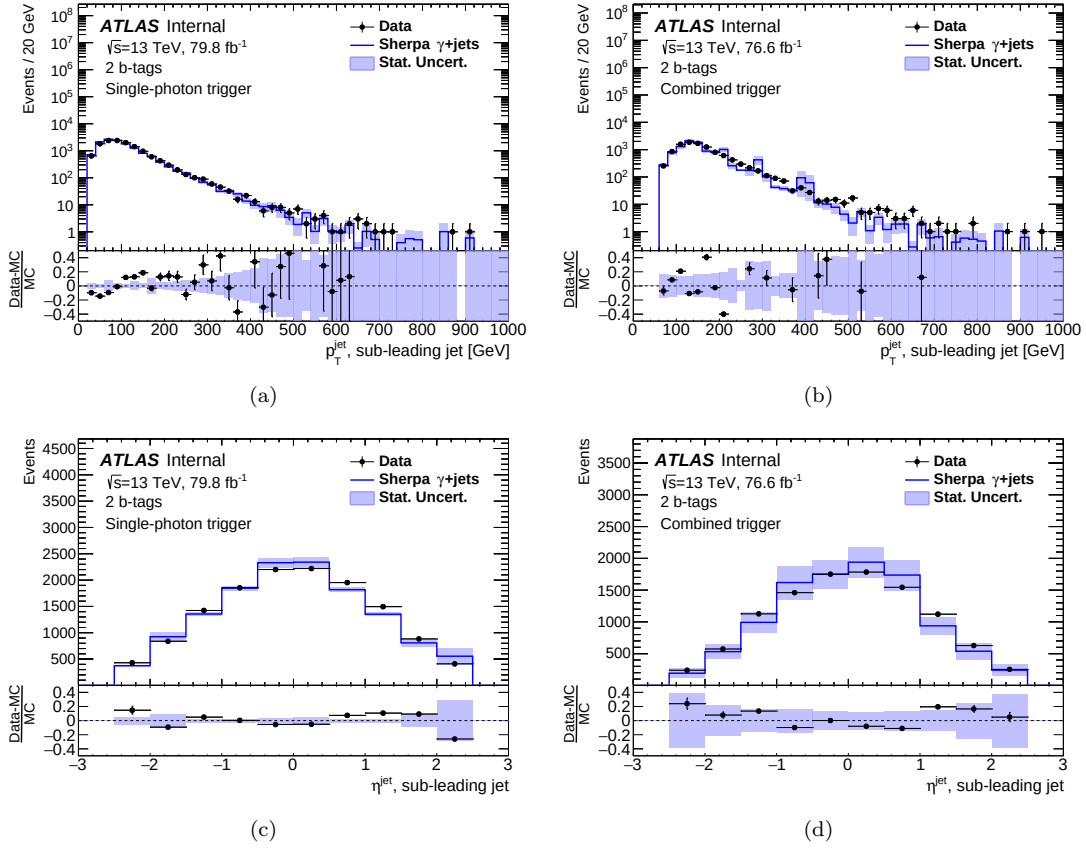


Figure B.3: Comparisons of data to MC for the distributions of p_T and η of the second-highest- p_T jet for the 2 b -tagged categories. Figs.(a) and (c) show the single-photon-trigger data while (b) and (d) show the combined-trigger data.

B.3 Signal modelling

All signal MC samples used in the analysis are plotted in figures B.4 through B.6. These show the peak visible in m_{jj} for each sample at the reconstructed level after passing all analysis cuts. The three figures show three different g_q coupling values for the Z' model. A Bukin fit [276] is performed to each peak to determine its width, and the results are found to range from around 13% for the lowest masses to 8% for the narrowest and highest masses. As all of these are within 15% width to mass ratio, this benchmark is appropriate for this fitting and bump-hunt based search.

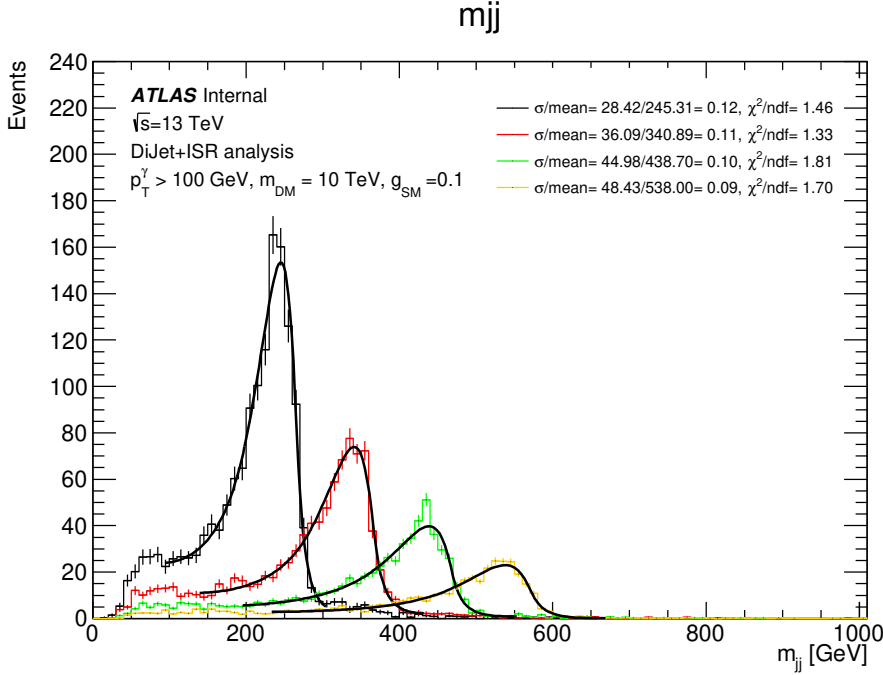


Figure B.4: Fits to signal masses in simulated Z' samples with $g_q = 0.1$. The signals have nominal masses of 250, 350, 450, and 550 GeV from left to right.

The cross sections for the Z' benchmark signal samples are shown in units of picobarns in figure B.7. As the figure makes clear, smaller coupling values of the signal to standard model quarks equate to a smaller cross-section for the simulated process, $pp \rightarrow Z' + \gamma \rightarrow qq\gamma$.

The number of signal events due to a new process of cross-section times k -factor times filter efficiency σ and branching ratio BR which would be expected in the dataset can be computed as follows:

$$N_{sig} = \mathcal{L} \cdot \sigma \cdot \text{BR} \cdot A \cdot \epsilon. \quad (\text{B.1})$$

As this shows, the relevant efficiencies and acceptances must be taken into account in order to correctly assess the amount of signal expected for a model with a given cross-section. The relevant factors which affect this analysis are as follows:

- **Kinematic acceptance** Fraction of events at truth level which pass analysis selection cuts, $a_{\text{kin}} = n_{\text{truth}}/n_{\text{tot}}$

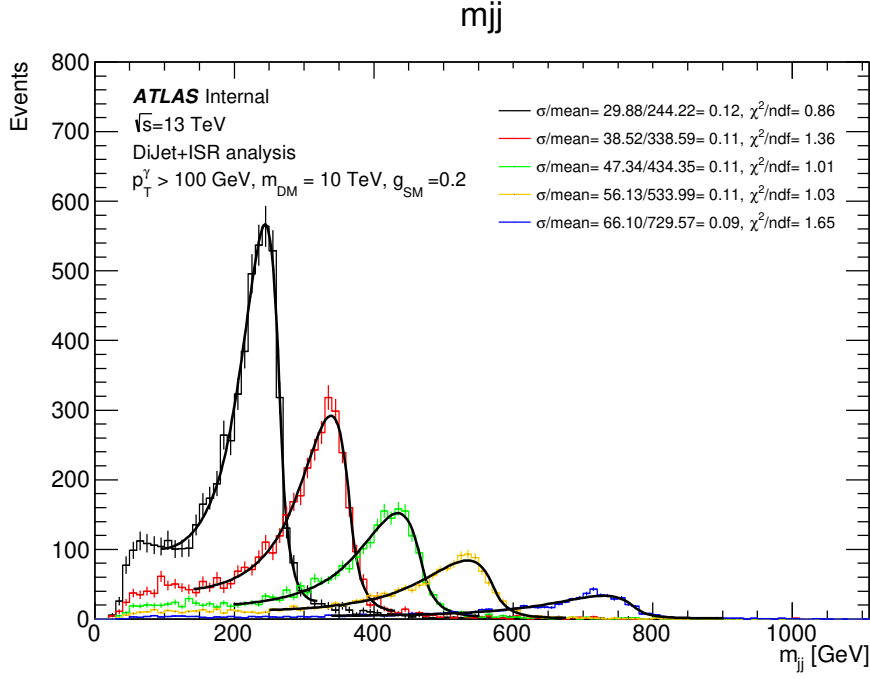


Figure B.5: Fits to signal masses in simulated Z' samples with $g_q = 0.2$. The signals have nominal masses of 250, 350, 450, 550, and 750 GeV from left to right.

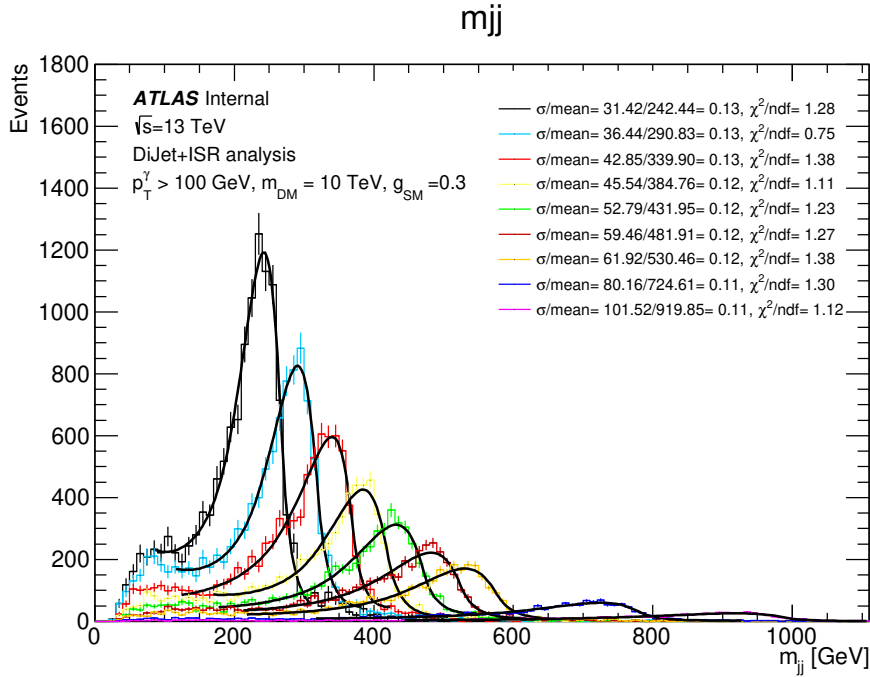


Figure B.6: Fits to signal masses in simulated Z' samples with $g_q = 0.3$. The signals have nominal masses of 250, 300, 350, 400, 450, 500, 550, 750, and 950 GeV from left to right.

- **Photon efficiency** Efficiency of photon identification and reconstruction. This factor is included in the reco-level efficiency.
- **Jet efficiency** Efficiency of jet reconstruction. This is 1 in ATLAS for all practical

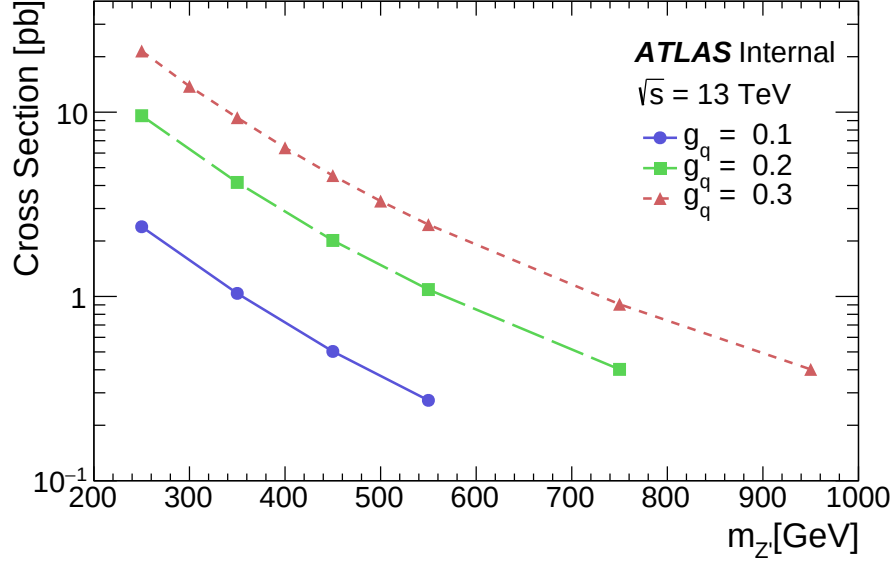


Figure B.7: Cross-sections of Z' benchmark model for all coupling values used in the analysis. Values displayed are in picobarns.

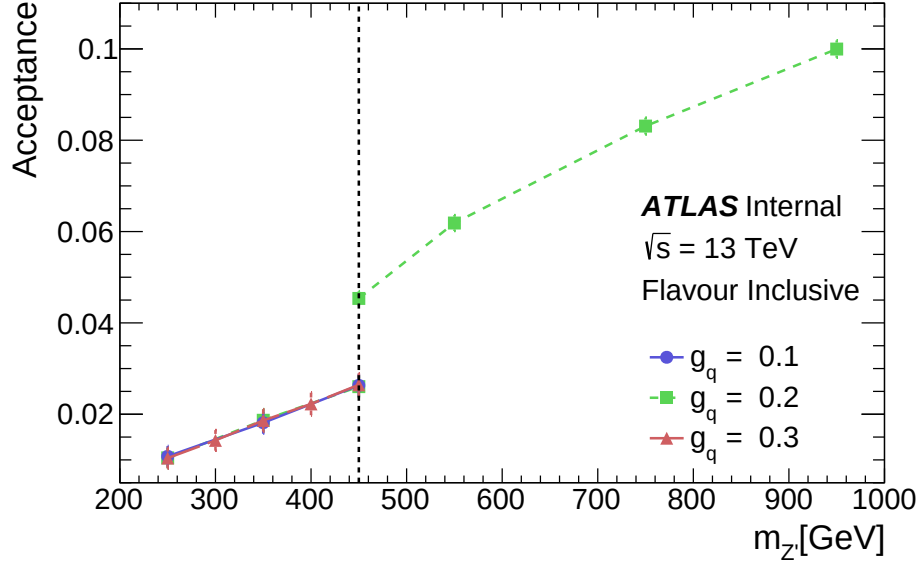
purposes.

- **b -tagging efficiency** Number of jets surviving the b -tagging process. This is a function of both tagging efficiency for real b -jets and mistag rate for light and c -jets, and is included in the reco-level efficiency.
- **Trigger efficiency** Efficiency of the photon reconstruction in the trigger. This factor is included in the reco-level efficiency.

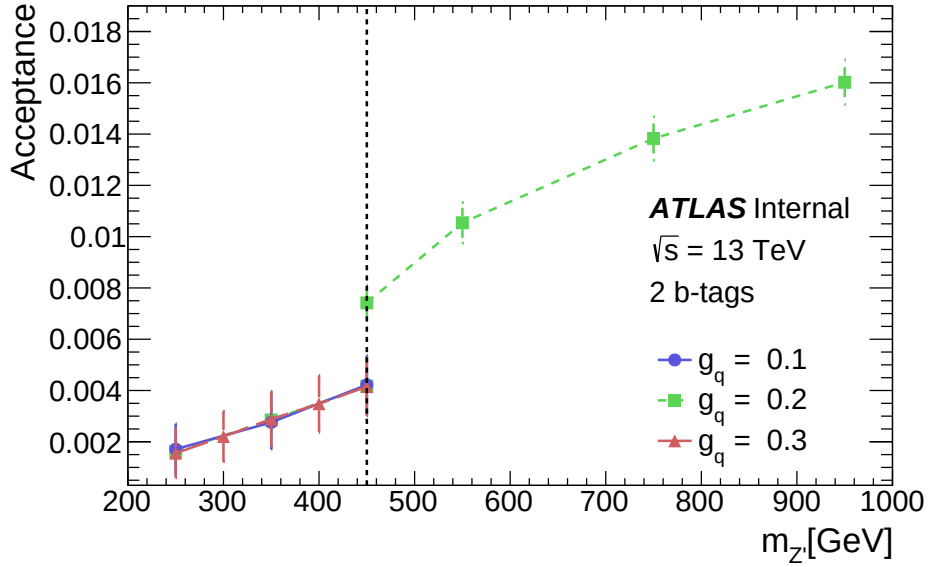
These do not need to be computed individually, but can in fact be measured as two quantities, a single fiducial acceptance and a single efficiency per signal point and channel. The acceptance is measured by finding the fraction of events which pass the kinematic analysis selection cuts (that is, excluding trigger requirement) at truth level. But the acceptances of the single photon trigger selection and compound trigger selection can't be directly compared with one another because the filter efficiencies for the two samples differ substantially. To remove the ATLAS MC-specific generator dependence of these numbers and compare the true kinematic-level acceptance, the curves are multiplied by the filter efficiency of each sample. The resulting ATLAS-independent acceptance curves are shown in figure B.8. Mass points below 450 GeV are shown using the samples with filter cut at photon $p_T = 100$ GeV and the single photon trigger selection, while mass points above 450 GeV are shown using the samples with filter cut at photon $p_T = 50$ GeV and the compound trigger selection.

The efficiency is defined as the ratio of number of reconstruction-level events which pass all analysis requirements to number of truth-level events which pass the kinematic requirements, and thus accounts for trigger, ID, and tagging efficiencies. These quantities are shown for each signal point in figure B.9.

The visible cross section for the Z' model is then given by $\sigma \cdot k \cdot \epsilon_{\text{filter}}$ multiplied by the two acceptance and efficiency values from the relevant plot at each mass point. The branching ratio is incorporated in the cross section value in this case, since only



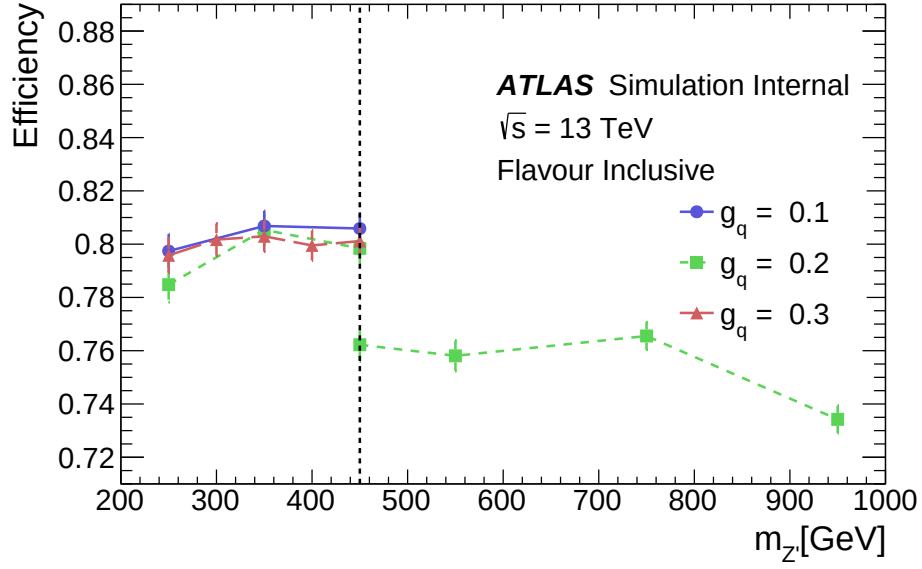
(a) Inclusive selection



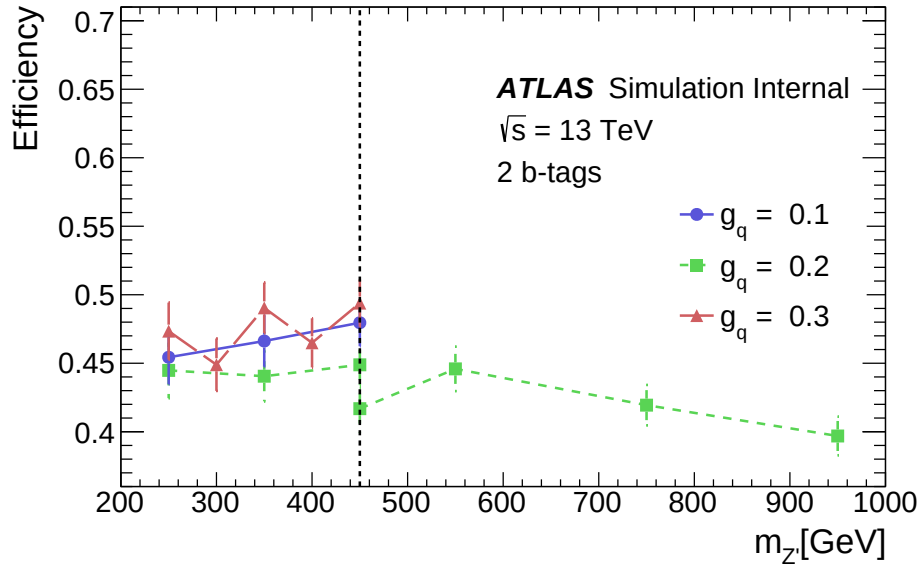
(b) 2- b -tagged selection

Figure B.8: Kinematic acceptance of the Z' benchmark model for all coupling values considered in the analysis. The acceptance quantities are multiplied by the filter efficiency for each sample to remove the otherwise hidden impact of the different photon p_T cuts at generator level. The single photon trigger selection and appropriate samples are used below 450 GeV while the compound trigger selection and appropriate samples are used above that point.

events resulting in a jet final state are generated. An interpolation between the points is performed logarithmically in Z' mass and appears as straight lines in the figures.



(a) Inclusive selection



(b) 2- b -tagged selection

Figure B.9: Efficiency of the Z' benchmark model for all mass points and coupling values considered in the analysis.

B.4 Mass binning

169	180	191	203	216	229	243	257	272
287	303	319	335	352	369	387	405	424
443	462	482	502	523	544	566	588	611
634	657	681	705	730	755	781	807	834
861	889	917	946	976	1006	1037	1068	1100
1133	1166	1200	1234	1269	1305	1341	1378	1416
1454	1493	1533	1573	1614	1656	1698	1741	1785
1830	1875	1921	1968	2016	2065	2114	2164	2215
2267	2320	2374	2429	2485	2542	2600	2659	2719
2780	2842	2905	2969	3034	3100	3167	3235	3305
3376	3448	3521	3596	3672	3749	3827	3907	3988
4070	4154	4239	4326	4414	4504	4595	4688	4782
4878	4975	5074	5175	5277	5381	5487	5595	5705
5817	5931	6047	6165	6285	6407	6531	6658	6787
6918	7052	7188	7326	7467	7610	7756	7904	8055
8208	8364	8523	8685	8850	9019	9191	9366	9544
9726	9911	10100	10292	10488	10688	10892	11100	
11312	11528	11748	11972	12200	12432	12669	12910	13156

Table B.5: Actual binning for the photon ISR channels, in units of GeV, as inherited from [\[145\]](#).

B.5 Results for tests of fitting in MC spectra and in a statistically non-sensitive dataset

Functional form	Channel (inclusive)	Fit type	χ^2 p-value
our4param	Single photon trigger	global	0.0
our4param	Single photon trigger	SWiFt, whw=22	0.002
our4param	Single photon trigger	SWiFt, whw=18	< 0.012
our4param	Single photon trigger	SWiFt, whw=16	< 0.019
our4param	Single photon trigger	SWiFt, whw=14	< 0.061
our5param	Single photon trigger	global	0.042
our5param	Single photon trigger	SWiFt, whw=22	0.132
our5param	Single photon trigger	SWiFt, whw=18	0.148
our5param	Single photon trigger	SWiFt, whw=16	0.171
UA2	Single photon trigger	global	< 0.01
UA2	Single photon trigger	SWiFt, whw=18	< 0.01
UA2	Single photon trigger	SWiFt, whw=16	< 0.01
UA2	Single photon trigger	SWiFt, whw=9	0.48
our4param	Combined trigger	global	0.852
our5param	Single photon trigger	global	0.856
UA2	Single photon trigger	global	0.079

Table B.6: Summary of the MC-based fitting tests, showing the χ^2 p-value for different fitting configurations.

Functional form	Channel (inclusive)	Fit type	χ^2 p-value	BH p-value
our4param	Combined trigger	SWiFt, whw=18	0.052	0.60
our5param	Combined trigger	SWiFt, whw=18	0.052	0.49
UA2	Combined trigger	SWiFt, whw=16	0.056	0.58
our4param	Single γ trigger	global	0.85	0.94
our5param	Single γ trigger	global	0.86	0.94
UA2	Single γ trigger	global	0.079	0.35

Table B.7: Summary of the fitting tests in data, showing the χ^2 and BumpHunter p-values for different fitting configurations.

Functional form	Channel (ABCD)	Fit type	χ^2 p-value
our5param	Single γ trigger	SWiFt, whw=17, fit range $m_{jj} < 1$ TeV	0.137
UA2	Single γ trigger	SWiFt, whw=14, fit range $m_{jj} < 1$ TeV	0.116
our5param	Single γ trigger	SWiFt, whw=15, fit range $m_{jj} < 0.8$ TeV	0.123
our4param	Single γ trigger	SWiFt, whw=15, fit range $m_{jj} < 0.8$ TeV	0.186
UA2	Single γ trigger	SWiFt, whw=14, fit range $m_{jj} < 0.8$ TeV	0.094

Table B.8: Summary of the fitting tests in an ABCD-scaled 2-tagged spectrum derived from data, showing the χ^2 p-value for different fitting configurations.

B.6 Systematics

B.6.1 Uncertainties applied to the background estimate

Fit uncertainty and function choice uncertainty

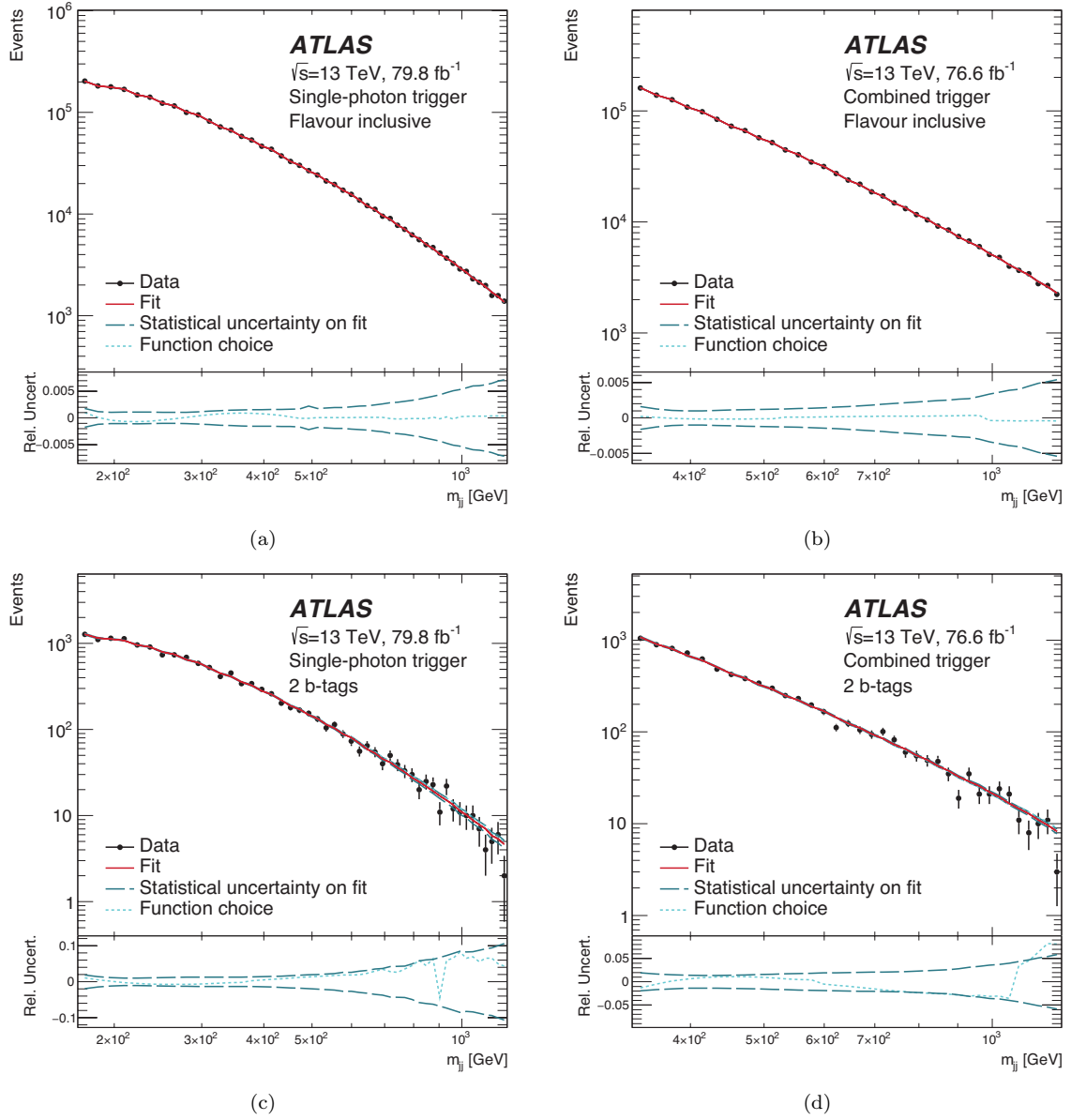


Figure B.10: Fit uncertainty and function choice uncertainty determined from data for each of the four categories: flavour inclusive using the single-photon trigger [a](#), flavour inclusive using the combined trigger [b](#), b -tagged with the single-photon trigger [c](#), and b -tagged with the combined trigger [d](#). The solid red line shows the fit-based background estimate. The dark blue lines depict the $\pm 1\sigma$ statistical uncertainty on the background estimate. The single light blue line represents the uncertainty due to the choice of fit function and its direction. At the bottom of each figure, a ratio panel shows the sizes of these uncertainties relative to the nominal fit result.

B.6.2 Uncertainties applied to the signal

Jet energy scale and resolution

An example of the variation due to the each nuisance parameter is given in figure B.11 for the Z' of mass 450 GeV and coupling $g_q = 0.2$. JES NP 1 has the largest effect. All three uncertainties act not on the acceptance but rather on the peak location, moving it to higher or lower m_{jj} as events move between bins.

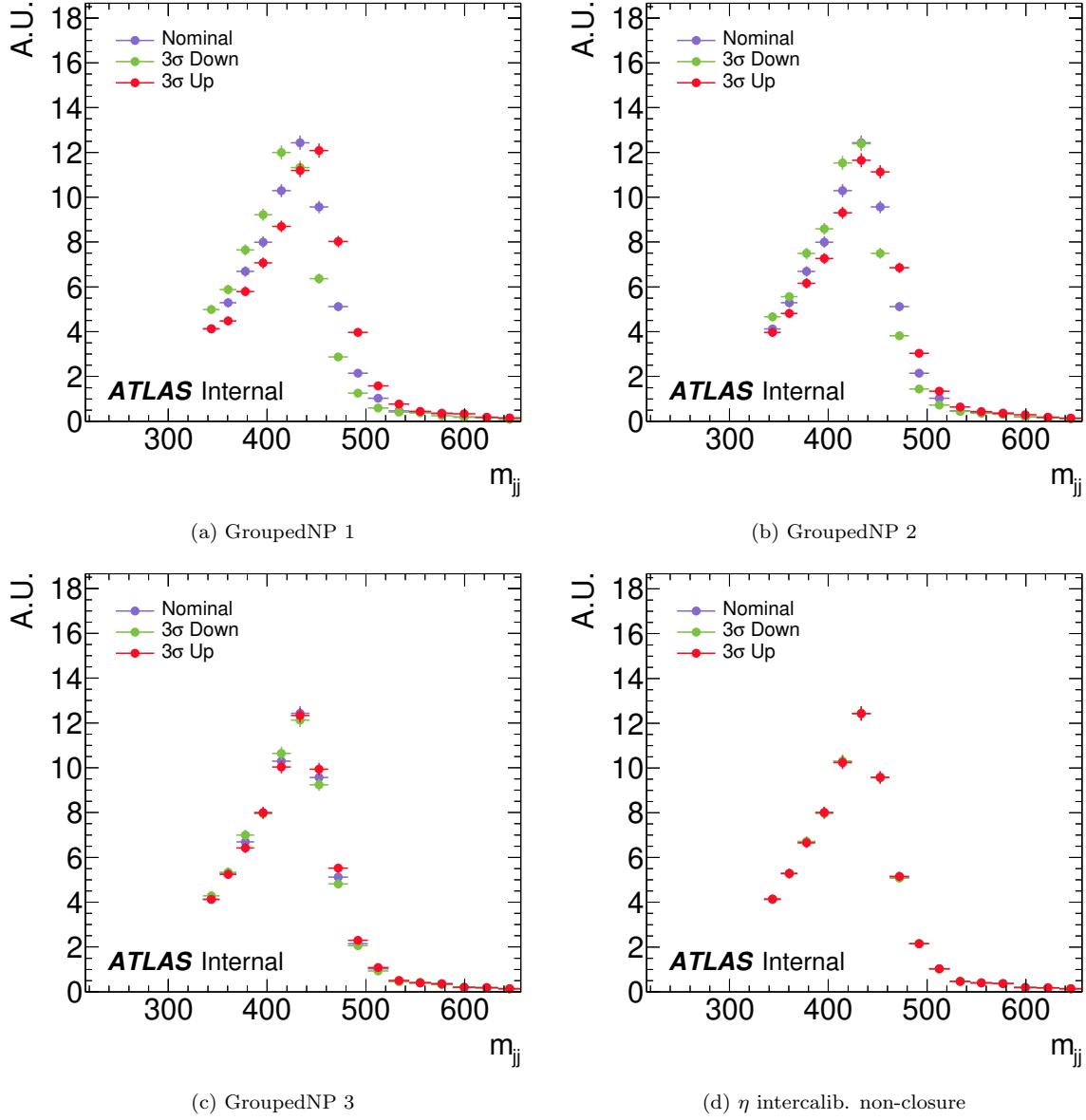


Figure B.11: Impact of $\pm 3\sigma$ variation in each of the four strongly reduced JES systematics. The Z' point with mass 450 GeV and coupling $g_q = 0.2$ is used as an illustrative example. The combined trigger and inclusive selection are applied.

The impact of JES in the 2 b -tagged channels is similarly modelled, but the smaller statistics make the impact more difficult to assess. Examples of the JES components for the same signal point with mass 450 GeV and coupling $g_q = 0.2$ but in the b -tagged channel are shown in figure B.12.

The uncertainty on the jet energy resolution (JER) is calculated by varying signal

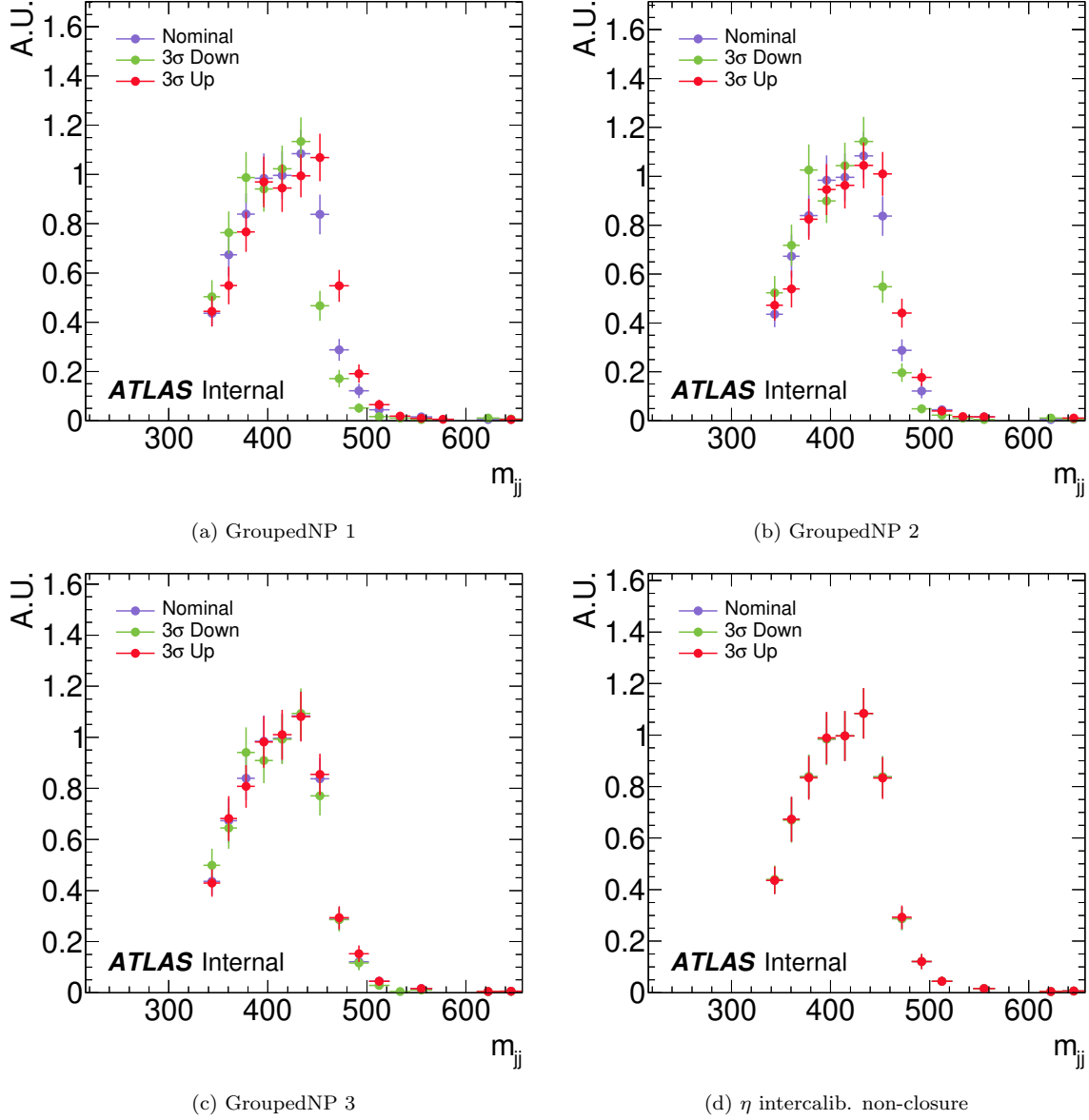
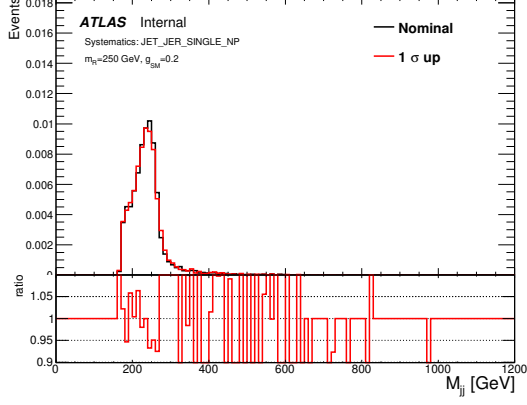


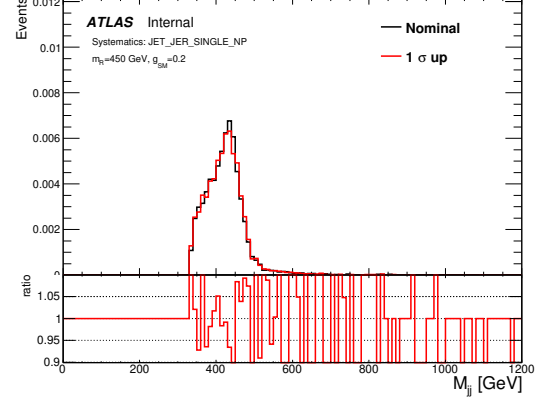
Figure B.12: Impact of $\pm 3\sigma$ variation in each of the four strongly reduced JES systematics. The Z' point with mass 450 GeV and coupling $g_q = 0.2$ is used as an illustrative example. The combined trigger and 2 b -tagged selection are applied.

templates according to JetEtMiss recommendations. Unlike the JES, the effect is not to change the signal peak location, but rather to widen the peak somewhat. Figure B.13 shows the effects of varying the JER on two sample signal templates, while figure B.14 overlays the effects bin by bin for all signal samples to look at large-scale trends. Both figures use 10 GeV bin widths.

To make sense of the points in figure B.14, the binning is increased to 50 GeV and the weighted average effect between all samples is taken as the value in each bin. A linear fit is performed to the resulting distribution. Based on the fits, a flat 3% JER uncertainty will be applied in both channels. Figure B.15 shows the variation due to JER averaged across all channels in these large bins with the linear fit overlaid.

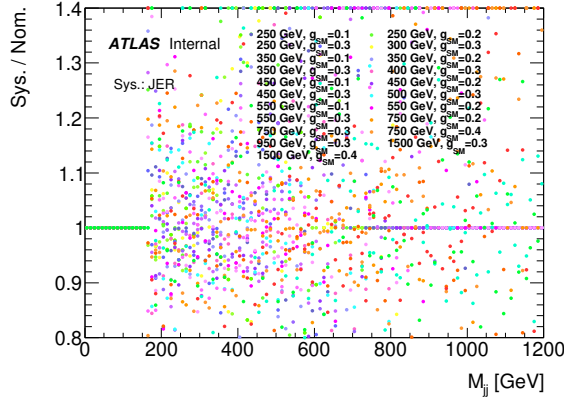


(a) 250 GeV Z' , $g_q = 0.2$

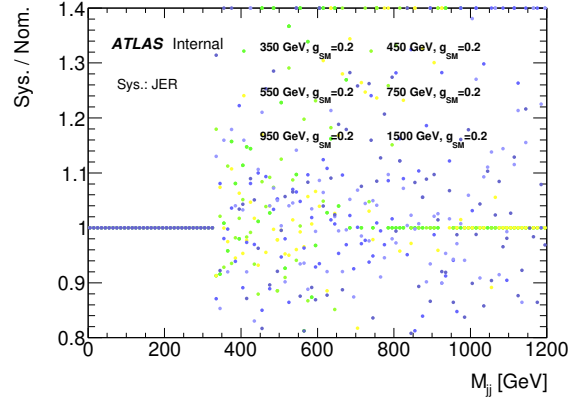


(b) 450 GeV Z' , $g_q = 0.2$

Figure B.13: Impact of JER variation on two representative signal samples. The impact of the uncertainty is, on average, to widen the peak somewhat, but the statistical effects are substantial.

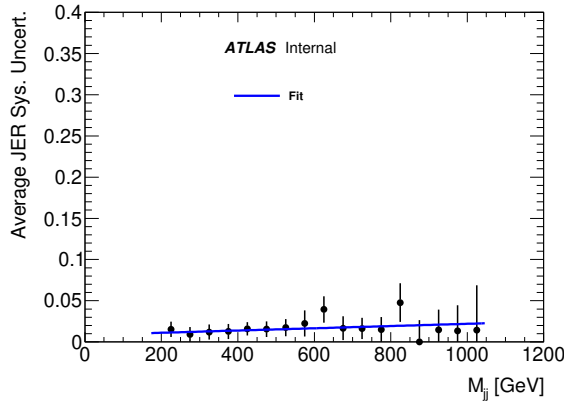


(a) Single photon trigger

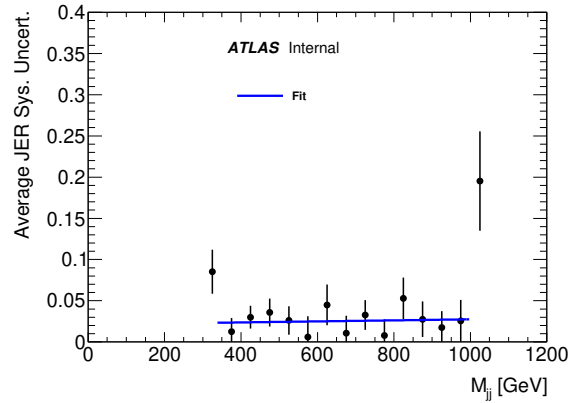


(b) Combined trigger

Figure B.14: Impact of JER variation on all signal samples for the single photon trigger (B.14a) and combined trigger (B.14b). Statistical fluctuations in this fine binning make patterns hard to distinguish.



(a) Single photon trigger



(b) Compound trigger

Figure B.15: Impact of JER variation on the bin-by-bin average of all signal samples for the single photon trigger (B.15a) and combined trigger (B.15b). By rebinning to 50 GeVbins, statistical fluctuations are suppressed, and the resulting points show a simple linear dependence on m_{jj} . A linear fit to each is shown. These plots support the use of a 3% flat uncertainty on JER in both channels.

Photon ID, energy scale and resolution

For these uncertainties, the simplified correlation scheme is used, reducing the various input uncertainties to two nuisance parameters corresponding to overall photon energy scale and resolution. Both of these uncertainties can affect signal acceptance but they do not affect signal shape. The impact on a representative Z' point (450 GeV, $g_q = 0.2$) is shown in figure B.16, and it can be seen that the effects alter the normalisation of the sample but not the peak shape or location.

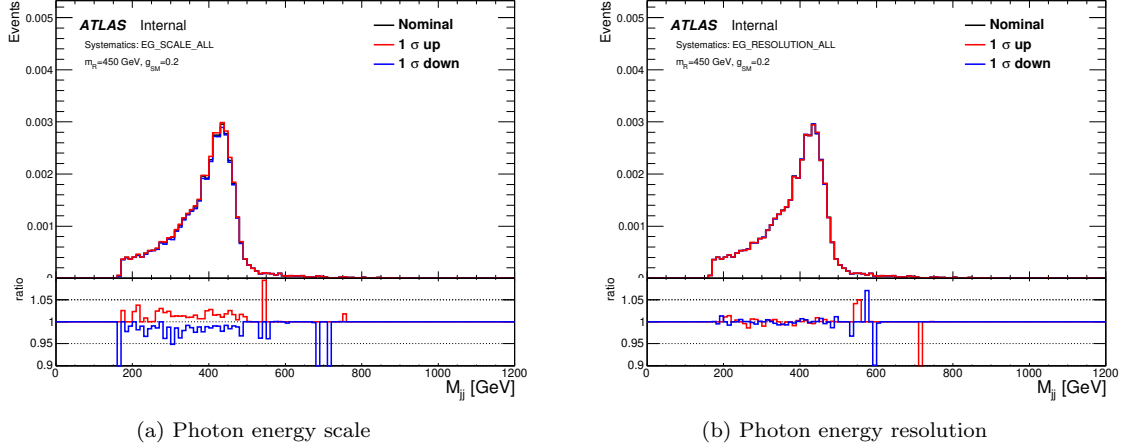


Figure B.16: Impact on a representative Z' signal MC sample of $\pm 1\sigma$ variations in the the photon energy scale (B.16a) and photon energy resolution (B.16b) uncertainties. The selected sample has mass 450 GeV and $g_q = 0.2$ and the single photon trigger inclusive selection is applied. The uncertainties are not found to have a meaningful effect on signal shape or peak location, but instead change the signal normalisation (equivalent to the acceptance).

Since the uncertainties evaluated within each sample are statistically limited, a method was sought for deriving a value of the uncertainty which could be applied to all signal samples. To this end, the variation in each signal point due to the systematics were plotted together to understand the overall behaviour and determine if it could be used to derive a statistics-robust evaluation of the uncertainty as a function of m_{jj} . These results are shown in figure B.17 for the energy scale and in figure B.18 for the energy resolution.

The photon ID scale factor uncertainty are assessed using the same technique as the previous uncertainties in order to determine a single consistent treatment across the signal samples. Figure B.19 shows the impact of the systematic across all signal samples for the inclusive selection.

To remove the statistical fluctuations and understand the overall trend in the photon uncertainties, the sum in quadrature of the three photon-related uncertainties per signal sample is taken, and a per bin weighted average of these total uncertainties for the different signal samples is then obtained. A linear fit is performed to the resulting points. This fit to the weighted average is shown in figure B.20a and is overlaid on the total uncertainties for the individual signals in Figure B.20b. The linear fit shows that the size of the uncertainty does not change with m_{jj} so a single flat acceptance uncertainty of 2.0% may be used in this channel. Figure B.21 shows the equivalent plots for the combined trigger, again using the inclusive channel. In this case, where the impact of the photon on the selection is somewhat smaller, a flat acceptance uncertainty of 1.4% is selected instead.

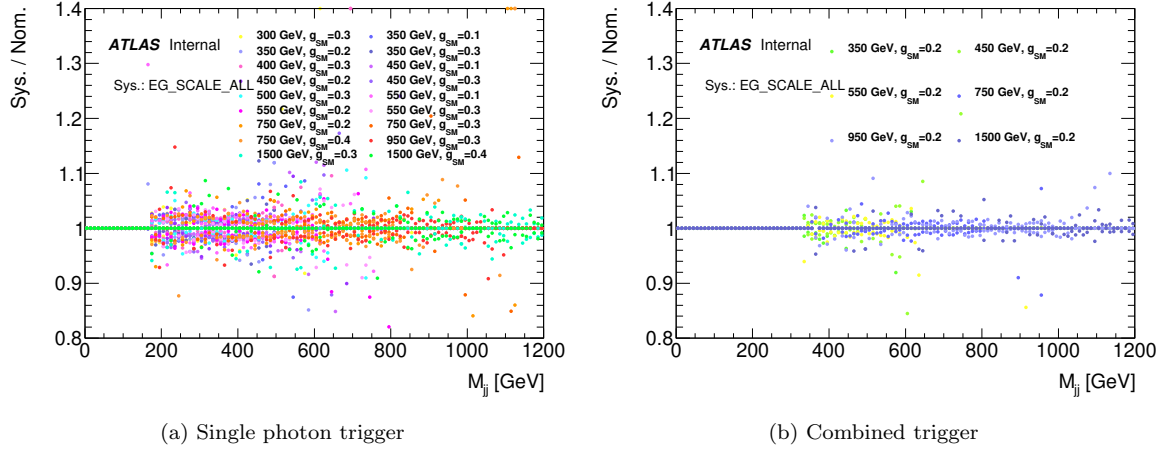


Figure B.17: Overlay of the photon energy scale uncertainties for all signal samples using the inclusive selection with the single photon trigger (B.17a) and combined trigger (B.17b).

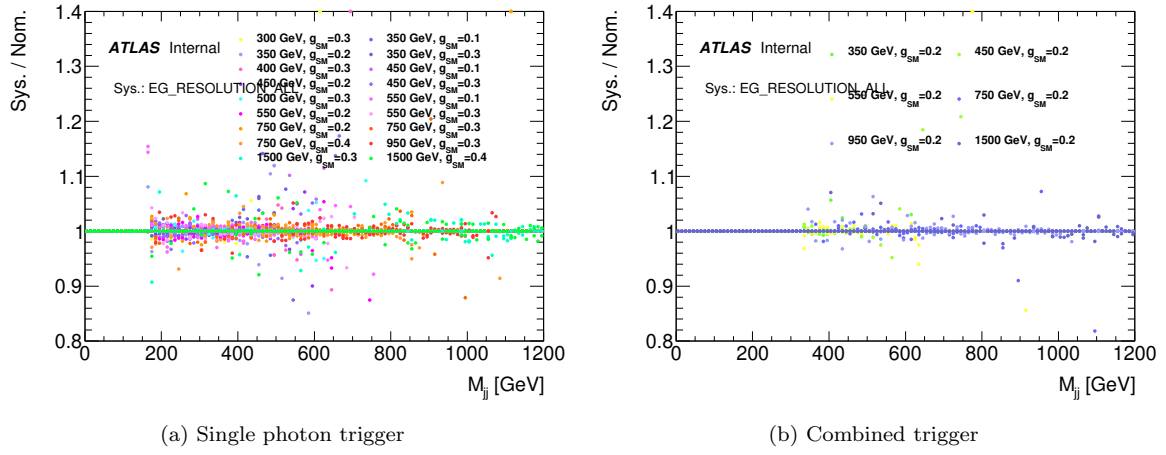


Figure B.18: Overlay of the photon energy resolution uncertainties for all signal samples using the inclusive selection with the single photon trigger (B.18a) and combined trigger (B.18b).

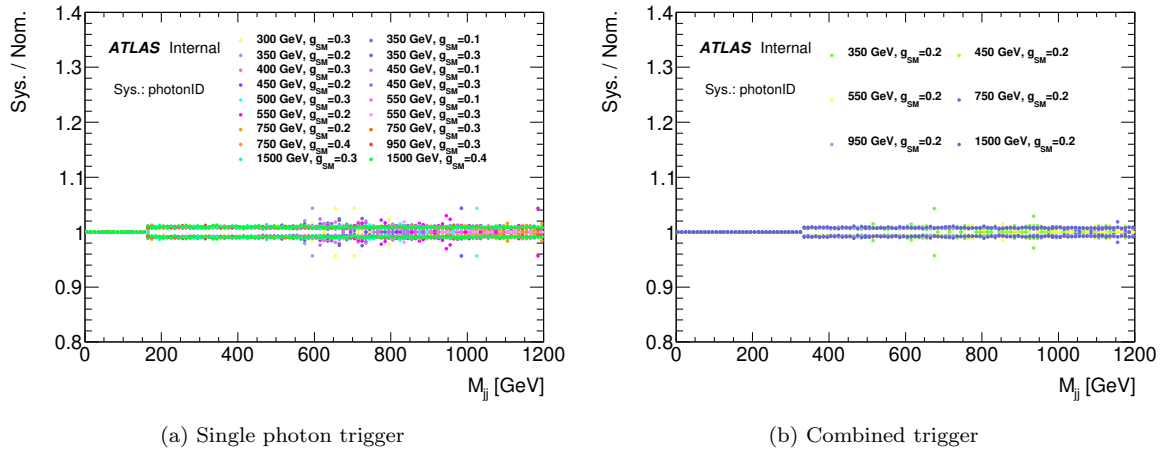


Figure B.19: Overlay of the photon ID scale factor uncertainties for all signal samples using the inclusive selection with the single photon trigger (B.19a) and combined trigger (B.19b).

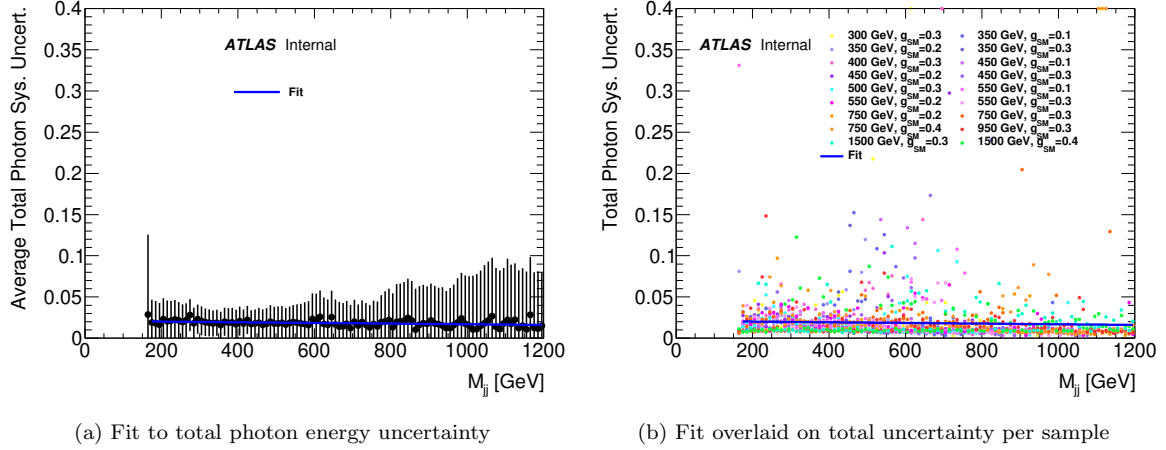


Figure B.20: The total photon energy uncertainty is obtained by summing the energy scale, energy resolution, and ID scale factor uncertainties in quadrature, for all signal samples using the single photon trigger and inclusive selection. A weighted average of the results in each bin across the various signal samples is then fitted and shown in B.20a. The resulting fit is overlaid on the total uncertainty for each signal separately in B.20b. This demonstrates that a 2% uncertainty, flat as a function of m_{jj} , is appropriate for the photon related uncertainties.

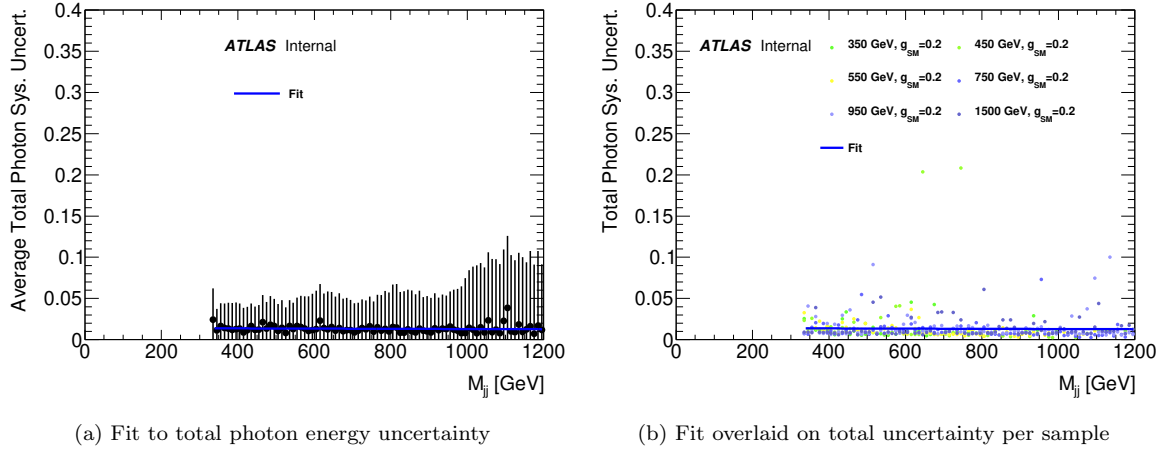


Figure B.21: The total photon energy uncertainty is obtained by summing the energy scale, energy resolution, and ID scale factor uncertainties in quadrature, for all signal samples using the combined trigger and inclusive selection. A weighted average of the results in each bin across the various signal samples is then fitted and shown in B.21a. The resulting fit is overlaid on the total uncertainty for each signal separately in B.21b. This demonstrates that a 1.4% uncertainty, flat as a function of m_{jj} , is appropriate for the photon related uncertainties.

Trigger efficiency

Figures B.22 and B.23 show the trigger efficiency versus m_{jj} for each trigger, overlaid with a horizontal line fitted to the data points in each. No obvious dependence of the efficiency on m_{jj} is visible; the apparent approach to full efficiency at high mass is an effect of the decreasing statistics. Based on these fits, an uncertainty of 3% is applied in the compound trigger channel to account for trigger inefficiency. No such uncertainty is applied for the single photon trigger where the efficiency is essentially 100%.

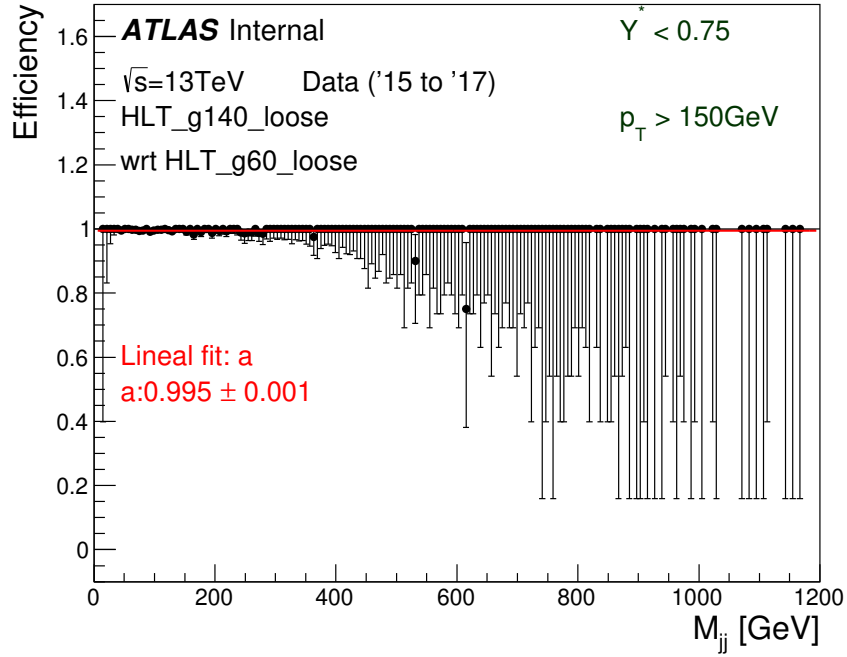


Figure B.22: Trigger efficiency as a function of m_{jj} for the single photon trigger. 99.5% efficiency is achieved across the full mass range so no uncertainty is required.

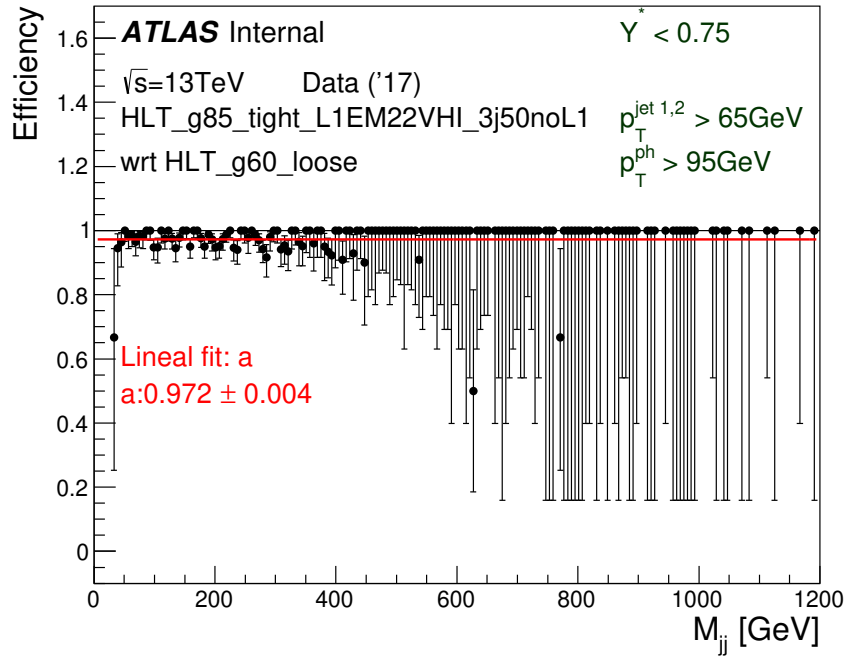


Figure B.23: Trigger efficiency as a function of m_{jj} for the compound trigger. This trigger achieves only $\sim 97\%$ efficiency across the entire observable mass range. A 3% uncertainty is therefore applied to the compound trigger channels to account for this inefficiency.

b -tagging scale factors

Approximately 25 individual scale factor uncertainties are provided by the flavour-tagging CP group and signal templates varied according to each have been produced. Since each of the 25 uncertainties is very small, a conservative simplification is made by taking the sum in quadrature of all of them and applying the result parameterised by a single nuisance parameter. The impact of that nuisance parameter was determined in the following way: first the impact on each signal sample was assessed to ensure it changed only normalisation and not shape. Next the impact bin by bin of each individual scale factor uncertainty was plotted for all signal samples, to ensure the size of the effect depended only on m_{jj} and not on the individual sample being considered. Finally the quadrature sum of the impact of all 25 uncertainties was averaged across the signal samples and a parameterisation found for it which could be used on each sample, thereby producing an uncertainty robust against statistical fluctuations in the individual samples.

Figure B.24 shows the impact of the two largest scale factor uncertainties (FT_EFF_Eigen_B_0 and FT_EFF_Eigen_B_1) on a representative signal sample with mass 450 GeV and $g_q = 0.2$. The single photon trigger is used and the 2 b -tagged selection applied.

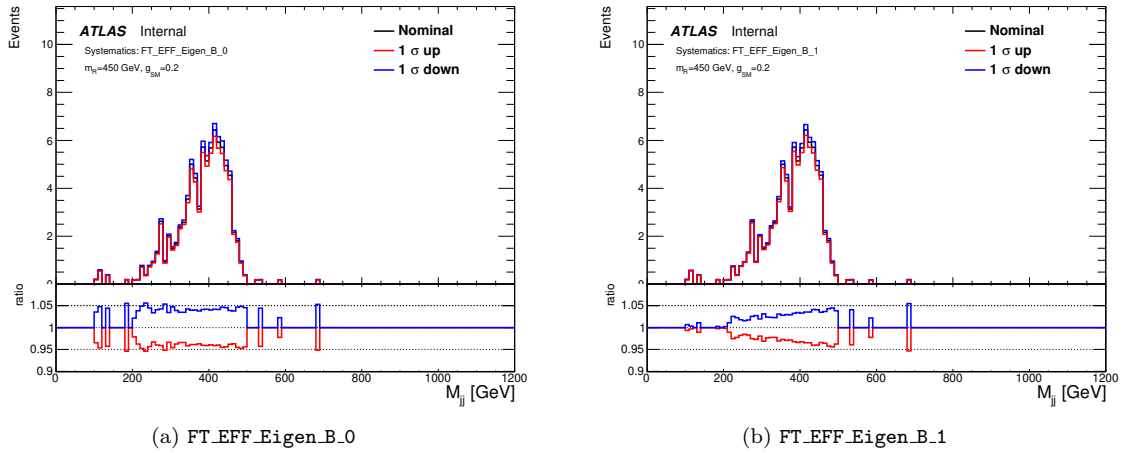


Figure B.24: Impact on a representative Z' signal MC sample of $\pm 1\sigma$ variations in the the FT_EFF_Eigen_B_0 (B.24a) and FT_EFF_Eigen_B_1 (B.24b) b -tagging scale factor uncertainties. The selected sample has mass 450 GeV and $g_q = 0.2$. The uncertainties are not found to have a meaningful effect on signal shape or peak location, but instead change the signal normalisation (equivalent to the acceptance).

The overlay of bin-by-bin uncertainty sizes for the four largest uncertainties are given in figure B.25 for the single photon trigger and the 2 b -tagged selection.

The total b -tagging scale factor uncertainty is shown for all signal samples in figure B.26. The total uncertainty is relatively flat until about m_{jj} of 300 GeV, when it begins to increase in a fairly linear way. To assess this m_{jj} dependence in more detail, a weighted average of the values in each bin is plotted, and a linear fit is performed from 300 GeV to 1200 GeV. A flat value of 5% can be used from 170 GeV to 300 GeV. The result of the fit to the average total uncertainty for the single photon trigger channel above 300 GeV is shown in figure B.27a. Figure B.27b overlays the same fit result on the total uncertainty in the compound trigger channel to demonstrate that it is appropriate for use in both cases, although it is very slightly more conservative than a dedicated fit would be in the compound trigger channel. Finally, Figure B.28 shows the fit result overlaid on the collection of the total uncertainty per bin for each signal sample separately.

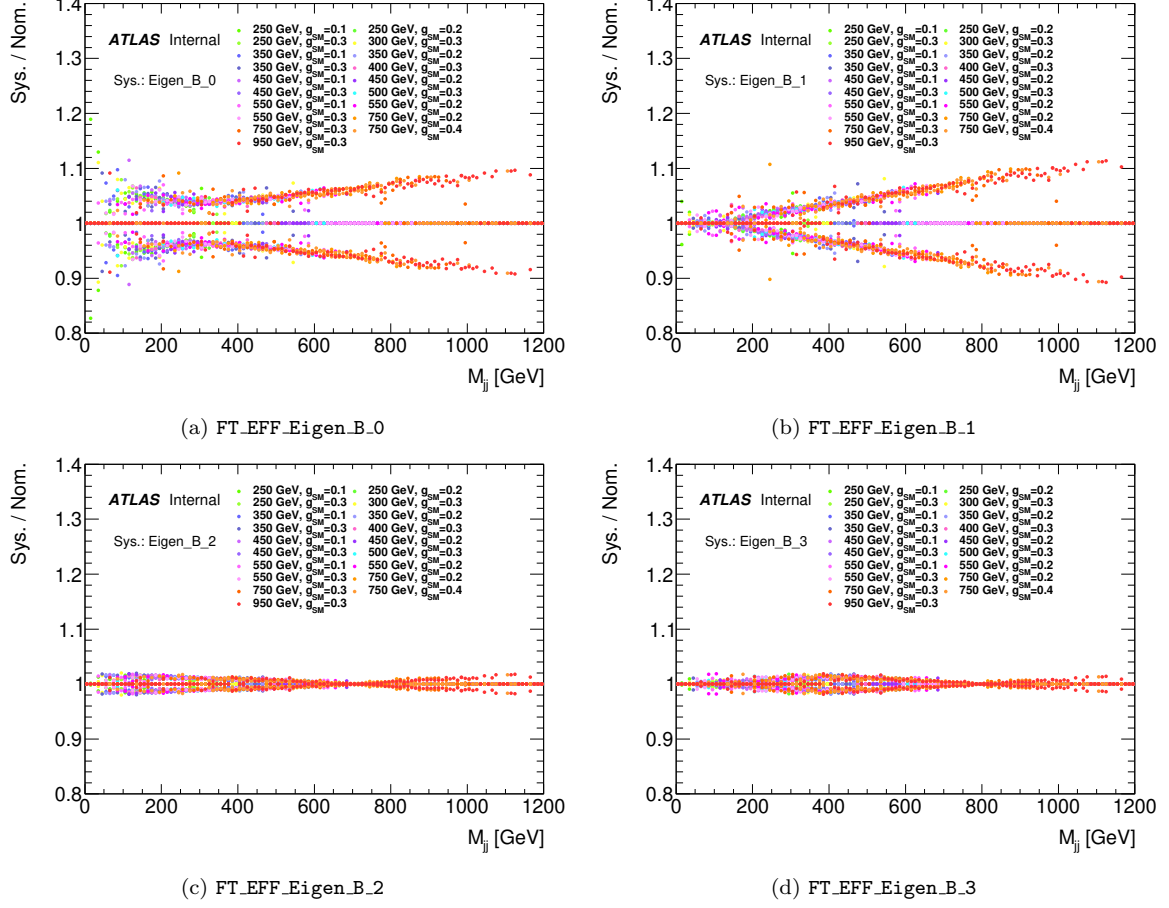


Figure B.25: Overlay of the four largest b -tagging scale factor uncertainties for all signal samples using the single photon trigger and the 2 b -tagged selection.

Thus the total b -tagging uncertainty used in both single photon trigger and compound trigger 2 b -tagged channels is 5% for $m_{jj} < 300$ GeV and $0.0001115(m_{jj} - 300) + 0.05$ for $300 \text{ GeV} < m_{jj} < 1200$ GeV.

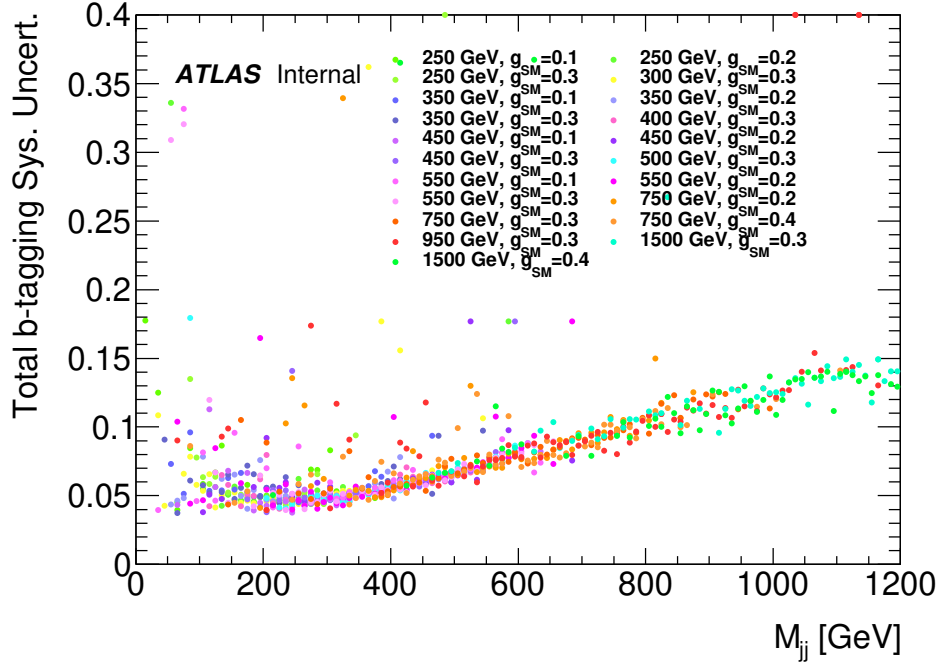


Figure B.26: Sum in quadrature of the 25 b -tagging scale factor uncertainties for every signal sample using the single photon trigger and 2 b -tagged selection. The total uncertainty is relatively flat as a function of m_{jj} until roughly 300 GeV, then increases to a maximum size of approximately 15%.

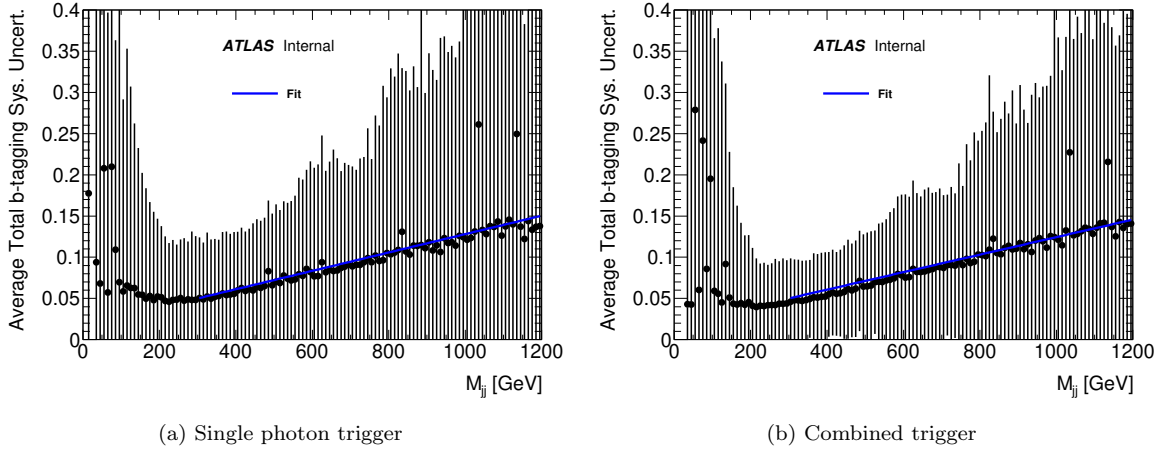
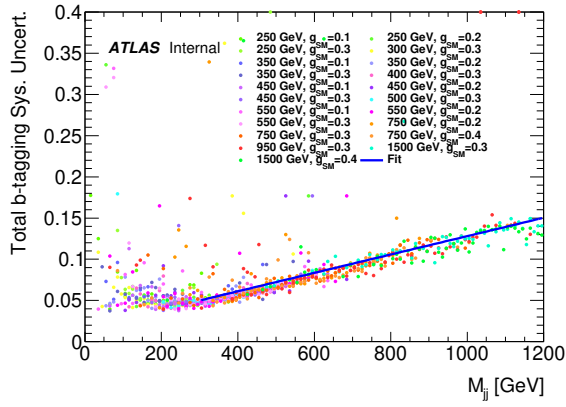
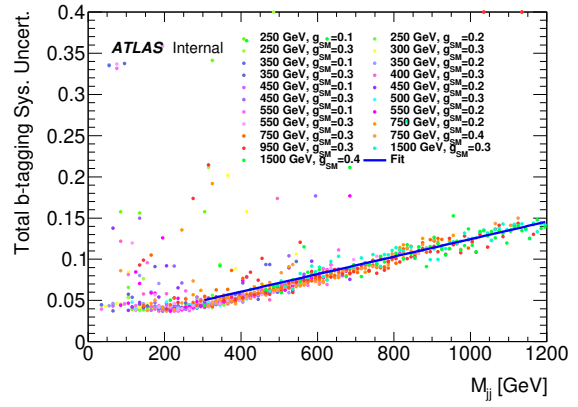


Figure B.27: Weighted average of the total b -tagging scale factor uncertainty across all signal samples in each m_{jj} bin. A linear fit is made to the total uncertainty for $300 \text{ GeV} < m_{jj} < 1200 \text{ GeV}$. The lower edge of the fit is fixed to 5% to match the flat uncertainty which will be used below 300 GeV. The fit is performed in the single photon trigger 2 b -tagged channel (B.27a) and is compared to the combined trigger 2 b -tagged channel to validate its use in both cases (B.27b).



(a) Single photon trigger



(b) Compound trigger

Figure B.28: The fit result calculated from the weighted average across all signal samples is overlaid on the total uncertainty separated by signal sample. The single photon trigger result is given in B.28a and the combined trigger result is in B.28b.

PDF choice and parameters

PDF uncertainties largely affect the normalisation of the signal rather than the shape of its distributions. To determine the effect, events are generated using the ensemble of PDFs provided by the NNPDF group using [175]. The differences in acceptance are calculated for each member of the ensemble and, following the PMG recommendation [176], the standard deviation of all acceptance variations is assigned as a systematic uncertainty. For this purpose, the mass distribution after the analysis selection and all relevant weights as a function of mediator mass is calculated for each pdf variation and shown in figure B.29. Comparing this result with the total weighted number of events before the analysis selection, the relative acceptance for each PDF variation is computed and shown in figure B.30. The results shown that the systematic uncertainty is less than 1% everywhere. Thus a 1% flat systematic was applied on the signal normalization.

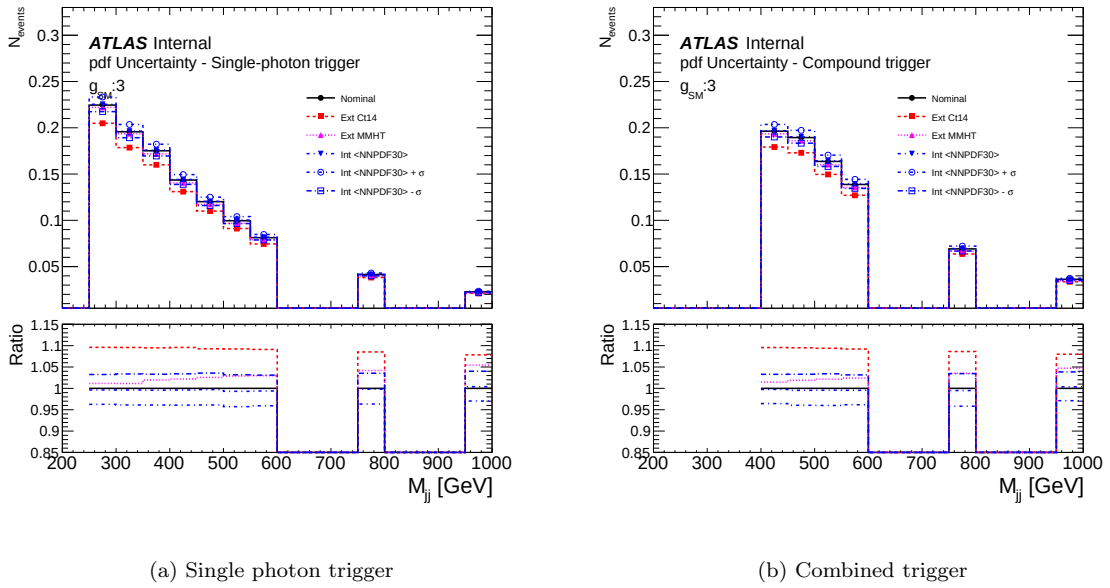


Figure B.29: The mass distribution after the analysis selection as a function of mediator mass for each PDF variation. Z' samples with coupling $g_q = 0.3$ are shown. The combined trigger selection is on the right and the single trigger selection is on the left; in each case the inclusive selection is used for the sake of statistics.

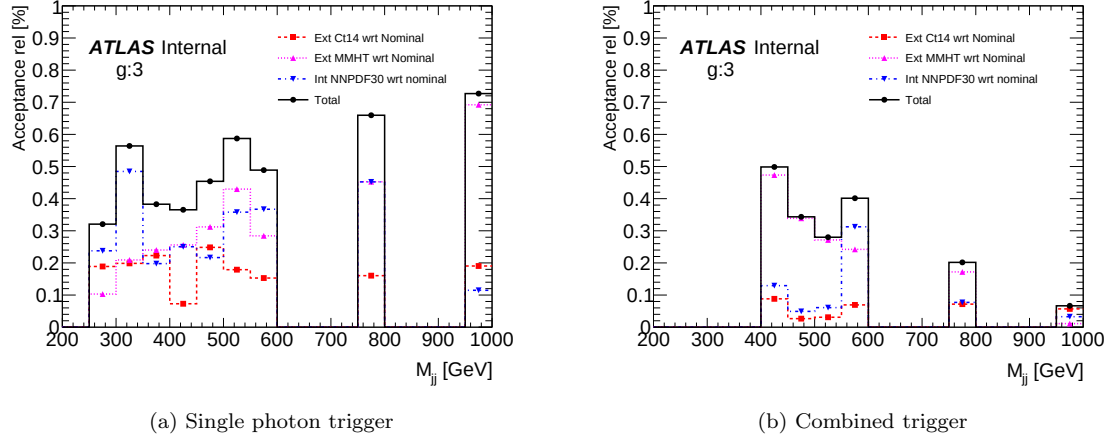


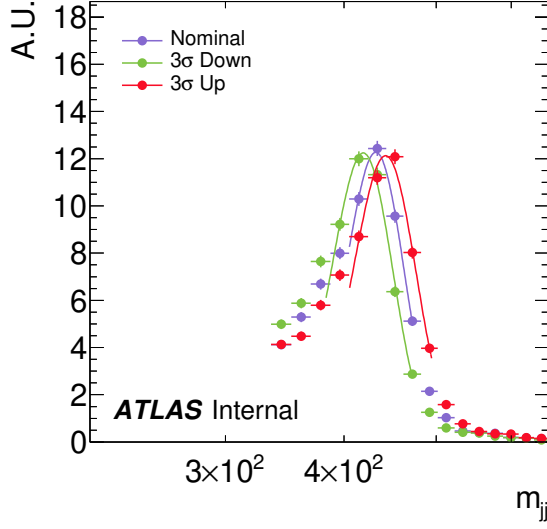
Figure B.30: The relative acceptance for each PDF variation with respect to the nominal PDF choices. Z' samples with coupling $g_q = 0.3$ are shown. The combined trigger selection is on the right and the single trigger selection is on the left; in each case the inclusive selection is used for the sake of statistics.

JES uncertainty for model-independent limits

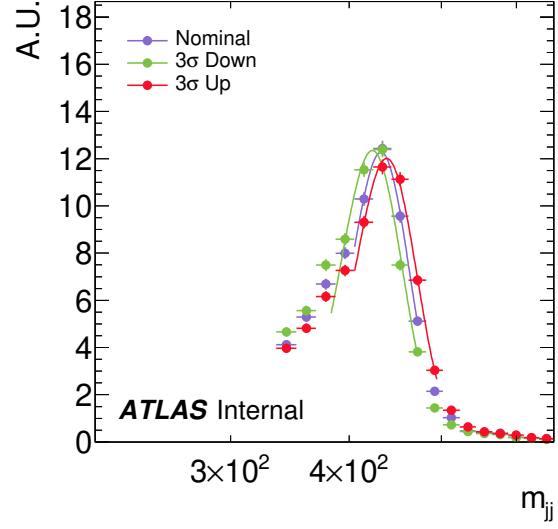
The acceptance uncertainties due to JER, photon energy scale and resolution, b -tagging scale factors, and luminosity can all be applied to Gaussian shaped signals in exactly the same way as to the Z' samples. The PDF uncertainty is not applied to Gaussian limits at all, since it is a theory-dependent uncertainty.

To simulate the effects of JES on a real signal for use with the Gaussians, the impact on the m_{jj} value of the signal peak due to the uncertainty must be measured and can then be applied to move the mean of the Gaussian template. To this end, a Gaussian fit is performed to the core of each signal template as well as to the $\pm 3\sigma$ variations in each JES uncertainty component. An example of these fits to the same templates shown in figure B.11 is given in figure B.31.

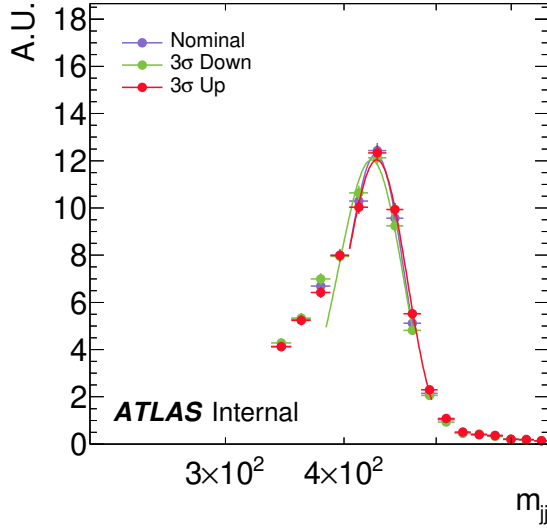
The equivalent fit is repeated for each point and the resulting shift in the fitted mean location is added in quadrature across the four independent nuisance parameters. These results are then summarised in figures B.32 and B.33. The Z' coupling values with the largest number of mass points are shown, but the other couplings behave similarly. The fits are less reliable in the 2 b -tagged channel due to the very low statistics, and in particular tend to fail for the $+3\sigma$ variations due to the shape of the signal. Thus the larger shifts in the -3σ direction should be taken as the more reliable estimate of the uncertainty size. In every case, the shift in the mean is found to be $\leq 2\%$. Therefore this value is chosen for use in the model-independent Gaussian limits.



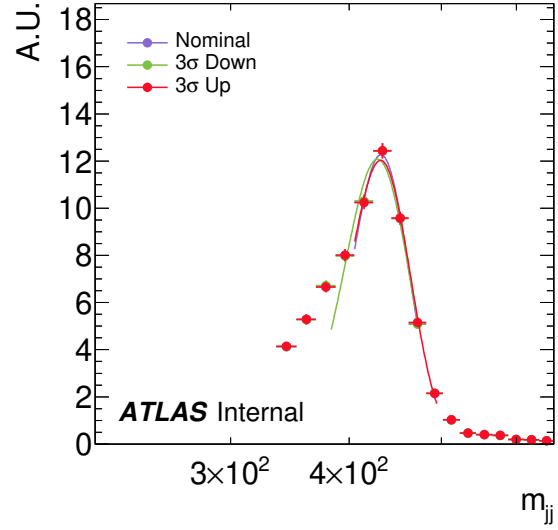
(a) GroupedNP 1



(b) GroupedNP 2

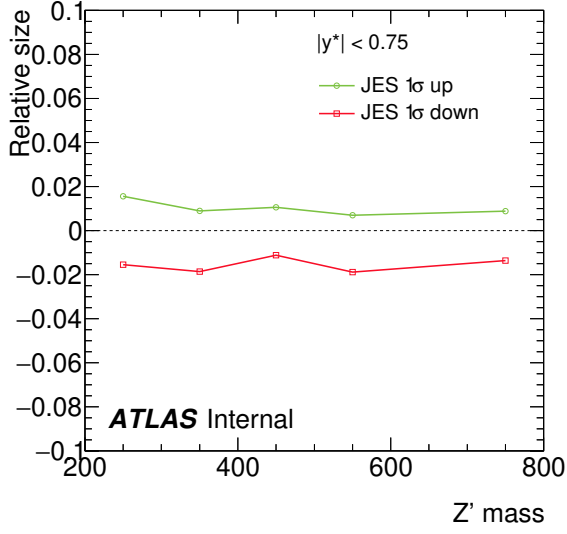


(c) GroupedNP 3

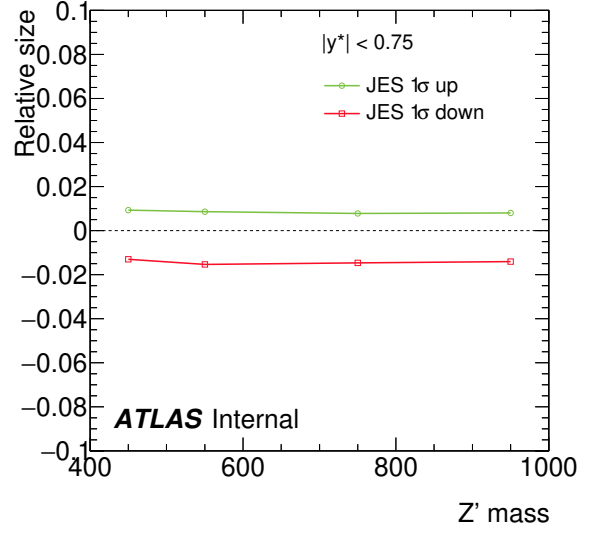


(d) η intercalib. non-closure

Figure B.31: Fits to the nominal and $\pm 3\sigma$ variations in each of the four strongly reduced JES systematics. The Z' point with mass 450 GeV and coupling $g_q = 0.2$ is used as an illustrative example. The combined trigger and inclusive selection are applied. The impact on the mean of the Gaussians is seen to be relatively small.

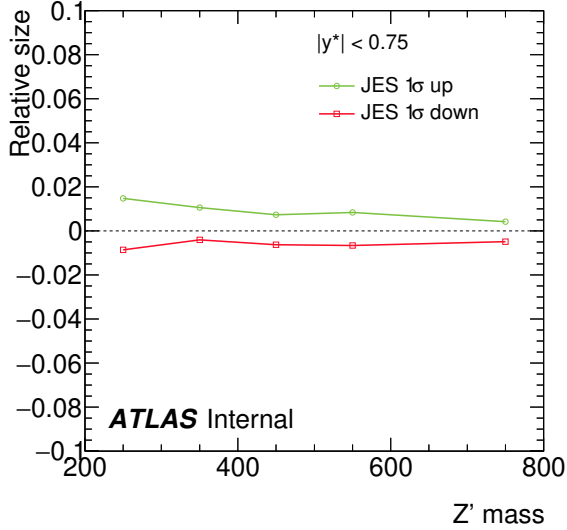


(a) Single photon trigger

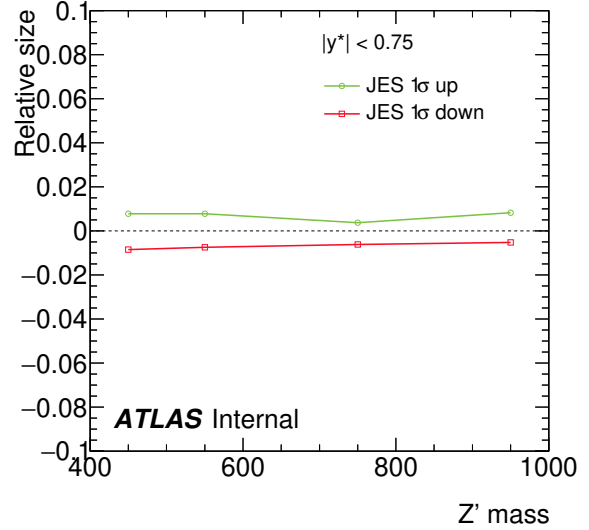


(b) Combined trigger

Figure B.32: Impact of $\pm 1\sigma$ in the total JES on the mean location of a Z' signal peak. The inclusive selection is used.



(a) Single photon trigger



(b) Combined trigger

Figure B.33: Impact of $\pm 1\sigma$ in the total JES on the mean location of a Z' signal peak. The 2 b -tagged selection is used. The fits, particularly to the upward variations, suffer from low statistics and therefore the inclusive channel provides a better measure of the JES impact.

Appendix C

Search for top quark decay to a charged Higgs boson and a b -quark

C.1 Analysis yields for backgrounds and signal

	4j-ex, 2b-ex, 1b-70%	4j-ex, 3b-ex	4j-ex, 4b-in
Single-top	1887.41 ± 611.306	1281.48 ± 431.431	19.9244 ± 10.295
$t\bar{t} + \geq 1b$	4957.47 ± 2113.14	8163.58 ± 3341.59	237.865 ± 52.2725
$t\bar{t} + \geq 1c$	5617.03 ± 3487.3	2943.97 ± 1787.35	13.828 ± 18.3601
$t\bar{t} + light$	31450.8 ± 3907.59	14636.9 ± 2516.46	14.9814 ± 15.0328
topEW	82.538 ± 13.1435	90.4308 ± 14.0888	5.7389 ± 1.01663
ttH	58.3502 ± 6.65559	114.345 ± 12.968	6.85066 ± 0.989806
W+jets light	704.47 ± 229.448	692.099 ± 267.647	7.1673 ± 2.66322
Z+jets light	149.858 ± 47.7329	157.171 ± 50.964	2.82184 ± 0.93943
Dibosons	44.3532 ± 16.9223	45.985 ± 16.1369	2.775 ± 1.05494
$H^+ \rightarrow c\bar{b}$ 110 GeV	2675.88 ± 112.579	4281.73 ± 165.259	122.448 ± 11.1429
Total	47628.1 ± 6245.22	32407.7 ± 4896.01	434.4 ± 63.1997

Table C.1: Predicted yields in the 4j-ex regions. The prediction is shown before the fit is performed. Also shown is the signal expectations for $t\bar{t} \rightarrow WbH^+b$ assuming $\mathcal{B}(H^+ \rightarrow c\bar{b}) = 1.0$. The $t\bar{t} \rightarrow WbWb$ background is normalised to the SM prediction. The quoted uncertainties are the sum in quadrature of statistical and systematic uncertainties on the yields.

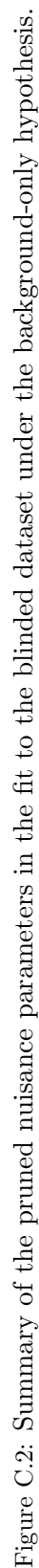
	5j-ex, 2b-ex, 1b-70%	5j-ex, 3b-ex	5j-ex, 4b-in
Single-top	1311.63 ± 457.843	1062.41 ± 385.157	46.4262 ± 22.9272
$t\bar{t} + \geq 1b$	6972.99 ± 2911.76	11999.6 ± 4479.01	782.54 ± 292.055
$t\bar{t} + \geq 1c$	6644.78 ± 4164.29	3579.55 ± 2131.49	36.578 ± 23.0534
$t\bar{t} + light$	20672.5 ± 3557.88	9663.01 ± 2334.73	16.475 ± 13.5492
topEW	152.264 ± 24.2357	178.712 ± 27.7932	21.2825 ± 3.4367
ttH	147.632 ± 16.5542	277.104 ± 30.8294	45.234 ± 5.44315
W+jets light	538.254 ± 168.135	364.977 ± 205.308	16.6604 ± 5.82129
Z+jets light	113.126 ± 35.8883	102.343 ± 31.5365	4.55115 ± 1.46367
Dibosons	52.7224 ± 23.2255	39.7719 ± 18.2511	1.94088 ± 0.921245
$H^+ \rightarrow c\bar{b}$ 110 GeV	1863.33 ± 77.0715	2991.51 ± 114.692	126.653 ± 10.0774
Total	38469.2 ± 6652.52	30259 ± 5711.92	1098.34 ± 297.961

Table C.2: Predicted yields in the 5j-ex regions. The prediction is shown before the fit is performed. Also shown is the signal expectations for $t\bar{t} \rightarrow WbH^+b$ assuming $\mathcal{B}(H^+ \rightarrow c\bar{b}) = 1.0$. The $t\bar{t} \rightarrow WbWb$ background is normalised to the SM prediction. The quoted uncertainties are the sum in quadrature of statistical and systematic uncertainties on the yields.

	6j-in, 2b-ex, 1b-70%	6j-in, 3b-ex	6j-in, 4b-in
Single-top	1010.87 ± 425.756	934.282 ± 434.665	79.3809 ± 45.8691
$t\bar{t} + \geq 1b$	10133.1 ± 4651.75	17887.6 ± 7616.72	2344.01 ± 827.859
$t\bar{t} + \geq 1c$	8048.27 ± 5565.79	4287.79 ± 2567.08	62.2041 ± 51.5105
$t\bar{t} + light$	13521.3 ± 5086.9	6282.15 ± 2991.83	21.5149 ± 31.8587
topEW	332.907 ± 53.1808	400.701 ± 62.1704	74.3216 ± 11.7772
ttH	336.473 ± 37.5941	650.571 ± 71.8236	173.003 ± 19.9731
W+jets light	525.104 ± 167.955	478.612 ± 149.025	30.7849 ± 9.67588
Z+jets light	94.1918 ± 29.3879	98.2311 ± 30.2775	7.16832 ± 2.26369
Dibosons	48.9388 ± 24.3787	42.0253 ± 20.6772	3.49284 ± 1.81495
$H^+ \rightarrow c\bar{b}$ 110 GeV	1237.92 ± 53.8151	1967.62 ± 77.5382	145.915 ± 10.5031
Total	35289.1 ± 9183.79	33029.6 ± 8767.82	2941.8 ± 837.822

Table C.3: Predicted yields in the 6j-in regions. The prediction is shown before the fit is performed. Also shown is the signal expectations for $t\bar{t} \rightarrow WbH^+b$ assuming $\mathcal{B}(H^+ \rightarrow c\bar{b}) = 1.0$. The $t\bar{t} \rightarrow WbWb$ background is normalised to the SM prediction. The quoted uncertainties are the sum in quadrature of statistical and systematic uncertainties on the yields.

C.2 Summary of the pruned nuisance parameters



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